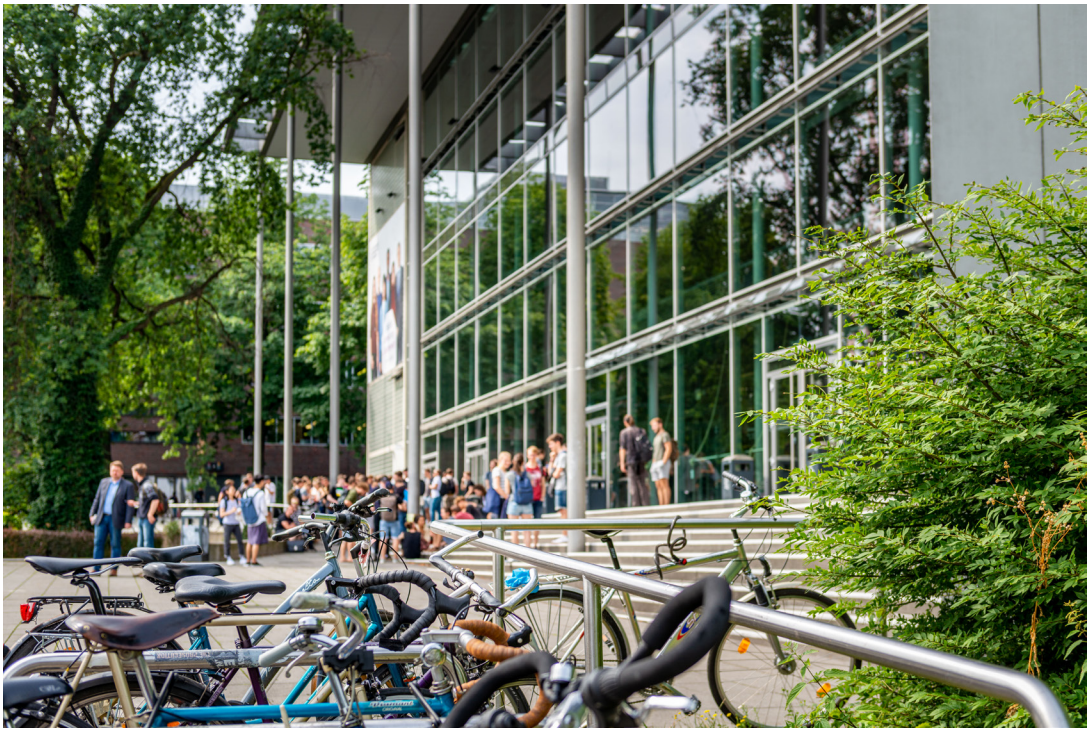
Deutsche Physikalische Gesellschaft DPG

DPG-Frühjahrstagung
(DPG Spring Meeting)

of the Condensed Matter Section (SKM)

together with the further divisions
Environmental Physics, Physics Education, Quantum Information

as well as the Working Groups
Accelerator Physics; Climate; Equal Opportunities; Industry and Business; Physics, Modern IT and Artificial Intelligence; Young DPG; Young Leaders in Physics



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8 – 13 March 2026

Technische Universität Dresden

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Content

Greeting 4

Organisation

Organiser 6
Local Organiser 6

Scientific Organisation

Chair of the Condensed Matter Section 6
Chairs of the Participating Divisions of the DPG 6
Chairs of the Participating Working Groups of the DPG 6
Symposia 7

Conference Information

Conference Venue 9
Conference Office / Information Desk 9
Lecture Rooms 9
Presentations 10
Oral Presentations 10
Poster Presentations 10
Notice Board 10
Communication / Internet Access 10
Public Working Area 11
Cloakroom 11
Lost and Found Property 11
Catering 11
Coffee Breaks 11
Snacks 11
Lunch 11
Wilhelm and Else Heraeus Communication Programme 11
CO_2 Compensation for the DPG Conferences 11
Acknowledgement 11
SAY CHEESE! 12
Liability Exclusion 12

Social Events

Welcome Evening 12
Opening of the Conference 12
Einstein Slam 12
Ceremonial Session with Award Ceremony 12
jDPG Pub Crawl 13
Exhibition of Scientific Instruments and Literature 13
Public Evening Talk 13
Members' Assemblies of the Divisions 13

Sponsors 14
Synopsis of the Daily Programme 16
Plenary Talks 56
Prize Talks 58
Plenary Special Talks 59
Tutorials 61

Symposia

AI and Data Challenges behind Emerging Self-Driving Laboratories (SYAI) 65
Fluids with Broken Time-Reversal Symmetry: Odd/Hall Viscosity between Active Matter and Electron Flows (SYBS) 67
Beyond Transistors: Material-Based Edge Computing Paradigms (SYBT) 69
Designing Quantum Materials with Light: From Floquet to Cavity Engineering (SYFC) 71
Guest Country Symposium France: Soft, Active and Alive: Emergent Properties in Living Matter (SYGF) 73
Interacting Degrees of Freedom in Ultrathin Quantum Films (SYQF) 75
The Sustainability Challenge: A Decade of Transformation (SYSC) 77
SKM Dissertation Prize 2026 (SYSD) 80
Tipping Points in Social and Climate Systems (SYTP) 82

Programme of the Divisions of SKM

BP Biological Physics 84
CPP Chemical and Polymer Physics 147
DS Thin Films 225
DY Dynamic and Statistical Physics 251
HL Semiconductor Physics 329
FM Crystalline Solids and their Microstructure 357
MA Magnetism 429
MM Metal and Material Physics 526
O Surface Science 573
SOE Physics of Socio-economic Systems 699
TT Low Temperature Physics 714
DD Physics Education 863
QI Quanteninformation 886
UP Environmental Physics 918

Working Groups

AKBP Accelerator Physics 926
AKC Equal Opportunities 939
AIW Industry and Business 941
AKjDPG Young DPG 943
AKPIK Physics, Modern IT and Artificial Intelligence 945

Job Market 953
Index of Authors 955
Index of Exhibitors 1001
Exhibition Maps 1010
Campus Map 1012
Timetable of the Conference 1013

Dear Conference Guests,

On behalf of the German Physical Society (DPG), I would like to warmly welcome you to the DPG Spring Meeting of the Condensed Matter Section (SKM) at Dresden University of Technology. Dresden is an important and long-established venue for DPG Spring Meetings. This support from Dresden University of Technology, renowned for its outstanding science and research, is also invaluable in strengthening the visibility and appreciation of physics in society and politics.

I am particularly pleased that France, represented by the Société Française de Physique (SFP), is our guest country at this conference in Dresden. To mark this special occasion, various prominent events will be held during the conference to promote scientific exchange and networking with our French partners. All conference participants are cordially invited to attend these events!

Our DPG Spring Meetings, which attract several thousands participants each year, have been very successful for decades – and they are also regularly among the largest physics conferences in Europe! That alone is a great achievement by all those involved. This year's outstanding conference programme in Dresden, with its wide range of topics, is also of inestimable importance for communication aimed at strengthening the perception and appreciation of physics in our society: it impressively demonstrates the strength of physics research and the special social responsibility that comes with it, namely to contribute to solutions for major global challenges through scientific findings from basic research.

I am also delighted that numerous companies from industry and business regularly show great interest in the DPG Industry and Book Exhibition. For this reason, this exhibition will also take place at our conference in Dresden. The exhibition also offers conference participants the opportunity to network with representatives from industry and business in a relaxed conference atmosphere through direct personal exchange, while also helping companies to attract skilled talents.

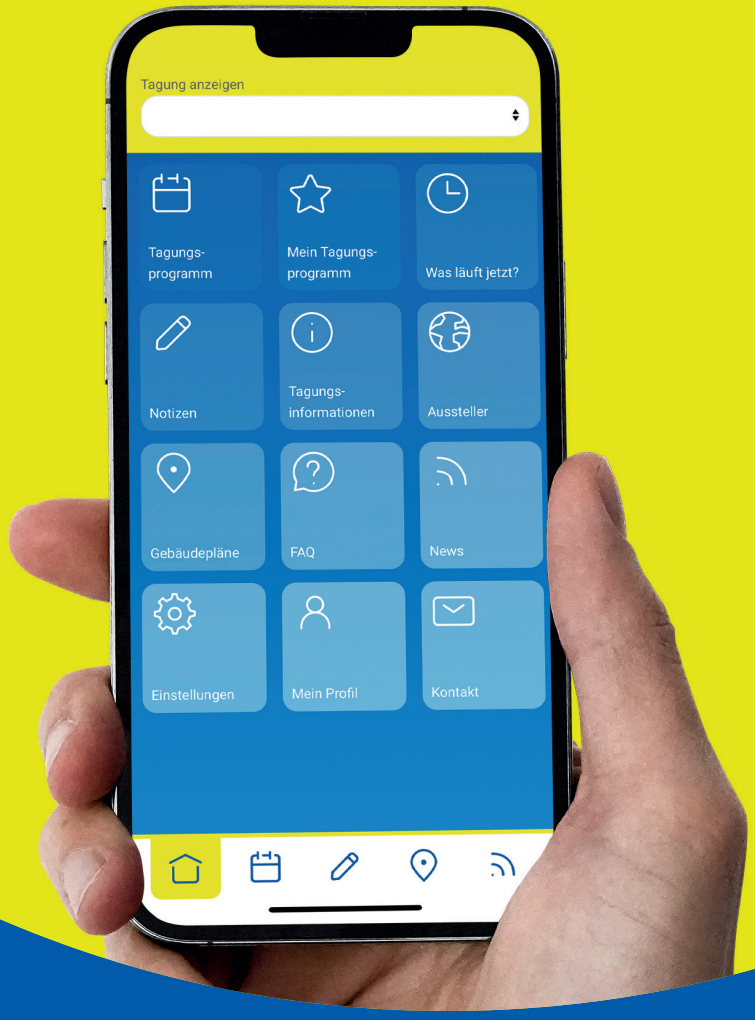
I would also like to point out that the DPG's communication focus for 2026 is artificial intelligence in the context of physics. Our goal is to promote discussion within physics and raise public awareness of the relevance of physics to AI research and development – and, last but not least, of the importance of AI in physics studies. Our DPG Spring Meeting in Dresden, with the participation of the Working Group on "Physics, Modern IT, and Artificial Intelligence" (AKPIK), offers ideal opportunities for discussions on these aspects as well.

The success of this Spring Meeting is only possible with the greatest commitment of many persons. I would like to express my sincere thanks to everyone involved. First of all, I would like to thank Dresden University of Technology for their hospitality and support. Many thanks also to the Wilhelm und Else Heraeus-Stiftung for generously supporting all DPG Spring Meetings. I would also like to thank the spokespersons of the DPG Condensed Matter Section, Prof. Sarah Köster and Prof. Elke Scheer, and the chairpersons of participating DPG Divisions and Working Groups for organising the excellent scientific programme. My special thanks go to the local organising committee at TU Dresden, headed by Prof. Jochen Geck, Institute of Solid State and Materials Physics. Finally, I would like to thank the DPG Head Office for its great support of all Spring Meetings.

Prof. Dr. Klaus Richter

President
Deutsche Physikalische Gesellschaft e. V.

DPG



Laden im App Store

JETZT BEI Google Play

Navigate the Spring Meeting with the DPG App!

The DPG app informs you about the conference programme, the venues and the exhibitors. Features such as your personal conference calendar and detailed floor plans simplify finding your way around the conference!

for iOS

for Android

Explore conference contributions on the new DPG Map.

CURRENTLY IN BETA

Dive into our network visualization and find related contributions.

Visit our platform at map.dpg-verhandlungen.de

Organisation

Organiser

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Homepage www.dpg-physik.de

Local Organiser

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Technische Universität Dresden
Institut für Festkörper- und Materialphysik
Haecklstraße 3, 01062 Dresden
Phone +49 (0) 351 463 37589
Email dresden26@dpg-tagungen.de

Scientific Organisation

Chair of the Condensed Matter Section (SKM)

Prof. Dr. Sarah Köster
Institut für Röntgenphysik
Universität Göttingen
Friedrich-Hund-Platz 1, 37077 Göttingen
Phone +49 (0) 551 39 29429
Email sarah.koester@uni-goettingen.de

Chairs of the Participating Divisions of the DPG:

(BP)	Biological Physics	–	Prof. Dr. Kristian Franze (kristian.franze@fau.de)
(CPP)	Chemical and Polymer Physics	–	Prof. Dr. Christine M. Papadakis (papadakis@tum.de)
(DD)	Physics Education	–	Prof. Dr. Susanne Heinicke (susanne.heinicke@uni-muenster.de)
(DS)	Thin Films	–	Prof. Dr. Stefan Krischok (stefan.krischok@tu-ilmenau.de)
(DY)	Dynamics and Statistical Physics	–	Prof. Dr. Carsten Beta (carsten.beta@uni-potsdam.de)
(FM)	Functional Materials	–	Dr.-Ing. Jan Schultheiß (jan.schultheiss@ntnu.no)
(HL)	Semiconductor Physics	–	Prof. Dr. Rudolf Bratschitsch (rudolf.bratschitsch@uni-muenster.de)
(MA)	Magnetism	–	Prof. Dr. Claudia Felser (claudia.felser@cpfs.mpg.de)
(MM)	Metal and Material Physics	–	Prof. Dr. Astrid Pundt (astrid.pundt@kit.edu)
(O)	Surface Science	–	Prof. Dr. Wolf Widdra (widdra@physik.uni-halle.de)
(QI)	Quantum Information	–	Prof. Dr. Christoph Marquardt (christoph.marquardt@fau.de)
(SOE)	Physics of Socio-economic Systems	–	Dr. Philipp Hövel (phoevel@physik.tu-berlin.de)
(TT)	Low Temperature Physics	–	Prof. Dr. Stefan Kehrein (stefan.kehrein@theorie.physik.uni-goettingen.de)
(UP)	Environmental Physics	–	Dr. Stefanie Falk (stefanie.falk@kit.edu)
(VA)	Vacuum Science and Technology	–	Dr. Stylianos Varoutis (stylianos.varoutis@kit.edu)

Chairs of the Participating Working Groups

(AGK)	Climate	–	Prof. Dr. Karim Zantout (zantout@dpg-mail.de)
(AGYouLeap)	Young Leaders in Physics	–	Dr. Aisha Aqeel (aisha.aqeel@uni-a.de) Dr. Lucas Kreuzer (lucas.kreuzer@frm2.tum.de)
(AKBP)	Accelerator Physics	–	Prof. Dr. Ulrich Schramm (u.schramm@hzdr.de)
(AKC)	Equal Opportunities	–	OStR Agnes Sandner (akc@dpg-physik.de)
(AKPIK)	Physics, Modern IT and Artificial Intelligence	–	Dr. Arash Rahimi-Iman (arash.rahimi-iman@physik.jlug.de)
(AIW)	Industry and Business	–	Dr. Hans-Georg Grothues (hg.grothues@dlr.de)
(AKjDPG)	Young DPG	–	Pauleo Nimtz (nimtz@jdpg.de)

Symposia

SYAI – AI and Data Challenges behind Emerging Self-Driving Laboratories
SYBS – Fluids with Broken Time-Reversal Symmetry: Odd/Hall Viscosity between Active Matter and Electron Flows
SYBT – Beyond Transistors: Material-Based Edge Computing Paradigms
SYFC – Designing Quantum Materials with Light: From Floquet to Cavity Engineering
SYGF – Guest of honour symposium France: Soft, Active and Alive: Emergent Properties in Living Matter
SYQF – Interacting Degrees of Freedom in Ultrathin Quantum Films
SYSC – The Sustainability Challenge: A Decade of Transformation
SYSD – SKM Dissertation Prize 2026
SYTP – Tipping Points in Social and Climate Systems

Organisation of the Exhibition of Scientific Instruments and Literature

DPG-Ausstellungs-, Kongreß- und Verwaltungsgesellschaft mbH (DPG-GmbH)
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Website www.dpg-gmbh.de

Programme

The scientific programme consists of **4,788** contributions:

11	Plenary Talks
1	Evening Talk
8	Prize Talks
1	Ceremonial Talk
4	Lunch Talks
255	Invited Talks
68	Topical Talks
3,157	Contributions
13	Tutorials
1,264	Posters
6	Discussions

The programme stated in this document corresponds to the status of January 30, 2026 and will not be updated!

Professional and personal development with the DPG

CAREER DEVELOPMENT TRAINING

DPG Akademie

Enhance your methodological and personal skills with practical training and seminars designed to elevate your career.

MORE INFO

STRATEGIC CAREER PLANNING

PIB (Physicists in the Workplace)

Discover valuable guidance and unique insights while networking in the inspiring setting of the Conference Centre and DPG Head Office.

MORE INFO

LEADERSHIP SKILLS DEVELOPMENT

Leading for Tomorrow

Acquire essential leadership skills to thrive in academia, industry and science management.

MORE INFO

STREAMLINED CAREER TRANSITION

DPG Mentoring

Experienced mentors support your career planning (with a focus on industry and business) and accompany you on your journey.

MORE INFO

CONNECTING MINDS

WTT Forum

Connecting students, researchers, founders and industry in DeepTech, spin-offs, joint ventures and startups — a hub for exchange and inspiration.

MORE INFO

Information for Participants

The conference will be held March 8 – 13, 2026.

Guest Country at the Conference
For the 2026 edition of the Spring Meeting of the Condensed Matter Section we are very happy to welcome France, represented by the Société Française de Physique (SFP), as our guest country.

On this special occasion, we will feature a number of events during the conference. We invite all conference participants to join these events and use the opportunity to strengthen their networks with our neighbours.

Conference Information

Mutual Respect at Conferences
All participants are requested to contribute to a conference that values respect and a spirit of open communication. Please be mindful in your interactions with other participants – whether during individual sessions or elsewhere during the conference, and consider that individuals with diverse backgrounds may be sensitive to different forms and manifestations of social behavior, scientific criticism, and appreciation. Also note that any form of encroaching behaviour has no place at the DPG's meetings. Do not hesitate to contact the conference's awareness team, the conference office or the local conference organisers in the event of disturbances. The conference organiser will take appropriate action.

Conference Venue
Technische Universität Dresden (TUD)
Campus Südvorstadt
Bergstraße 64
01069 Dresden

The conference will take place on the campus Südvorstadt of the TUD. The central activities like registration etc. will take place in the Lecture Hall Center (HSZ) of the TUD (Bergstraße 64). For a detailed map of the campus and the buildings please see "Maps" at the end of this document. The position of the lecture rooms on the campus can be found at the campus navigator of TU Dresden *https://navigator.tu-dresden.de/* or the DPG-App.

Conference Office / Information Desk
The conference office and the information desk are located in the Lecture Hall Center, HSZ E01. The opening hours are the following:

		Registration	**Information Desk**
Sunday	March 08	15:00 – 19:00	15:00 – 20:00
Monday	March 09	08:00 – 18:00	08:00 – 20:00
Tuesday	March 10	08:00 – 16:00	08:00 – 18:00
Wednesday	March 11	08:00 – 16:00	08:00 – 18:00
Thursday	March 12	08:00 – 16:00	08:00 – 18:00
Friday	March 13	08:00 – 12:00	08:00 – 15:00

You will receive your name tag, a receipt for your conference fee, the login password for using WiFi as well as food and drink vouchers for the Welcome Evening (Sunday 18:30-21:30). The name tag must be worn visibly during the entire conference.
The organisers, staff of the conference desk and student assistants will be identifiable by colored name tags and T-shirts. Please contact them if you have any questions. Do not hesitate to come to the information desk and inquire about all necessary information concerning the conference, orientation in Dresden, accommodation, restaurants, going out and cultural events.

Lecture Rooms
The lecture rooms will be signposted by abbreviations for the respective buildings and the room number. The campus map and location of the buildings are printed at the end of this document.

Abbr.	**Building**		
BAR	Barkhausen-Bau	POT	Gerhard-Potthoff-Bau
BEY	Beyer-Bau	SCH	Georg-Schumann-Bau
CHE	Chemiegebäude (Chemistry Building)	TRE	Trefftz-Bau
REC	Recknagel-Bau	Tent A	Tent behind the Lecture Hall Center / Exhibition
GER	von-Gerber-Bau	Tent C	Mommsenstr. 10 (in front of the 'Alte Mensa' Mommsenstraße)
GÖR	Görges-Bau	WIL	Willers-Bau

HÜL	Hülsse-Bau	ZEU	Zeuner-Bau
HSZ	Hörsaalzentrum (Lecture Hall Center)	MER	Merkel-Bau

Presentations
Scientific presentations will be held either as oral presentations or posters. Presentations are typically held in English.

Oral Presentations
Speakers are requested to provide their presentations electronically. All lecture rooms are equipped with a projector ("beamer") with HDMI input.

Laptops as well as necessary hdmi adapters must be provided by the speakers. Furthermore, please bring a copy of your presentation in pdf or pptx format on a USB flash drive.

All laptops must be set up and connected with the projector before the start of the respective session. All rooms will be opened at latest 30 minutes prior to the session. Speakers are requested to be in the lecture room at least 20 minutes prior to the start of the session, to report to the chairperson as well as the technical staff, to ensure that the laptops handshake with the projector, and to receive a brief introduction to the equipment in the lecture room.

Poster Presentation
Sites for poster sessions are named and located as follows:

P1	Tent A behind the Lecture Hall Center (Exhibition Tent)
P2	Tent C Mommsenstraße 10 (in front of the Mensa 'Mommsenstraße')
P4	Room HSZ/0304, 3rd floor
P5	Room ZEU/0250, 2nd floor

Posters must fit within a rectangle 90 cm wide and 120 cm high (DIN A0), portrait format!

The poster boards will be marked with the number according to the scientific programme. Authors are asked to mount their poster when the poster board is prepared with the corresponding poster number. Usually this will be arranged in the morning, or one hour before the session when there are several poster sessions per day. Each poster should display the number according to the scientific programme.

For the mounting of the poster please use the prepared "power strips" at the poster frame or contact the available student staff. Please make sure to use only power strips for mounting the poster (residue-free removing). The presenting authors should be available for discussion at their poster during for at least half of the poster session and should announce by a note this time at the poster.

The posters have to be removed after the poster session. Any posters remaining on display walls after the poster session will be removed and disposed of without requesting your permission. The conference management accepts no liability for the posters.

Notice Board
All changes to the conference programme (i.e. cancellation of presentations, change of rooms, etc.) are transferred directly to the online version of the programme which is available in different formats (sorted by publication date, filterable by conference parts and as an rss-feed). Please use the form *dresden26.dpg-tagungen.de/programme/notice-board-form* to notify changes or cancellations. All changes are also displayed in the DPG app so that the displayed programme is always up-to-date.

Communication / Internet Access
EDUROAM
The TU Dresden is member of the eduroam-network. Users from eduroam institutions, who have registered for eduroam, can use WLAN at the TU Dresden without local registration in Dresden. Eduroam in Dresden is possible with WLAN SSID eduroam.

WiFi in the buildings of TU-Campus
For internet access at TU Dresden, please use your individual login-password on your registration document. Please search for and connect to the network named "VPN/WEB". After you have been connected, please visit any website with your browser to get redirected to the login page of the network. Enter your username and password and click on "Login". Afterwards you should be able to access the internet. This connection is not encrypted.

Public Working Area
Public working rooms which you can use as workspace are located in BEY/0117, BEY/0E25 and MER/0003.

Cloakroom
In the basement of the Lecture Hall Centre (HSZ) you will find a cloakroom free of charge managed by student assistants. The opening hours are as follows:

Sunday	March 08	15:00 — 21:30
Monday	March 09	08:00 — 21:30
Tuesday	March 10	08:00 — 20:30
Wednesday	March 11	08:00 — 20:30
Thursday	March 12	08:00 — 22:00
Friday	March 13	08:00 — 14:00

Lost and Found Property
Please bring found items to the Lecture Hall Center, room E03 (next to the information desk). There you can also get your lost property back.

Catering

Coffee Breaks
Coffee and tea are offered for free during the breaks in nearly all conference locations (see also in the legend of the campus map). You want to actively contribute to protect our climate and environment? Then please bring your own cup or use your paper cup several times. Thank you!

Snacks
You can get coffee, tea, refreshments and snacks as indicated in the campus map at the:

• Tent B behind the Lecture Hall center	Monday to Thursday, 08:00 – 15:00; Friday 08:00 – 14:00
• Restaurant of the Leibniz-Institute IFW Dresden	Monday to Friday, 08:00 – 15:00
• „insgrüne coffeebar“ in the Georg-Schumann-Bau (SCH)	Monday to Friday, 10:00 – 15:00
• Cafeteria & Mensa ‘Alte Mensa’, Mommsenstraße 13	Monday to Thursday, 08:00 – 16:00; Friday 08:00 – 15:00
• Cafeteria & Mensa Zeltschlösschen, Nürnberger Str. 55	Monday to Friday, 08:00 – 15:30
• Cafeteria & Mensa Siedepunkt, Zellescher Weg 17	Monday to Friday, 11:00 – 14:30

as well as at Bergstr. 68 „FIRAT-Kebap-Haus“ and Münchner Str. „DERSIM-Dürüm-Kebab-Haus“ and bakery „Möbius“.

Lunch
The Mensa Zeltschlösschen, Mensa Siedepunkt and the ‘Alte Mensa’ Mommsenstraße offer plenty of opportunities for lunch at moderate prices (self-payment). The IFW restaurant offers regular meals for a limited number of conference participants.

Wilhelm and Else Heraeus Communication Programme
Important notes for participants who apply for a grant in the WEH Communication Programme:
When registering at the conference office, you will receive your receipt of the conference fee along with a certificate for the WE-Heraeus Communication Programme. Please keep this document safe. Participation in the conference must be certified at the conference office with a stamp on the WEH receipt on the day of departure. You have the possibility to leave the stamped certificate with the staff members of the DPG (recommended!) or submit it to the DPG head office *weh@dpg-physik.de* by April 3, 2026 at the latest. For more detailed information refer to *weh.dpg-physik.de.*

The Deutsche Physikalische Gesellschaft thanks the Wilhelm and Else Heraeus Foundation for the generous financial support of young academic talents. We hope that young physicists will continue to seize the offered opportunity for active scientific communication at scientific conferences. A total of about 44,800 young academics were supported by this programme so far.

CO_2 Compensation for the DPG Conferences
By decision of its council, the DPG will compensate for fossil CO_2 emissions resulting from mobility for DPG conferences and committee meetings.

Acknowledgement
The Deutsche Physikalische Gesellschaft (DPG) and the local organisers want to thank the following institutions for supporting the conference:

- the Wilhelm and Else Heraeus Foundation, Hanau
- the TU Dresden
- the official sponsors of the DPG-Frühjahrstagung
- and all staff, who make the success of the conference possible.

SAY CHEESE!
The DPG Spring Meetings are basically public to the press. Please note: On behalf of DPG, photos and videos will be recorded during the Spring Meetings. In the context of public relations, these recordings (as the case may be) will be published on our website, in social media or within prints of the DPG for example.

Liability Exclusion
Participants are asked to look carefully after their wardrobe, valuables, laptops, and other belongings. The organisers decline any liability.

Social Events (in chronological order)

Welcome Evening
On Sunday, March 8, 18:30 – 21:30 the Welcome Evening will be held in the 'Alte Mensa', Mommsenstraße 13. Snacks, beer and soft drinks will be served. Do not miss the opportunity to register (15:00 – 19:00) before the official beginning of the conference and to meet people in an informal atmosphere. When registering for the conference you will receive your badge and food and drink vouchers for the Welcome Evening. Please wear your badge which you have received at the registration.

Opening of the Conference
A short opening address will be given by the chair of the Condensed Matter Section (SKM) on Monday, March 9 from 8:25 until 8:30 in HSZ/AUDI.

Einstein Slam
Monday, March 9, 20:00, HSZ/AUDI
Einstein Slam is the competitive art of making complex science accessible to a broad audience. There are just 10 minutes for every attendee to present their self-made performance. The event will finish with a public poll in order to evaluate if a particular contribution was either instructive and amusing or rather should have never been performed. All presentations will be given in English. For more information please refer to *www.einstein-slam.de*.

Ceremonial Session with Award Ceremony
On Tuesday, March 10, at 16:00 the Ceremonial Session with Award Ceremony will take place in HSZ/AUDI. The programme is as follows:

Music
"*SCHOOKO DUO*"

Welcome
Prof. Dr. Jochen Geck, TU Dresden
Local Organiser

Speech
Prof. Dr. Klaus Richter
President of the Deutsche Physikalische Gesellschaft e.V.

Music

Award Ceremony

Walter-Schottky-Prize 2026
to Dr. Marcel Reutzel, Georg-August-Universität Göttingen / Philipps-Universität Marburg

Gaede-Prize 2026
to Dr. Anna Rosławska, MPI für Festkörperforschung, Stuttgart

Dissertation Prize of the Condensed Matter Section 2026
(The Laureate will be announced after the SKM-Dissertations-Prize Symposium)

Music

Ceremonial Lecture
Prof. Dr. Frank Wilhelm-Mauch, Forschungszentrum Jülich GmbH
"*Quantum computers as large research instruments – what can we expect and how do we develop them?*"

jDPG Pub Crawl
Tuesday, March 9, 20:00
Meeting Point: in front of the Hörsaalzentrum HSZ (Bergstraße side)
On Tuesday evening, the young DPG invites to a pub crawl through Dresden. Next to the opportunity to be on a move outside and network with others, the members of the local regional group will tell about the Dresden physics, the life in the city and other facts worth knowing.

Exhibition of Scientific Instruments and Literature
From Tuesday to Thursday there will be an exhibition of Scientific Instruments and Literature. The exhibition will take place in the exhibition tents A (beside the Lecture Hall Centre) and C (Mommsenstraße 10). More than 130 companies (see list of exhibitors at the end of this document) will present their products. Opening hours are from 09:30 to 18:00 (Thursday until 15:00). All conference participants are welcome to attend the exhibition. The entrance is free.

Public Evening Talk (in german language)
Wednesday, March 11, 19:00 – 20:00, HSZ/AUDI
Prof. Dr. Michèle Heurs, Leibniz Universität Hannover, will speak about "*Gravitationswellenastronomie — quo vadis?*"
The public evening talk is open for the interested public and all conference participants. The entrance is free.

Members' Assemblies of the Divisions and Working Groups
During the DPG Spring Meeting, Members' Assemblies of the DPG divisions and working groups take place. Please refer to the scientific programme for the time and place of the meetings.

Sponsors of the DPG Spring Meeting Dresden

Main Sponsors:

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WITTENSTEIN group

CFM
INSIGHT.DATA.CLARITY.

Cryo andmore

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EUROPE

SPECSGROUP

THORLABS

Zurich
Instruments

Sponsors

magnitude
GENERATING FIELDS FOR SCIENCE AND TECHNOLOGY

MenloSystems

Park
SYSTEMS

Sumitomo
(SHI) Cryogenics of Europe GmbH

Schäfter+Kirchhoff

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SINCE 1963

Springer

WILEY

ELSEVIER

Quantum Valley
Lower Saxony

Deutsche Physikalische Gesellschaft DPG

DPG-FRÜHJAHRSTAGUNG DRESDEN 2026

Physik und Beruf

Jobbörse

in Kooperation mit Wiley VCH

Wo arbeiten Physiker:innen?

Di – Mi, 11:00 – 16:00 Uhr

HSZ/0405

Industrietag

Woran arbeiten Physiker:innen?

Mittwoch, 14:00 – 18:00 Uhr

H4

Mehr Informationen auf Seite 43

Industrieausstellung

Womit arbeiten Physiker:innen?

Di – Mi, 09:30 – 18:00 Uhr

Zelte A + C

Mehr Informationen auf Seite 13

Lunch Talks

Wie arbeiten Physiker:innen?

Mo – Do, 13:00 – 13:45 Uhr

HSZ/0002, HSZ/0003, HSZ/0004

Mehr Informationen auf Seite 59

Bei den Angeboten von „Physik und Beruf“ sind alle Tagungsteilnehmenden herzlich willkommen!

Sunday, March 8, 2026

TUT

Sessions

16:00	HSZ/0002	TUT 1	**Hands-on Tutorial: HyperSpy – Multidimensional data analysis using Python**
16:15	HSZ/0002	TUT 1.2	Hands-On Session 1: General usage HyperSpy/RosettaSciIO •Jonas Lähnemann
16:45	HSZ/0002	TUT 1.3	lumiSpy for luminescence spectroscopy •Aidan Campbell
17:15	HSZ/0002	TUT 1.4	Hyperspy for Electron Energy-loss Spectroscopy •Hannah Nerl
17:45	HSZ/0002	TUT 1.5	Using pyXem for magnetic and structural analysis of 4D-STEM data •Magnus Nord
16:00	BEY/0137	TUT 2	**Tutorial des Fachverbands Didaktik der Physik**
16:00	BEY/0137	TUT 2.1	Rethinking University Teaching: Creating interactive and sustainable learning environments in lectures •Susanne Heinicke
16:00	HSZ/0003	TUT 3	**Tutorial: Machine Learning Use Cases in Materials Science**
16:00	HSZ/0003	TUT 3.1	Welcome Remarks Arbeitskreis Physik, moderne Informationstechnologie und Künstliche Intelligenz •Arash Rahimi-Iman
16:05	HSZ/0003	TUT 3.2	A practical machine learning case study in materials science: Stumbling blocks, lucky breaks, and helpful colleagues •Max Grossmann, •Malte Grunert
16:50	HSZ/0003	TUT 3.3	Machine Learning-based Analysis of Electron Microscopy Images: Preprocessing and Synthetic Data Generation •Amir Omidvarnia
17:35	HSZ/0003	TUT 3.4	Machine Learning-based Analysis of Electron Microscopy Images: Segmentation •Amir Omidvarnia
16:00	HSZ/0004	TUT 4	**Tutorial: Physics of Behavior**
16:00	HSZ/0004	TUT 4.1	Physics of Behavior •Greg Stephens
17:15	HSZ/0004	TUT 4.2	Physics of Behavior •Antonio Carlos Costa
16:00	TRE/PHYS	TUT 5	**Hands-On Tutorial: Magnetic Structure Determination Using Fullprof and SARAh Representation Analysis**
16:00	TRE/PHYS	TUT 5.1	Recent advances and challenges in magnetic structure determination •Dmytro Inosov
16:30	TRE/PHYS	TUT 5.2	Hands-On Tutorial: Magnetic Structure Determination Using Fullprof and SARAh Representation Analysis •Matthias Frontzek
16:00	TRE/MATH	TUT 6	**Hands on Tutorial: Linking large language models with digital workflows for materials science simulations**
16:00	TRE/MATH	TUT 6.1	Hands on Tutorial: Linking large language models with digital workflows for materials science simulations •Jörg Neugebauer

18:30	Mensa Mommsenstraße	**Welcome Evening** (for registered participants)

Monday, March 9, 2026

Plenary Talks

08:30	HSZ/AUDI	PV I	Cavity-altered superconductivity •Dmitri Basov
14:00	HSZ/AUDI	PV II	Towards Intelligent Matter: Energy-Efficient In-Materio Computing •Karin Everschor-Sitte
14:00	HSZ/0002	PV III	Simulating the Hubbard model with moiré semiconductors •Jie Shan

Prize Talk

13:00	HSZ/0002	PRV I	Driven Quantum Materials: Controlling Emergent Phenomena away from Equilibrium •Andrea Cavalleri (Laureate of the Stern-Gerlach-Medal)

Lunch Talk, Discussion

13:00	HSZ/AUDI	PSV I	Sustainability! And now? – Opportunities for young researchers •Roxana Scharpegge
13:00	HSZ/0004	PSV II	Physics Meets Statistics: Advancing Data Analytics in Semiconductor Manufacturing •Sarah Fischbach

SYFC

Invited Talks

09:30	HSZ/AUDI	SYFC 1.1	Subcycle videography of strong-field controlled band structures •Rupert Huber
10:00	HSZ/AUDI	SYFC 1.2	Engineering Quantum Materials through Structured Cavity Vacuum Fluctuations •Angel Rubio
10:30	HSZ/AUDI	SYFC 1.3	Floquet engineering of quantum materials: from semiconductors to semimetals •Shuyun Zhou
11:15	HSZ/AUDI	SYFC 1.4	(Quantum) Light Control of Materials •Dante Kennes
11:45	HSZ/AUDI	SYFC 1.5	Lightwave-driven electrons in a Floquet topological insulator •Peter Hommelhoff

Session

09:30	HSZ/AUDI	SYFC 1	Designing Quantum Materials With Light: from Floquet to Cavity Engineering

SYSC

Invited Talks

15:00	HSZ/AUDI	SYSC 1.1	Open-Endedness and Community-Based Approaches to Sustainability Challenges •Hiroki Sayama
15:30	HSZ/AUDI	SYSC 1.2	Education as a Social Tipping Element: Evidence from Climate and Physics Education Research •Thomas Schubatzky
16:00	HSZ/AUDI	SYSC 1.3	Mechanistic and Material Perspectives on Enzymatic Hydrolysis of Semicrystalline Polyesters •Birte Höcker
16:45	HSZ/AUDI	SYSC 1.4	Decarbonization Options for Industry •Uwe Riedel
17:15	HSZ/AUDI	SYSC 1.5	Impacts of Cosmic Dust and Space Debris in the Terrestrial Atmosphere •John Plane

Session

15:00	HSZ/AUDI	SYSC 1	The Sustainability Challenge: A Decade of Transformation

Monday, March 9, 2026

SYSD

Invited Talks

09:30	HSZ/0002	SYSD 1.1	Stochastic-Calculus Approach to Non-equilibrium Statistical Physics •Cai Dieball
10:00	HSZ/0002	SYSD 1.2	Nonuniform magnetic spin textures for sensing, storage and computing applications •Sabri Koraltan
10:30	HSZ/0002	SYSD 1.3	Anomalous Quantum Oscillations beyond Onsager's Fermi Surface Paradigm •Valentin Leeb
11:00	HSZ/0002	SYSD 1.4	Coherent Control Schemes for Semiconductor Quantum Systems •Eva Schöll
11:30	HSZ/0002	SYSD 1.5	On stochastic thermodynamics under incomplete information: Thermodynamic inference from Markovian events •Jann van der Meer

Session

09:30	HSZ/0002	SYSD 1	SKM Dissertation Prize Symposium 2026

BP

Invited Talks

11:15	BAR/SCHÖ	BP 1.7	Modeling and inference of magnetotactic motility in complex environments •Stefan Klumpp
09:30	BAR/0205	BP 3.1	The unreasonable effectiveness of computational models in biological patterning and morphogenesis •Michel Milinkovitch
15:00	BAR/SCHÖ	BP 4.1	The Multi-faceted Role of Cholesterol in Cellular Membranes and Lipid Nanoparticles •Rainer Böckmann
17:15	BAR/0106	BP 8.3	Constructing synthetic life-like vesicle systems by integration of artificial metabolic reaction networks •Laura Heinen
16:45	BAR/0205	BP 9.1	Breaking the photobleaching limit in single-molecule FRET with nanophotonic DyeCycling. •Sonja Schmid

Sessions

09:30	BAR/SCHÖ	BP 1	Active Matter I
09:30	BAR/0106	BP 2	Computational Biophysics I
09:30	BAR/0205	BP 3	Tissue Mechanics I
15:00	BAR/SCHÖ	BP 4	Computational Biophysics II
15:00	BAR/0205	BP 5	Membranes, Vesicles and Synthetic Life-like Systems I
15:00	ZEU/0160	BP 6	Active Matter II
15:00	P5	BP 7	Poster Session I
16:45	BAR/0106	BP 8	Systems and Networks Biophysics
16:45	BAR/0205	BP 9	Single Molecule Biophysics

CPP

Invited Talks

09:30	ZEU/LICH	CPP 3.1	Theory and Modeling of Fluid Adsorption and Transport in Nanoporous Materials •Benoit Coasne
09:30	ZEU/0255	CPP 4.1	Exploration of Cathode Materials for Li-S Batteries •Yan Lu
09:30	ZEU/0260	CPP 5.1	Cleaning of dusty surfaces •Doris Vollmer
11:15	ZEU/LICH	CPP 6.1	Hierarchical Porosity Meets Nanoconfined Water: Toward Water-Driven Functional Materials •Patrick Huber

Monday, March 9, 2026

CPP

15:00	ZEU/LICH	CPP 9.1	Why Polymers Swell or Collapse: Molecular Insights into Cosolute Effects •Nico van der Vegt
15:00	ZEU/0255	CPP 12.1	Multifunctional films by tailoring chemistry and morphology of polymer brushes at the nanoscale •Petra Uhlmann
16:30	ZEU/0255	CPP 12.6	Thin-film and interface properties in energy conversion devices unveiled by X-rays •Marcus Bär
15:00	ZEU/0260	CPP 13.1	Modelling and simulation of pH-sensitive polyelectrolyte microgels •Stefanie Schneider
17:15	ZEU/0260	CPP 16.1	Understanding the Passivation Properties of Solid Electrolyte Interphases (SEIs) in Batteries: Generator-Collector Experiments combined with a Transport and Reaction Model •Bernhard Roling

Sessions

09:30	BAR/SCHÖ	CPP 1	Active Matter I
09:30	MER/0002	CPP 2	Sustainability: Challenges and Solutions
09:30	ZEU/LICH	CPP 3	French-German Session: Membranes and Porous Materials I
09:30	ZEU/0255	CPP 4	Energy Storage Materials and Devices I
09:30	ZEU/0260	CPP 5	Wetting, Fluidics and Liquids at Interfaces and Surfaces I
11:15	ZEU/LICH	CPP 6	French-German Session: Membranes and Porous Materials II
11:30	ZEU/0255	CPP 7	Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods I
11:30	ZEU/0260	CPP 8	Wetting, Fluidics and Liquids at Interfaces and Surfaces II
15:00	ZEU/LICH	CPP 9	French-German Session: Simulation Methods and Modeling of Soft Matter I
15:00	ZEU/0118	CPP 10	Droplets, Wetting, and Microfluidics
15:00	ZEU/0160	CPP 11	Active Matter II
15:00	ZEU/0255	CPP 12	French-German Session: 2D Materials, Thin Films and Interfaces I
15:00	ZEU/0260	CPP 13	Charged Soft Matter, Polyelectrolytes and Ionic Liquids
17:15	ZEU/LICH	CPP 14	French-German Session: Simulation Methods and Modeling of Soft Matter II
17:15	ZEU/0255	CPP 15	Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods II
17:15	ZEU/0260	CPP 16	Energy Storage Materials and Devices II
19:00	P5	CPP 17	Poster I

DS

Sessions

09:30	REC/C213	DS 1	Organic Thin Films
15:00	HSZ/0003	DS 2	Focus Session: Tunable Correlations in van der Waals Quantum Materials I
15:00	REC/C213	DS 3	Thin Film Properties I: Methods
16:30	REC/C213	DS 4	Thin Film Properties II

DY

Invited Talks

09:30	ZEU/0114	DY 7.1	Fast Rare Events in Exit Times Distributions of Jump Processes •Raffaella Burioni
11:15	ZEU/0114	DY 7.6	Large deviations in resetting Brownian motions •Satya Majumdar
10:30	ZEU/0118	DY 8.5	Mean-field approach to finite-size fluctuations in coupled oscillator systems •Oleh Omelchenko
15:00	ZEU/0114	DY 15.1	Monte Carlo Simulation Methods for Rare-Event Sampling •Wolfhard Janke
17:00	ZEU/0160	DY 17.8	Topological transition in filamentous cyanobacteria: from motion to structure •Marco Mazza

Monday, March 9, 2026

DY

Sessions

09:30	HSZ/0003	DY 2	Focus Session: New Routes to Localization and Quantum Non-Ergodicity I
09:30	HSZ/0101	DY 3	Quantum-Critical Phenomena
09:30	BAR/SCHÖ	DY 4	Active Matter I
09:30	GÖR/0226	DY 5	Focus Session: Physics of Behavior
09:30	HÜL/S186	DY 6	Machine Learning in Dynamics and Statistical Physics I
09:30	ZEU/0114	DY 7	Focus Session: Large Deviations and Rare Events I
09:30	ZEU/0118	DY 8	Nonlinear Dynamics, Synchronization, and Chaos
09:30	ZEU/0160	DY 9	Statistical Physics far from Thermal Equilibrium I
09:30	ZEU/0260	DY 10	Wetting, Fluidics and Liquids at Interfaces and Surfaces I
11:30	ZEU/0260	DY 11	Wetting, Fluidics and Liquids at Interfaces and Surfaces II
15:00	CHE/0089	DY 12	Focus Session: Relaxation Timescales in Open Quantum Systems
15:00	CHE/0091	DY 13	Focus Session: New Routes to Localization and Quantum Non-Ergodicity II
15:00	HÜL/S186	DY 14	Machine Learning in Dynamics and Statistical Physics II
15:00	ZEU/0114	DY 15	Focus Session: Large Deviations and Rare Events II
15:00	ZEU/0118	DY 16	Droplets, Wetting, and Microfluidics
15:00	ZEU/0160	DY 17	Active Matter II

FM

Invited Talk

15:00	BEY/0138	FM 4.1	(Anti)Ferroelectric HfZrO2: from non volatile memory to energy storage applications •Bertrand Vilquin

Sessions

09:30	BEY/0138	FM 2	Energy Materials
09:30	POT/0151	FM 3	Focus Session: Novel mechanisms of ferroic switching
15:00	BEY/0138	FM 4	Focus Session: (Anti)ferroic states – Non-conventional states I
15:00	BEY/0E40	FM 5	Focus Session: Holistic structural and safety assessment of battery materials and cells

HL

Invited Talks

09:30	POT/0051	HL 2.1	Intrinsically stretchable polymers and devices for biosensing applications •Ulrike Kraft
10:00	POT/0051	HL 2.2	Complexity in Organic Mixed Ionic Electronic Conductors and its Application in Neuromorphic Computing •Hans Kleemann
10:30	POT/0051	HL 2.3	Organic Neuromorphic Interfaces for Biohybrid Systems: Material and Structural Biomimicry of Synaptic Plasticity •Francesca Santoro
11:15	POT/0051	HL 2.4	Fully-organic flexible detectors for real-time dose monitoring during radio/proton therapy •Beatrice Fraboni
11:45	POT/0051	HL 2.5	Organic LEDs and photodetectors for light-based diagnostics and therapy •Caroline Murawski
09:30	POT/0251	HL 4.1	X-ray nanodiffraction studies of lead-halide perovskite supercrystals •Ivan Zaluzhnyy
15:00	POT/0251	HL 11.1	Quantum Repeater Hardware made from Silicon Carbide •Jörg Wrachtrup
15:30	POT/0251	HL 11.2	Diamond based quantum sensing for drug testing •Romana Schirhagl
16:00	POT/0251	HL 11.3	The oxygen-related ST1 centre in diamond: a room temperature coherently controllable electron spin •Sebastien Pezzagna

Monday, March 9, 2026

HL

16:45	POT/0251	HL 11.4	Silicon quantum emitters emitting in the optical telecommunication range for scalable quantum photonic circuits •Yonder Berencén
17:15	POT/0251	HL 11.5	Advances in materials processing for quantum sensing •Adam Gali

Sessions

09:30	POT/0006	HL 1	Optical Properties I
09:30	POT/0051	HL 2	Focus Session: Biocompatible Organic Semiconductors for Artificial Intelligence
09:30	POT/0081	HL 3	2D Materials I – Excitonic properties
09:30	POT/0251	HL 4	Perovskite and Photovoltaics: Synthesis and Performance
10:30	TRE/MATH	HL 5	2D Materials: Electronic structure, excitations, etc. I
15:00	HSZ/0003	HL 6	Focus Session: Tunable Correlations in van der Waals Quantum Materials I
15:00	HSZ/0204	HL 7	2D Materials beyond graphene: Growth, structure and substrate interaction
15:00	POT/0006	HL 8	Ultra-fast Phenomena I
15:00	POT/0051	HL 9	Oxide Semiconductors: Growth and Fabrication
15:00	POT/0081	HL 10	2D Materials II – Electronic and transport properties
15:00	POT/0251	HL 11	Focus Session: Quantum Emitters in 3D Semiconductors
16:45	POT/0051	HL 12	Heterostructures, Interfaces and Surfaces: Photonics
16:45	POT/0081	HL 13	2D Materials III – Interlayer excitons

MA

Invited Talks

09:30	POT/0151	MA 4.1	From ML to Kinetics: Modeling the Switching in Ferroelectric Wurtzites •Andrew Rappe
10:00	POT/0151	MA 4.2	Topological order parameter switching •Sergey Artyukhin
10:30	POT/0151	MA 4.3	Optical Control of Ferroaxial Order via Circular Phonon Excitation •Zhiyang Zeng
15:00	POT/0112	MA 10.1	Multi-field analysis of magnetic materials: Phase-field based simulations of magnetic domains and phase transition •Mobina Alaeddini
15:20	POT/0112	MA 10.2	Realistic Modelling of Finite Temperature Electron Transport Properties in Ferromagnets •Fabian Engelke
15:55	POT/0112	MA 10.3	Exploring magneto- and multicaloric materials for room and cryogenic temperature applications •Benedikt Beckmann
16:20	POT/0112	MA 10.4	Nonlinear magnon dynamics: From the discovery of Floquet magnons to CMOS-compatible magnon computing •Christopher Heins
16:45	POT/0112	MA 10.5	The geometric memory of quantum wave functions •Niclas Heinsdorf
17:10	POT/0112	MA 10.6	Altermagnets and Odd-parity-wave Magnets •Anna Birk Hellenes

Sessions

09:30	HSZ/0004	MA 2	Altermagnets I
09:30	POT/0112	MA 3	Complex Magnetic Oxides
09:30	POT/0151	MA 4	Focus Session: Novel mechanisms of ferroic switching
09:30	POT/0351	MA 5	Surface Magnetism and Topological Insulators
09:30	POT/0361	MA 6	Magnetic Imaging Techniques I
09:30	P2	MA 7	Poster Magnetism I
15:00	HSZ/0002	MA 8	Altermagnets II
15:00	HSZ/0004	MA 9	Magnonics I
15:00	POT/0112	MA 10	INNOMAG e.V. Prizes 2026 (Diplom-/Master and Ph.D. Thesis)
15:00	POT/0151	MA 11	Electron Theory of Magnetism and Correlations
15:00	POT/0351	MA 12	Terahertz Spintronics
15:00	POT/0361	MA 13	Magnetic Heuslers and Semiconductors

Monday, March 9, 2026

MM

Invited Talks, Topical Talks

09:30	SCH/A251	MM 2.1	Deep-Learning and Generative AI for the Discovery of Electron-Phonon Superconductors •Richard Hennig
10:15	SCH/A216	MM 4.1	Photoelectric properties of dislocations in SrTiO3 single crystals •Marin Alexe
10:15	SCH/A251	MM 5.1	Machine Learning for Materials Discovery: from Big Data to Predictive Insights •Silvana Botti
11:45	SCH/A251	MM 5.5	Leveraging data science technologies to enable AI-driven materials design •Tilmann Hickel
15:00	SCH/A251	MM 6.1	Transformation-induced plasticity in zirconia ceramics: simulations and experiments •David Rodney
15:45	SCH/A251	MM 9.1	Atomistic simulations in the ternary Fe-O-H system: interatomic potential development and applications •Baptiste Bienvenu

Sessions

09:30	SCH/A251	MM 2	Invited Talk: Richard Hennig
10:15	SCH/A215	MM 3	Mechanical Properties and Alloy Design I
10:15	SCH/A216	MM 4	Materials for the Storage and Conversion of Energy I
10:15	SCH/A251	MM 5	Topical Session: Physics-driven Artificial Intelligence for Materials I
15:00	SCH/A251	MM 6	Invited Talk: David Rodney
15:45	SCH/A215	MM 7	Mechanical Properties and Alloy Design II
15:45	SCH/A216	MM 8	Materials for the Storage and Conversion of Energy II
15:45	SCH/A251	MM 9	Topical Session: Physics-driven Artificial Intelligence for Materials II

O

Invited Talks, Topical Talk

09:30	TRE/PHYS	O 1.1	Vortices, inter-band coupling and inelastic QPI in two band superconductors •Wulf Wulfhekel
11:00	HSZ/0201	O 2.3	Superconducting Fermi arcs. •Andrii Kuibarov
10:30	HSZ/0403	O 5.1	Can the mineral-water interface save the world? Mineral carbonation, enhanced weathering and negative emissions •Philip Pogge von Strandmann
11:30	HSZ/0403	O 5.4	Machine learning exploration of water binding and ice nucleation at silicate and carbon surfaces •Mie Andersen
10:30	TRE/MATH	O 7.1	Magnetic Order in 2D Materials Beyond Bulk Constraints •Jeison Fischer
11:00	WILL/A317	O 8.3	Controlling nanostructures on surfaces via intermolecular interactions •Yunjun Cao
15:00	TRE/MATH	O 14.1	Spin and time-resolved ARPES and the orbital angular momentum of light •Mauro Fanciulli
15:00	WILL/A317	O 15.1	Tuning Spin-1/2 Interactions in Graphene: From Long-Range Coupling to Altermagnetic Order •Beatriz Viña-Bausá

Sessions

09:30	TRE/PHYS	O 1	Topical Talk Wulfhekel
10:30	HSZ/0201	O 2	Electronic structure of surfaces: Spectroscopy, surface states I
10:30	HSZ/0204	O 3	Scanning probe techniques: Method development I
10:30	HSZ/0401	O 4	Metal & Semiconductor substrates: Adsorption and reaction of small molecules I
10:30	HSZ/0403	O 5	Focus Session: Mineral-water interfaces I
10:30	TRE/PHYS	O 6	Organic molecules on inorganic substrates: Adsorption and growth I
10:30	TRE/MATH	O 7	2D Materials: Electronic structure, excitations, etc. I
10:30	WILL/A317	O 8	Nanostructures at surfaces:1D, 2D, networks I

Monday, March 9, 2026

O

15:00	HSZ/0201	O 9	Organic molecules on inorganic substrates: electronic, optical and other properties I
15:00	HSZ/0204	O 10	2D Materials beyond graphene: Growth, structure and substrate interaction
15:00	HSZ/0401	O 11	Metal & Semiconductor substrates: Adsorption and reaction of small molecules II
15:00	HSZ/0403	O 12	Scanning probe microscopy: light matter interaction at atomic scales
15:00	TRE/PHYS	O 13	Solid-liquid interfaces: Reactions and electrochemistry I
15:00	TRE/MATH	O 14	Ultrafast electron dynamics at surface and interfaces I
15:00	WILL/A317	O 15	Spins on surfaces at the atomic scale I
18:00	P2	O 16	Focus Session: Structure and Dynamics of Solvent at Electrochemical Interfaces – Poster
18:00	P2	O 17	Spins on surfaces at the atomic scale – Poster
18:00	P2	O 18	New methods: Theory – Poster
18:00	P2	O 19	Vacuum Science & Technology: Theory and Applications – Poster
18:00	P2	O 20	Electronic structure theory – Poster
18:00	P2	O 21	Surface magnetism – Poster
18:00	P2	O 22	Surface dynamics – Poster
18:00	P2	O 23	Catalysis and surface reactions – Poster
18:00	P2	O 24	Solid-liquid interfaces: Reactions and electrochemistry – Poster
18:00	P2	O 25	Solid-liquid interfaces: Structure, spectroscopy – Poster
18:00	P2	O 26	Plasmonics and nanooptics: Fabrication, characterization and applications – Poster
18:00	P2	O 27	Plasmonics and nanooptics: Light-matter interaction, spectroscopy – Poster
18:00	P2	O 28	Oxide and insulator surfaces: Structure, epitaxy and growth – Poster
18:00	P2	O 29	Oxides and insulators: Adsorption and reaction of small molecules – Poster
18:00	P2	O 30	Metal & Semiconductor substrates: Structure, epitaxy and growth – Poster
18:00	P2	O 31	Metal & Semiconductor substrates: Adsorption and reaction of small molecules – Poster

SOE

Invited Talk

09:30	GÖR/0226	SOE 2.1	Memory and equilibrium in collective animal behaviour •Thierry Mora

Sessions

09:30	GÖR/0226	SOE 2	Focus Session: Physics of Behavior
09:30	MER/0002	SOE 3	Sustainability: Challenges and Solutions
18:00	P4	SOE 4	Poster Session

TT

Topical Talks

09:30	HSZ/0003	TT 1.1	Eigenstate thermalization in thermal first-order phase transitions •Maksym Serbyn
10:00	HSZ/0003	TT 1.2	Stabilizing Floquet orders to infinite time •Anushya Chandran
10:30	HSZ/0003	TT 1.3	Dynamical landscape of out of equilibrium emergent lattice gauge theories in two dimensions •Nilotpal Chakraborty
11:15	HSZ/0003	TT 1.4	Interference, topology, and new Hilbert-space routes to quantum non-ergodicity •Yi-Ping Huang
11:45	HSZ/0003	TT 1.5	Fock-space cages and their spectral signatures •Cheryne Jonay
15:00	HSZ/0003	TT 12.1	Charge confinement in twisted bilayer graphene •Christoph Stampfer
15:30	HSZ/0003	TT 12.2	Tuning Coulomb interactions and Hubbard bands in 1T-TaS_2 •Anna Galler
16:00	HSZ/0003	TT 12.3	Optical signatures of interlayer electron coherence in a bilayer semiconductor •Nadine Leisgang

Monday, March 9, 2026

TT

16:45	HSZ/0003	TT 12.4	Faithful modeling of quantum geometry and electronic correlations in van der Waals heterostructures •Ammon Fischer
17:15	HSZ/0003	TT 12.5	Mesoscale Atomic Engineering in a Crystal Lattice •Julian Klein
15:00	CHE/0089	TT 18.1	Markovian and non-Markovian approaches to quantum relaxation •Heinz-Peter Breuer
15:30	CHE/0089	TT 18.2	Asymptotic relaxation in quantum Markovian dynamics •Susana Huelga
16:00	CHE/0089	TT 18.3	Floquet engineering of open quantum Systems •André Eckardt
16:45	CHE/0089	TT 18.4	Nonequilibrium thermodynamics of time-dependent quantum transport •Janine Splettstoesser
17:15	CHE/0089	TT 18.5	Connecting time-nonlocal and time-local quantum master equations •Maarten Wegewijs

Sessions

09:30	HSZ/0003	TT 1	Focus Session: New Routes to Localization and Quantum Non-Ergodicity I
09:30	HSZ/0101	TT 2	Quantum-Critical Phenomena
09:30	HSZ/0103	TT 3	Correlated Electrons: Electronic Structure Calculations
09:30	HSZ/0105	TT 4	Graphene, 2D and Twisted Materials
09:30	CHE/0089	TT 5	Superconductivity: Sample Preparation and Characterization
09:30	CHE/0091	TT 6	Topological Superconductors
09:30	POT/0351	TT 7	Surface Magnetism and Topological Insulators
09:30	TRE/PHYS	TT 8	Topical Talk Wulfhekel
10:30	TRE/MATH	TT 9	2D Materials: Electronic structure, excitations, etc. I
11:00	HSZ/0103	TT 10	Correlated Electrons: Other Theoretical Topics
11:15	CHE/0091	TT 11	$PtBi_2$
15:00	HSZ/0003	TT 12	Focus Session: Tunable Correlations in van der Waals Quantum Materials I
15:00	HSZ/0101	TT 13	Correlated Electrons: Method Development I
15:00	HSZ/0103	TT 14	Superconductivity: Properties and Electronic Structure
15:00	HSZ/0105	TT 15	Topology: Majorana Physics
15:00	HSZ/0204	TT 16	2D Materials beyond graphene: Growth, structure and substrate interaction
15:00	BEY/0245	TT 17	Quantum Manybody Systems
15:00	CHE/0089	TT 18	Focus Session: Relaxation Timescales in Open Quantum Systems
15:00	CHE/0091	TT 19	Focus Session: New Routes to Localization and Quantum Non-Ergodicity II
15:00	POT/0081	TT 20	2D Materials II – Electronic and Transport Properties
15:00	POT/0151	TT 21	Electron Theory of Magnetism and Correlations
18:00	P1	TT 22	Superconductivity – Poster I
18:00	P1	TT 23	Correlated Electrons – Poster I

DD

Invited Talk

09:30	HÜL/S386	DD 2.1	Zukunft gestalten: Physik als Werkzeug zum Verstehen und Gestalten unserer Umwelt •Bianca Watzka

Sessions

09:30	HÜL/S386	DD 2	Eröffnung und Hauptvortrag I
10:45	SCH/A101	DD 3	Quantenphysik I
10:45	SCH/A252	DD 4	Digitale Medien I
10:45	SCH/A284	DD 5	Astronomie, Inklusion und Lernforschung
10:45	SCH/A285	DD 6	Lehrkräfteaus- und -fortbildung I
12:00	SCH/A101	DD 7	Quantenphysik II
12:00	SCH/A252	DD 8	Außerschulische Lernorte I
12:00	SCH/A284	DD 9	Neue Konzepte I
12:00	SCH/A285	DD 10	Hochschuldidaktik I

Monday, March 9, 2026

QI

Invited Talks

09:30	BEY/0245	QI 2.1	Advances in Frequency-Multiplexed Readout and Subsequent Qubit-State Reset •Benjamin Lienhard
15:00	BEY/0245	QI 4.1	Reducing Noise, Complexity, and Optimization Barriers in Quantum Simulations of Strongly Correlated Systems •Werner Dobrautz

Sessions

09:30	BEY/0137	QI 1	Quantum Computing and Algorithms I
09:30	BEY/0245	QI 2	Implementations I
15:00	BEY/0137	QI 3	Quantum Simulation
15:00	BEY/0245	QI 4	Quantum Manybody Systems

UP

Session

09:30	MER/0002	UP 1	Sustainability: Challenges and Solutions

AKBP

Topical Talks

09:30	SCH/A117	AKBP 1.1	Recent Developments at S-DALINAC •D. Schneider
10:00	SCH/A117	AKBP 1.2	Status of Source and Delivery of Spin-Polarized Electron Beams at ELSA •Michael Switka
11:00	SCH/A117	AKBP 2.1	From ELBE to DALI - Superconducting Electron Accelerators in Dresden •Andreas Wagner

Sessions

09:30	SCH/A117	AKBP 1	Electron Accelerators and Sources I
11:00	SCH/A117	AKBP 2	Electron Accelerators and Sources II
15:00	SCH/A117	AKBP 3	Diagnostics
16:45	SCH/A117	AKBP 4	Beam Dynamics

20:00	HSZ/AUDI	**Einstein Slam**

Tuesday, March 10, 2026

Plenary Talk

08:30	HSZ/AUDI	PV IV	Spins in Quantum Dots: The Quiet Revolution •Dorian Gangloff

Prize Talks

13:00	HSZ/0002	PRV II	Polymers / Soft Matter as Model Systems for Physics •Kurt Kremer (Laureate of the Max-Planck-Medal 2026)
13:00	HSZ/0004	PRV III	Optics of single molecules explored with sub-nm precision •Anna Rosławska (Laureate of the Gaede-Prize 2026)

Lunch Talk, Discussion

13:00	HSZ/AUDI	PSV III	Soft Science Skills – Self-branding for Scientists •Lucas Kreuzer, •Christian Kuttner, •Alexander Schlaich
13:00	HSZ/0003	PSV IV	Funding Opportunities for International Collaborations at the German Research Foundation •Joanna Kowalska

Ceremonial Session with Award Ceremony and Ceremonial Talk

16:00	HSZ/AUDI	PSV V	Quantum computers as large research instruments – what can we expect and how do we develop them? •Frank Wilhelm-Mauch

SYBS

Invited Talks

09:30	HSZ/AUDI	SYBS 1.1	Odd viscosity in three-dimensional fluids: flows, wakes, and eddies •Tali Khain
10:00	HSZ/AUDI	SYBS 1.2	Odd viscosity in two-dimensional hydrodynamic electron transport •Igor Gornyi
10:30	HSZ/AUDI	SYBS 1.3	Odd slip on chiral active surfaces •Andrej Vilfan
11:15	HSZ/AUDI	SYBS 1.4	Parity-odd transport in electron fluids •Johanna Erdmenger
11:30	HSZ/AUDI	SYBS 1.5	Curved Odd Elasticity •Piotr Surówka

Session

09:30	HSZ/AUDI	SYBS 1	Fluids with broken time-reversal symmetry: Odd/Hall viscosity between active matter and electron flows

BP

Invited Talks

11:15	BAR/0106	BP 11.7	Physics of bacterial adhesion: heterogeneity, patchiness, and surface interactions •Karin Jacobs
09:30	BAR/0205	BP 12.1	Tuning the Tracks: Functional Diversity Encoded in Microtubule Lattice States •Lukas Kapitein

Sessions

09:30	BAR/SCHÖ	BP 10	Active Matter III
09:30	BAR/0106	BP 11	Franco-German Session: Bacterial Biophysics I
09:30	BAR/0205	BP 12	Cytoskeleton I
14:00	ZEU/0160	BP 13	Active Matter IV
18:00	P2	BP 14	Poster Session II

CPP

Invited Talks, Topical Talks

09:30	ZEU/LICH	CPP 19.1	Surface adsorption and protonation equilibrium of atmospheric organics at the aqueous surface •Nønne Prisle

Tuesday, March 10, 2026

CPP

09:30	ZEU/0255	CPP 21.1	Molecular modelling of gas solubility and free volume trends in Si-functionalized ionic liquids •Kateryna Goloviznina
09:30	ZEU/0260	CPP 22.1	From Solution to Thin Films: Structure Formation Pathways in Organic Photovoltaic Films •Eva M. Herzig
14:00	HÜL/S386	CPP 26.1	Investigating lignin graphitisation depending on botanical source and extraction method •Pascale Launois
14:00	ZEU/LICH	CPP 27.1	Why water in plants survives negative pressure •Matej Kandu\v{c}
14:00	ZEU/0260	CPP 30.1	Solvent effects on amphiphile self-assembly in Deep Eutectic Solvents •Karen Edler

Sessions

09:30	BAR/SCHÖ	CPP 18	Active Matter III
09:30	ZEU/LICH	CPP 19	Focus Session: Water – from Atmosphere to Space I
09:30	ZEU/0160	CPP 20	Complex Fluids and Soft Matter
09:30	ZEU/0255	CPP 21	French-German Session: Simulation Methods and Modeling of Soft Matter III
09:30	ZEU/0260	CPP 22	Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics I
11:15	ZEU/LICH	CPP 23	Focus Session: Water – from Atmosphere to Space II
11:30	ZEU/0255	CPP 24	French-German Session: Simulation Methods and Modeling of Soft Matter IV
11:30	ZEU/0260	CPP 25	Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics II
14:00	HÜL/S386	CPP 26	French-German Session: 2D Materials, Thin Films and Interfaces II
14:00	ZEU/LICH	CPP 27	Focus Session: Water – from Atmosphere to Space III
14:00	ZEU/0160	CPP 28	Active Matter IV
14:00	ZEU/0255	CPP 29	Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods III
14:00	ZEU/0260	CPP 30	Complex Fluids, Colloids, Micelles and Vesicles I

DS

Invited Talks

09:30	REC/C213	DS 6.1	Soft X-ray Microscopy of Ferroic Thin Films •Tim A. Butcher
11:15	REC/C213	DS 6.6	Charge transfer at interfaces of free-standing oxide membranes and heterostructures •Felix Gunkel

Sessions

09:30	HSZ/0105	DS 5	Focus Session: Tunable Correlations in van der Waals Quantum Materials II
09:30	REC/C213	DS 6	Thin Oxides and Oxide Layers
10:00	REC/B214	DS 7	Thermoelectric and Phase Change Materials
14:00	REC/B214	DS 8	Transport Properties
14:00	REC/C213	DS 9	Thin Film Properties III: Oxides

DY

Invited Talks

09:30	HÜL/S186	DY 19.1	Mechanics of entangled fibers •Olivier Pouliquen
11:15	ZEU/0114	DY 21.7	Why Life Is Hot •Tanja Schilling
14:00	ZEU/0118	DY 28.1	Geometry of turbulent mixing in thermal convection •Jörg Schumacher
15:00	ZEU/0160	DY 29.5	Designing topological edge states in bacterial active matter •Kazumasa A. Takeuchi

Tuesday, March 10, 2026

DY

Sessions

09:30	BAR/SCHÖ	DY 18	Active Matter III
09:30	HÜL/S186	DY 19	Franco-German Session on Granular Matter I
09:30	ZEU/LICH	DY 20	Focus Session: Water – from Atmosphere to Space I
09:30	ZEU/0114	DY 21	Stochastic Thermodynamics
09:30	ZEU/0118	DY 22	Pattern Formation
09:30	ZEU/0160	DY 23	Complex Fluids and Soft Matter
11:15	ZEU/LICH	DY 24	Focus Session: Water – from Atmosphere to Space II
14:00	HÜL/S186	DY 25	Franco-German Session on Granular Matter II
14:00	ZEU/LICH	DY 26	Focus Session: Water – from Atmosphere to Space III
14:00	ZEU/0114	DY 27	Statistical Physics far from Thermal Equilibrium II
14:00	ZEU/0118	DY 28	Fluid Physics and Turbulence
14:00	ZEU/0160	DY 29	Active Matter IV

FM

Invited Talks

09:30	BEY/0138	FM 6.1	Robust Data Generation, Heuristics and Machine Learning for Materials Design •Janine George
14:00	BEY/0138	FM 9.1	Thin film combinatorial studies of functional magnetic materials •Nora Dempsey

Sessions

09:30	BEY/0138	FM 6	Focus Session: Materials Discovery I -- Material informatics
09:30	BEY/0E40	FM 7	Crystal Defects and Real Structure Physics in Diamond and Functional Materials I
09:30	POT/0112	FM 8	Multiferroics and Magnetoelectric Coupling
14:00	BEY/0138	FM 9	Focus Session: Materials Discovery II – High throughput searches for functional magnetic materials
14:00	BEY/0E40	FM 10	Crystal Defects and Real Structure Physics in Diamond and Functional Materials II
18:00	P4	FM 11	Poster Session Functional Materials

HL

Invited Talks

09:30	POT/0081	HL 16.1	Tailoring the performance of WSe_2 quantum emitters via cavity quantum electrodynamics and coherent driving •Ivan Solovev
10:00	POT/0081	HL 16.2	Deterministic single-photon emitters in 2D materials •Ursula Wurstbauer
10:30	POT/0081	HL 16.3	Resolving atomic and electronic structure of point defects in MoS_2 by first-principles calculations and scanning tunneling microscopy •Hannu-Pekka Komsa
11:15	POT/0081	HL 16.4	Polarization dynamics of isolated defects in hexagonal boron nitride •Serkan Ateş
11:45	POT/0081	HL 16.5	Defect-driven quantum emission in 2D materials •Magdalena Grzeszczyk

Sessions

09:30	HSZ/0105	HL 14	Focus Session: Tunable Correlations in van der Waals Quantum Materials II
09:30	POT/0006	HL 15	Organic Semiconductors: Optics and Photonics
09:30	POT/0081	HL 16	Focus Session: Quantum Emitters in 2D Semiconductors
09:30	POT/0251	HL 17	Quantum Dots and Wires: Rings, Wires and Transport
10:00	POT/0051	HL 18	Nanomechanical systems
10:30	HSZ/0201	HL 19	Graphene: Growth, structure and substrate interaction
18:00	P1	HL 20	Poster I

Tuesday, March 10, 2026

MA

Invited Talks

09:35	HSZ/0002	MA 14.1	Femtophonomagnetism •Sangeeta Sharma
10:20	HSZ/0002	MA 14.2	THz-driven dynamical ferroicity in paraelectric and diamagnetic perovskites •Martina Basini
10:50	HSZ/0002	MA 14.3	Angular momentum transfer and chiral phonons from first principles •Markus Weißenhofer
11:35	HSZ/0002	MA 14.4	Inertial Spin Dynamics: A Signature of Non-Markovian Interactions in Ferromagnets •Vivek Unikandanunni
12:05	HSZ/0002	MA 14.5	Atomistic simulations of ultrafast spin-lattice dynamics •Richard Evans
09:30	POT/0151	MA 18.1	Magnetic Cooling: From applications at room temperature to hydrogen liquefaction •T. Gottschall

Sessions

09:30	HSZ/0002	MA 14	PhD Focus Session: What about the lattice? Lessons from (ultrafast) magnetism
09:30	HSZ/0003	MA 15	Focus Session: Quantum Sensing with Solid State Spin defects I
09:30	HSZ/0004	MA 16	Skyrmions I
09:30	POT/0112	MA 17	Multiferroics and Magnetoelectric Coupling
09:30	POT/0151	MA 18	Caloric Effects in Ferromagnetic Materials
09:30	POT/0361	MA 19	Frustrated Magnets I
14:00	HSZ/0002	MA 20	Altermagnets III
14:00	HSZ/0004	MA 21	Skyrmions II
14:00	BEY/0138	MA 22	Focus Session: Materials Discovery II – High throughput searches for functional magnetic materials
14:00	POT/0151	MA 23	Cooperative Phenomena: Spin Structures and Magnetic Phase Transitions
14:00	POT/0361	MA 24	Weyl Semimetals

MM

Invited Talk

09:30	SCH/A251	MM 10.1	Chemically graded materials for accelerated exploration of the TRIP-TWIP Ti-alloy family •Lola Lilensten

Sessions

09:30	SCH/A251	MM 10	Invited Talk: Lola Lilensten
10:15	SCH/A215	MM 11	Structurally and Chemically Complex Alloys
10:15	SCH/A216	MM 12	Materials for the Storage and Conversion of Energy III / Functional Materials I
10:15	SCH/A251	MM 13	Data-driven Materials Science: Big Data and Workflows I
11:30	SCH/A315	MM 14	Liquid and Amorphous Materials I
14:00	SCH/A215	MM 15	Phase Transformations I
14:00	SCH/A216	MM 16	Functional Materials II
14:00	SCH/A251	MM 17	Data-driven Materials Science: Big Data and Workflows II
14:00	SCH/A315	MM 18	Liquid and Amorphous Materials II
18:00	P5	MM 19	Poster Session

O

Invited Talks, Topical Talk

09:30	TRE/PHYS	O 32.1	Excitons in molecular solids: from unitary films to donor-acceptor co-crystals •Gregor Witte
10:30	HSZ/0201	O 33.1	During-synthesis functionalization of graphene layers •Cristina Africh
10:30	HSZ/0403	O 36.1	Acidity in nanoconfinement from ab initio and NNPs simulations •Marialore Sulpizi

Tuesday, March 10, 2026

O

11:30	HSZ/0403	O 36.4	Living Interfaces: Dissolution and Precipitation Processes at Mineral-Brine Interfaces Revealed by AFM •Igor Siretanu
10:30	TRE/PHYS	O 37.1	Calculations of excited electronic states by converging on saddle points on the electronic energy surface •Hannes Jonsson
11:30	TRE/PHYS	O 37.4	Many-Body Theory meets Electrochemistry: Electronic Structure of Cathode Materials •Silke Biermann
11:00	WILL/A317	O 39.3	Electric double layer of platinum electrodes •Marc Koper
12:00	WILL/A317	O 39.6	First-principles modelling of electrochemical interfaces •Axel Groß
14:30	TRE/MATH	O 51.1	Ultrafast aqueous electric double-layer dynamics •Mischa Bonn
15:15	TRE/MATH	O 51.3	Interface-specific nonlinear THz spectroscopy •Chuanshan Tian
14:30	WILL/A317	O 52.1	Dynamics of catalytically active, atomically precise clusters on reducible oxide supports under the (fast) scanning tunneling microscope •Friedrich Esch

Sessions

09:30	TRE/PHYS	O 32	Topical Talk Witte
10:30	HSZ/0201	O 33	Graphene: Growth, structure and substrate interaction
10:30	HSZ/0204	O 34	Catalysis and surface reactions I
10:30	HSZ/0401	O 35	Organic molecules on inorganic substrates: Adsorption and growth II
10:30	HSZ/0403	O 36	Focus Session: Mineral-water interfaces II
10:30	TRE/PHYS	O 37	Electronic structure theory I
10:30	TRE/MATH	O 38	Ultrafast electron dynamics at surface and interfaces II
10:30	WILL/A317	O 39	Focus Session: Structure and Dynamics of Solvent at Electrochemical Interfaces I
14:00	P2	O 40	Ultrafast electron dynamics at surface and interfaces – Poster
14:00	P2	O 41	Topology and symmetry protected materials & Topological insulators – Poster
14:00	P2	O 42	Electronic structure of surfaces: Spectroscopy, surface states – Poster
14:00	P2	O 43	Scanning probe microscopy: light matter interaction at atomic scales – Poster
14:00	P2	O 44	Scanning probe techniques: Method development – Poster
14:00	P2	O 45	Organic molecules on inorganic substrates: Adsorption and growth – Poster
14:00	P2	O 46	Organic molecules on inorganic substrates: electronic, optical and other properties – Poster
14:30	HSZ/0201	O 47	New methods: Theory
14:30	HSZ/0204	O 48	Metal & Semiconductor substrates: Structure, epitaxy and growth
14:30	HSZ/0403	O 49	Plasmonics and nanooptics: Light-matter interaction, spectroscopy I
14:30	TRE/PHYS	O 50	Electronic structure theory II
14:30	TRE/MATH	O 51	Focus Session: Structure and Dynamics of Solvent at Electrochemical Interfaces II
14:30	WILL/A317	O 52	Oxide and insulator surfaces: Structure, epitaxy and growth I

SOE

Prize Talk, Invited Talk, Topical Talk

09:30	GÖR/0226	SOE 5.1	Network Science in Criminology: Insights from Empirical Case Studies •Masarah Paquet-Clouston
14:00	GÖR/0226	SOE 7.1	What's that noise? Why does it make a difference? And why am I thinking about it all the time? •Dirk Brockmann
14:45	GÖR/0226	SOE 7.2	How things spread: Complexity and criticality of inhomogeneous spreading models •Laurent Hébert-Dufresne (Laureate of the YSA 2026)

Sessions

09:30	GÖR/0226	SOE 5	Network Science
10:45	GÖR/0226	SOE 6	Mobility, Traffic Dynamics, Urban and Regional Systems
14:00	GÖR/0226	SOE 7	Award Session: Young Scientist Award for Socio- and Econophysics (YSA)

Tuesday, March 10, 2026

TT

Invited Talk, Topical Talks

09:30	HSZ/0003	TT 24.1	Exploring nanoscale van der Waals magnetism using single spin microscopy •Patrick Maletinsky
10:00	HSZ/0003	TT 24.2	Optically addressable spin defects in two-dimensional materials •Vladimir Dyakonov
10:30	HSZ/0003	TT 24.3	Nitrogen vacancy centers in diamond as novel sensing and imaging tool for magnetic nanostructures, in life science and chemistry •Elke Neu-Ruffing
11:15	HSZ/0003	TT 24.4	Electron spin, nuclear spin, and optical properties of transition-metal defects in silicon carbide with perspectives for quantum technologies •Guido Burkard
11:45	HSZ/0003	TT 24.5	Statics and dynamics of complex magnetic states in microstructures •Aurore Finco
09:30	HSZ/0105	TT 27.1	Simulating high-temperature superconductivity in a triangular moiré lattice •Kin Fai Mak

Sessions

09:30	HSZ/0003	TT 24	Focus Session: Quantum Sensing with Solid State Spin defects I
09:30	HSZ/0101	TT 25	f-Electron Systems
09:30	HSZ/0103	TT 26	Correlated Magnetism – Frustrated Systems
09:30	HSZ/0105	TT 27	Focus Session: Tunable Correlations in van der Waals Quantum Materials II
09:30	CHE/0089	TT 28	Superconducting Electronics: SQUIDs and other Josephson Circuits and Components
09:30	CHE/0091	TT 29	Unconventional Superconductors
09:30	POT/0151	TT 30	Caloric Effects in Ferromagnetic Materials
09:30	POT/0361	TT 31	Frustrated Magnets I
10:00	POT/0051	TT 32	Nanomechanical systems
11:00	HSZ/0105	TT 33	Correlated Magnetism – Dynamics and Spectroscopy
14:00	HSZ/0101	TT 34	Members' Assembly
14:00	POT/0151	TT 35	Cooperative Phenomena: Spin Structures and Magnetic Phase Transitions
14:00	POT/0361	TT 36	Weyl Semimetals
14:00	P2	TT 37	Ultrafast electron dynamics at surface and interfaces – Poster
14:00	P2	TT 38	Topology and symmetry protected materials & Topological insulators – Poster

DD

Invited Talk

09:30	HÜL/S386	DD 11.1	Lernen mit KI, Lernen über KI: Perspektiven für die Naturwissenschaftsdidaktik •Arne Bewersdorff

Sessions

09:30	HÜL/S386	DD 11	Hauptvortrag II
10:45	SCH/A101	DD 12	Praktika und Experimente
10:45	SCH/A252	DD 13	Digitale Medien II
10:45	SCH/A284	DD 14	Bildung für nachhaltige Entwicklung
10:45	SCH/A285	DD 15	Interesse I
12:00	SCH/A101	DD 16	Experimente
12:00	SCH/A252	DD 17	Außerschulische Lernorte II
12:00	SCH/A284	DD 18	BNE Workshop
12:00	SCH/A285	DD 19	Hochschuldidaktik II
14:00	P5	DD 20	Poster – Lehrkräfteaus- und -fortbildung
14:00	P5	DD 21	Poster – Außerschulische Lernorte
14:00	P5	DD 22	Poster – Astronomie
14:00	P5	DD 23	Poster – Bildung für nachhaltige Entwicklung
14:00	P5	DD 24	Poster – Digitale Medien
14:00	P5	DD 25	Poster – Experimente und Praktika
14:00	P5	DD 26	Poster – Hochschuldidaktik
14:00	P5	DD 27	Poster – Lehr- und Lernforschung
14:00	P5	DD 28	Poster – Neue Konzepte

Tuesday, March 10, 2026

DD

14:00	P5	DD 29	Poster – Nature of Science
14:00	P5	DD 30	Poster – Quantenphysik
14:00	P5	DD 31	Poster – Physikdidaktik und Inklusion
14:00	P5	DD 32	Poster – Sprache und Physikunterricht
14:00	P5	DD 33	Poster – Sonstiges
18:00	SCH/A101	DD 34	Mitgliederversammlung

QI

Invited Talk

09:30	BEY/0245	QI 6.1	Erbium dopants for quantum networks •Andreas Reiserer

Sessions

09:30	BEY/0137	QI 5	Quantum Computing and Algorithms II
09:30	BEY/0245	QI 6	Implementations II
09:30	BEY/0E17	QI 7	Quantum Thermodynamics
14:00	BEY/0137	QI 8	Implementations III
14:00	BEY/0245	QI 9	Decoherence and Open Systems I

UP

Invited Talks

10:15	MER/0002	UP 2.4	Klimakommunikation in der Schule? Mehr als nur darüber reden! •Michael Sach
11:15	MER/0002	UP 3.1	Supporting the monitoring and tracking of carbon dioxide and methane emissions with satellites •Dominik Brunner
14:00	MER/0002	UP 5.1	A path to seamless modelling of the convective atmospheric boundary layer •Mirjana Sakradzija

Sessions

09:30	MER/0002	UP 2	Climate Communication
11:15	MER/0002	UP 3	Air Quality, Exposure and Atmospheric Dynamics
13:00	MER/0002	UP 4	Members' Assembly
14:00	MER/0002	UP 5	Modelling and Prediction Across Scales

AKBP

Topical Talks

09:30	SCH/A117	AKBP 5.1	Generation and Acceleration of In-Target Gold Fission Fragments using the ATLAS-3000 Laser System •Laura D. Geulig
11:00	SCH/A117	AKBP 6.1	Efficient high energy and high-repetition-rate proton acceleration from cryogenic hydrogen foil targets •Stefan Assenbaum

Sessions

09:30	SCH/A117	AKBP 5	Plasma Accelerators, Ions I
11:00	SCH/A117	AKBP 6	Plasma Accelerators, Ions II
14:00	SCH/A117	AKBP 7	Ion and Medical Accelerators

AKPIK

Invited Talks

11:45	BEY/0127	AKPIK 3.4	Model-free training of optical neural networks based on multimode semiconductor lasers •Anas Skalli
12:15	BEY/0127	AKPIK 3.5	Virtual Reality Gamification for Photonics, AI and More •Arash Rahimi-Iman

Tuesday, March 10, 2026

AKPIK

14:00	BEY/0127	AKPIK 4.1	Beyond the Hype: Can AI Truly Transform Photonics? •Mehdi K. Hedayati
14:30	BEY/0127	AKPIK 4.2	Machine-learning assisted design of metasurfaces •Marco Rahm
			Sessions
09:30	BEY/0127	AKPIK 2	Machine Learning Prediction and Optimization Tasks
11:00	BEY/0127	AKPIK 3	Research with AI: Hardware, Software, Tools
14:00	BEY/0127	AKPIK 4	Focus: Deep Learning in Electromagnetics Research

JOB

			Invited Talks
11:00	HSZ/0405	JOB 1.1	d-fine GmbH: Entwicklung einer ERP-Software für Sanitätshäuser •Maximilian Sommer, •Philipp Banker-Busch
13:00	HSZ/0405	JOB 1.2	Ritzenhoefer GmbH: Agentic Journey •Andreas Ringleb, •Alice von Bassewitz
			Session
11:00	HSZ/0405	JOB 1	Job Market I

09:30	Tents A and C	**Exhibition of Scientific Instruments and Literature** (free entrance)

20:00	HSZ Main Entrance Bergstraße	**jDPG Pub Crawl**

Wednesday, March 11, 2026

Plenary Talks

08:30	HSZ/AUDI	PV V	Reimagining Physics Education for a Planet in Transformation •Giulia Tasquier
14:00	HSZ/AUDI	PV VI	Materials selection methods: a compass in the jungle •Yves Bréchet
14:00	HSZ/0002	PV VII	Stronger yet weaker: Long-range orientational order in 2D active matter •Hugues Chaté

Prize Talk

13:00	HSZ/0003	PRV IV	Fractionalisation, fractals and strong coupling QED in spin liquids •Roderich Moessner (Laureate of the Max-Born-Prize 2026)

Lunch Talk, Discussion

13:00	HSZ/AUDI	PSV VI	Career Paths: Academia or Industry? •Joanna Kowalska, •Elisabeth Trommer, •Jonas Schubert, •Annegret Rößler
13:00	HSZ/0002	PSV VII	The French Research Landscape in Physics •Elisabeth Giacobino

SYBT

Invited Talks

09:30	HSZ/AUDI	SYBT 1.1	Finding Neuromorphic Advantage with Magnetism •Johan Mentink
10:00	HSZ/AUDI	SYBT 1.2	Accelerating Neural Networks Computation with Ferroelectric Oxides •Laura Bégon-Lours
10:30	HSZ/AUDI	SYBT 1.3	a photonic approach to probabilistic computing •Wolfram Pernice
11:15	HSZ/AUDI	SYBT 1.4	Tackling Reliability and Scalability in Neuromorphic Computing via Noise-aware Learning •Eleni Vasilaki
11:45	HSZ/AUDI	SYBT 1.5	Bayesian nanodevices for trustworthy artificial intelligence •Damien Querlioz

Session

09:30	HSZ/AUDI	SYBT 1	Beyond Transistors: Material-Based Edge Computing Paradigms

SYGF

Invited Talks

15:00	HSZ/AUDI	SYGF 1.1	Liquid crystal geometries in type I collagen-based tissues •Nadine Nassif
15:30	HSZ/AUDI	SYGF 1.2	Self-organization of the cytoplasm by physical instabilities •Jan Brugues
16:00	HSZ/AUDI	SYGF 1.3	From morphogenesis to space partitioning by microtubules and molecular motors. •Manuel Thery
16:45	HSZ/AUDI	SYGF 1.4	More than the sum: how composite interfaces govern function •Alba Diz-Muñoz
17:15	HSZ/AUDI	SYGF 1.5	Swimming and Swarming of Intelligent Active Particles •Gerhard Gompper
17:45	HSZ/AUDI	SYGF 1.6	Perturbing the collective motion of fish with challenging environments •Aurélie Dupont

Session

15:00	HSZ/AUDI	SYGF 1	Guest Country Symposium France: Soft, Active and Alive: Emergent Properties in Living Matter (SYGF)

Wednesday, March 11, 2026

BP

Invited Talks

09:30	BAR/0205	BP 16.1	Illuminating mitochondrial permeabilisation in apoptosis •Ana J. Garcia Saez
10:30	BAR/0106	BP 18.1	Protein complex structure prediction, state-of-the-art and challenges •Ezgi Karaca
11:45	BAR/0106	BP 18.4	From Sparse Restraints to All-Atom Models: Integrative Reconstruction of Hidden GPCR Conformations •Matthias Elgeti
15:45	BAR/0106	BP 20.4	Solution scattering and MD simulation as quantitative probes of protein-specific and temperature-dependent hydration •Jochen S Hub
15:00	HÜL/S386	BP 21.1	Microbial Behavior in Context •Fernanda Pinheiro
16:15	HÜL/S386	BP 21.4	The navigability of fitness landscapes shaped by global and universal epistasis •Joachim Krug

Sessions

09:30	BAR/SCHÖ	BP 15	Computational Biophysics III
09:30	BAR/0205	BP 16	Membranes, Vesicles and Synthetic Life-like Systems II
09:30	ZEU/0114	BP 17	Statistical Physics of Biological Systems I
10:30	BAR/0106	BP 18	Focus session: Integrative Structural Modeling
11:45	ZEU/LICH	BP 19	Round Table Discussion: The Future of Neutrons in France and Germany
15:00	BAR/0106	BP 20	Protein Structure and Dynamics
15:00	HÜL/S386	BP 21	Focus Session: Sequence Spaces, Populations and Evolution
15:00	ZEU/0114	BP 22	Statistical Physics of Biological Systems II
15:00	ZEU/0255	BP 23	Biopolymers, Biomaterials and Bioinspired Functional Materials I
17:00	ZEU/0255	BP 24	Biopolymers, Biomaterials and Bioinspired Functional Materials II
18:30	BAR/0205	BP 25	Members' Assembly

CPP

Invited Talks, Topical Talk, Discussion

09:30	ZEU/0255	CPP 31.1	Hydrogels with a Pinch of Embodied Intelligence •Andreas Walther
09:30	ZEU/0260	CPP 32.1	Synchrotron X-Ray Studies on Structural Transitions in Water and Alcohol containing Ice Analogues •Christina M. Tonauer
10:00	ZEU/LICH	CPP 33.1	Shape-induced superstructure formation in concentrated ferrofluids •Sabrina Disch
11:45	ZEU/LICH	CPP 36.1	Round Table: Novel Opportunities for France/Germany Cooperation in Neutron Science •Julian Oberdisse, •Frank Schreiber, •Arnaud Desmedt, •Stephan Förster, •Jacques Jestin, •Pascale Launois, •Christian Pfleiderer, •Sabrina Disch
15:00	ZEU/LICH	CPP 37.1	Predicting molecular ordering in deposited molecular films •Denis Adrienko
15:00	ZEU/0255	CPP 38.1	Engineering, processing and application of recombinant spider silk proteins •Thomas Scheibel
15:00	ZEU/0260	CPP 39.1	A polarizable model for atomistic simulations of metals and graphitic material/liquid interfaces •Marialore Sulpizi
17:00	ZEU/0260	CPP 42.1	Mesopores filled with (poly)ionic liquids: phase transitions under confinement, and structure seen by SAXS and SANS •Julian Oberdisse

Sessions

09:30	ZEU/0255	CPP 31	Responsive and Adaptive Systems
09:30	ZEU/0260	CPP 32	Focus Session: Water – from Atmosphere to Space IV
10:00	ZEU/LICH	CPP 33	Complex Fluids, Colloids, Micelles and Vesicles II
11:00	ZEU/0260	CPP 34	Focus Session: Water – from Atmosphere to Space V

Wednesday, March 11, 2026

CPP

11:15	ZEU/0118	CPP 35	Glasses and Glass Transition
11:45	ZEU/LICH	CPP 36	Round Table Discussion: The Future of Neutrons in France and Germany
15:00	ZEU/LICH	CPP 37	Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics III
15:00	ZEU/0255	CPP 38	Biopolymers, Biomaterials and Bioinspired Functional Materials I
15:00	ZEU/0260	CPP 39	French-German Session: Nanomaterials, Composites and Hybrids I
17:00	ZEU/LICH	CPP 40	Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics IV
17:00	ZEU/0255	CPP 41	Biopolymers, Biomaterials and Bioinspired Functional Materials II
17:00	ZEU/0260	CPP 42	French-German Session: Nanomaterials, Composites and Hybrids II

DS

Invited Talk

15:00	REC/B214	DS 13.1	Tailored thermal treatments for multi-layer, multi-material polymer devices •Katherina Haase

Sessions

09:30	HSZ/0003	DS 10	Focus Session: Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects I
09:30	REC/B214	DS 11	Layer Deposition
09:30	REC/C213	DS 12	2D Materials I
15:00	REC/B214	DS 13	Layer Properties
15:00	REC/C213	DS 14	2D Materials II

DY

Invited Talks

09:30	ZEU/0160	DY 34.1	Active turbulence and odd viscosity in a colloidal chiral active system in bulk and in patterned environments •Marisol Ripoll
11:15	ZEU/0118	DY 37.1	Topological defects in 2D amorphous ensembles •Peter Keim
15:00	ZEU/0114	DY 40.1	Learning the statistical folding of bacterial chromosomes •Chase Broedersz

Sessions

09:30	CHE/0091	DY 30	Nonequilibrium Quantum Systems I
09:30	GÖR/0226	DY 31	Networks, From Topology to Dynamics – Part I
09:30	HÜL/S186	DY 32	Many-body Systems: Equilibration, Chaos, and Localization
09:30	ZEU/0114	DY 33	Statistical Physics of Biological Systems I
09:30	ZEU/0160	DY 34	Focus Session: Fluids with Broken Time-Reversal Symmetry – Odd/Hall Viscosity Between Active Matter and Electron Flows
09:30	ZEU/0260	DY 35	Focus Session: Water – from Atmosphere to Space IV
11:00	ZEU/0260	DY 36	Focus Session: Water – from Atmosphere to Space V
11:15	ZEU/0118	DY 37	Glasses and Glass Transition
15:00	HSZ/0105	DY 38	Nonequilibrium Quantum Systems II
15:00	GÖR/0226	DY 39	Networks, From Topology to Dynamics – Part II
15:00	ZEU/0114	DY 40	Statistical Physics of Biological Systems II
15:00	P5	DY 41	Poster: Nonlinear Dynamics, Granular Matter, and Machine Learning
15:00	P5	DY 42	Poster: Quantum Dynamics and Many-body Systems
15:00	P5	DY 43	Poster: Statistical Physics
15:00	P5	DY 44	Poster: Active Matter, Soft Matter, and Fluids

FM

Invited Talk

09:30	BEY/0138	FM 12.1	Shedding Light on Polar Topological Textures •Salia Cherifi-Hertel

Wednesday, March 11, 2026

FM

Sessions

09:30	BEY/0138	FM 12	German-French Focus Session: Materials Research in Polar Oxides – From Domain Engineering to Photonic and Electronic Devices I
10:15	SCH/A251	FM 13	Topical Session: Dislocations in Functional Materials I
15:00	BEY/0138	FM 14	Focus Session: Materials Research in Polar Oxides – From Domain Engineering to Photonic and Electronic Devices II
15:00	BEY/0E40	FM 15	Nanoscale Probing of Functional Properties
15:45	SCH/A251	FM 16	Topical Session: Dislocations in Functional Materials II

HL

Invited Talks

09:30	POT/0251	HL 25.1	Quantum dots for single-electron current sources •Johannes C. Bayer
10:00	POT/0251	HL 25.2	Optical readout of reconfigurable in-plane magnetic domains in CrSBr •Aleksandra Łopion
10:30	POT/0251	HL 25.3	Ferroelectric switching in Mn-doped epitaxial $BaTiO_3$ films and superlattices on silicon •Alfredo Blázquez Martínez
11:15	POT/0251	HL 25.4	Tunability of quantized Hall plateaus •Serkan Sirt
11:45	POT/0251	HL 25.5	How to achieve high gain in organic photodetectors? •Johannes Benduhn
15:00	POT/0081	HL 30.1	Dual proximity engineering of spin-orbit and magnetic effects in graphene heterostructures •Christoph Kastl

Sessions

09:30	HSZ/0101	HL 21	Focus Session: Quantum Sensing with Solid State Spin defects II
09:30	POT/0006	HL 22	Biocompatible Organic Semiconductors
09:30	POT/0051	HL 23	Transport Properties
09:30	POT/0081	HL 24	2D Materials IV – Emerging materials and properties
09:30	POT/0251	HL 25	Focus Session: Young Semiconductor Forum
09:30	P1	HL 26	Poster II
10:30	TRE/MATH	HL 27	2D Materials: Electronic structure, excitations, etc. II
15:00	HSZ/0401	HL 28	Topology and symmetry protected materials & Topological insulators
15:00	POT/0006	HL 29	Quantum Transport and Quantum Hall effects
15:00	POT/0081	HL 30	2D Materials V – Magnetic, spintronic, and topological properties
15:00	POT/0251	HL 31	Materials and Devices for Quantum Technology I
15:00	REC/C213	HL 32	2D Materials 2
16:30	POT/0006	HL 33	Nitrides I – Growth and fabrication
16:30	POT/0051	HL 34	Quantum Dots and Wires: Telecom Wavelength
16:30	POT/0251	HL 35	Optical Properties II
17:30	POT/0081	HL 36	2D Materials VI – Optoelectronic properties

MA

Invited Talks

09:30	HSZ/0002	MA 25.1	Coherent phononic control of chirality •Michael Först
10:00	HSZ/0002	MA 25.2	Towards a modern theory of chiralization (and can chiral phonons help us get there?) •Nicola Spaldin
11:15	HSZ/0002	MA 25.5	Observation and control of chiral phonons in non-centrosymmetric materials •Hiroki Ueda
09:30	HSZ/0004	MA 27.1	Towards sub-10fs magnetization switching •Quentin Remy
09:30	POT/0112	MA 29.1	Exploring the interplay between spin and chirality •Angela Wittmann

Wednesday, March 11, 2026

MA

15:00	POT/0112	MA 35.1	Magneto-optic Kerr effects of higher order in magnetization in thin films of different crystal orientations •Timo Kuschel

Sessions

09:30	HSZ/0002	MA 25	Focus Session: Chiral phonons and crystals coupled to magnetic order I
09:30	HSZ/0003	MA 26	Focus Session: Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects I
09:30	HSZ/0004	MA 27	Ultrafast Magnetization Effects I
09:30	HSZ/0101	MA 28	Focus Session: Quantum Sensing with Solid State Spin defects II
09:30	POT/0112	MA 29	Spin Transport and Orbitronics, Spin-Hall Effects I
09:30	POT/0151	MA 30	Functional Antiferromagnetism
09:30	POT/0361	MA 31	Frustrated Magnets II
14:00	HZDR	MA 32	Excursion: Current and Future High-Field THz User Facilities at HZDR
15:00	HSZ/0002	MA 33	Altermagnets IV
15:00	HSZ/0004	MA 34	Computational Magnetism I
15:00	POT/0112	MA 35	Spintronics (other effects)
15:00	POT/0151	MA 36	Molecular Magnetism and Magnetic Particles / Clusters I
15:00	POT/0351	MA 37	Non-Skyrmionic Magnetic Textures
15:00	POT/0361	MA 38	Ultrafast Magnetization Effects II
18:00	P2	MA 39	Poster Magnetism II

MM

Invited Talk, Topical Talks

09:30	SCH/A251	MM 20.1	Neural Network Atomistic Modeling of Dislocation Plasticity in Ceramics •Shigenobu Ogata
15:00	SCH/A251	MM 24.1	Recent advances in processing of rare-earth free MnBi magnets by severe plastic deformation •Andrea Bachmaier
15:45	SCH/A251	MM 27.1	Dislocations in perovskite oxides: similarities and differences •Pierre Hirel

Sessions

09:30	SCH/A251	MM 20	Topical Talk: Shigenobu Ogata
10:15	SCH/A215	MM 21	Phase Transformations II
10:15	SCH/A216	MM 22	Data-driven Materials Science: Big Data and Workflows III
10:15	SCH/A251	MM 23	Topical Session: Dislocations in Functional Materials I
15:00	SCH/A251	MM 24	Invited Talk: Andrea Bachmaier
15:45	SCH/A215	MM 25	Interface Controlled Properties, Nanomaterials, and Microstructure Design I
15:45	SCH/A216	MM 26	Transport in Materials: Diffusion, Charge, or Heat Conduction I
15:45	SCH/A251	MM 27	Topical Session: Dislocations in Functional Materials II
17:15	SCH/A251	MM 28	MM Members Assembly

O

Invited Talks, Topical Talk

09:30	TRE/PHYS	O 53.1	Single-Atom Catalysis: Insights From Model Systems •Gareth S. Parkinson
11:00	HSZ/0204	O 55.3	Cationic Mixing in Ultrathin Oxide Films: How substrate and oxygen conditions control nanoalloying. •Jacek Goniakowski
10:30	HSZ/0403	O 57.1	From Plasmonic Near-Fields to Electron Dynamics - A Photoemission Perspective •Pascal Dreher
10:30	WILL/A317	O 60.1	Disentangling the origins of spin polarization in (inverse) photoemission from solid surfaces •Jürgen Henk

Wednesday, March 11, 2026

O

15:00	HSZ/0403	O 64.1	Cantilever based Scanning Force Microscopy: Ultimate Sensitivity and Quantitative Imaging of Nanoscale Spin Textures •Hans J. Hug
16:30	HSZ/0403	O 64.6	Single-spin sensing: A molecule-on-tip approach •Laurent Limot
15:00	TRE/MATH	O 66.1	Ultrafast exciton dynamics in 2D semiconductors and electric field gated devices •Jan Philipp Bange
15:00	WILL/A317	O 67.1	New frontiers of one step model of photoemission for quantum materials •Jan Minar

Sessions

09:30	TRE/PHYS	O 53	Topical Talk Parkinson
10:30	HSZ/0201	O 54	Nanostructured surfaces and thin films
10:30	HSZ/0204	O 55	Oxide and insulator surfaces: Structure, epitaxy and growth II
10:30	HSZ/0401	O 56	Scanning probe techniques: Method development II
10:30	HSZ/0403	O 57	Plasmonics and nanooptics: Light-matter interaction, spectroscopy II
10:30	TRE/PHYS	O 58	Organic molecules on inorganic substrates: Adsorption and growth III
10:30	TRE/MATH	O 59	2D Materials: Electronic structure, excitations, etc. II
10:30	WILL/A317	O 60	Focus Session: Unoccupied States by Inverse Photoemission I
15:00	HSZ/0201	O 61	Organic molecules on inorganic substrates: electronic, optical and other properties II
15:00	HSZ/0204	O 62	Graphene: Electronic structure, excitations, etc.
15:00	HSZ/0401	O 63	Topology and symmetry protected materials & Topological insulators
15:00	HSZ/0403	O 64	Surface Magnetism
15:00	TRE/PHYS	O 65	Solid-liquid interfaces: Reactions and electrochemistry II
15:00	TRE/MATH	O 66	Ultrafast electron dynamics at surface and interfaces III
15:00	WILL/A317	O 67	Focus Session: Unoccupied States by Inverse Photoemission II
18:00	P2	O 68	Nanostructured surfaces and thin films – Poster
18:00	P2	O 69	Nanostructures at surfaces:1D, 2D, networks – Poster
18:00	P2	O 70	2D materials: Stacking and heterostructures – Poster
18:00	P2	O 71	2D Materials: Electronic structure, excitations, etc. – Poster
18:00	P2	O 72	2D Materials beyond graphene: Growth, structure and substrate interaction – Poster
18:00	P2	O 73	Graphene: Growth, structure and substrate interaction – Poster
18:00	P2	O 74	Graphene: Electronic structure, excitations, etc. – Poster

SOE

Invited Talk

09:30	GÖR/0226	SOE 8.1	Dynamics and Structure in Temporal Networks •Natasa Djurdjevac Conrad

Sessions

09:30	GÖR/0226	SOE 8	Networks, From Topology to Dynamics I
11:30	GÖR/0226	SOE 9	Economic Models
15:00	GÖR/0226	SOE 10	Networks, From Topology to Dynamics II
15:45	GÖR/0226	SOE 11	Polarization
17:15	GÖR/0226	SOE 12	Statistical Physics of Politics
18:00	GÖR/0226	SOE 13	Members' Assembly

TT

Topical Talks

09:30	HSZ/0003	TT 39.1	Unconventional Superconductivity in Infinite-layer Samarium Nickelates •Danfeng Li
10:00	HSZ/0003	TT 39.2	Recent insights into infinite-layer nickelate heterostructures from x-ray spectroscopy •Eva Benckiser
10:30	HSZ/0003	TT 39.3	Theory of infinite-layer nickelate superconductors •Karsten Held

Wednesday, March 11, 2026

TT

11:15	HSZ/0003	TT 39.4	Disorder and distortions: what electrons tell us about nickelate superconductivity •Berit H. Goodge
11:45	HSZ/0003	TT 39.5	Superconducting gap structure and bosonic mode in $La_2PrNi_2O_7$ thin films at ambient pressure •Hai-Hu Wen
15:00	HSZ/0003	TT 50.1	Josephson Quantum Tunneling at Odd Parity •Julia S. Meyer
15:30	HSZ/0003	TT 50.2	Superconducting qubits and amplifiers resilient to Tesla-scale magnetic fields •Ioan Pop
16:00	HSZ/0003	TT 50.3	Josephson metamaterials as near-quantum-limited microwave amplifiers •Nicolas Roch
16:45	HSZ/0003	TT 50.4	Second Order Topological Insulators probed with mesoscopic physics •Sophie Gueron
17:15	HSZ/0003	TT 50.5	Proximity superconductivity in chiral Kagome antiferromagnets •Piet Brouwer

Sessions

09:30	HSZ/0003	TT 39	Focus Session: Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects I
09:30	HSZ/0101	TT 40	Focus Session: Quantum Sensing with Solid State Spin defects II
09:30	HSZ/0103	TT 41	Topological Semimetals
09:30	HSZ/0105	TT 42	Other Transport Topics
09:30	CHE/0089	TT 43	Superconducting Electronics: Qubits
09:30	CHE/0091	TT 44	Nonequilibrium Quantum Systems I
09:30	HÜL/S186	TT 45	Many-body Systems: Equilibration, Chaos, and Localization
09:30	POT/0112	TT 46	Spin Transport and Orbitronics, Spin-Hall Effects I
09:30	POT/0361	TT 47	Frustrated Magnets II
10:30	TRE/MATH	TT 48	2D Materials: Electronic structure, excitations, etc. II
10:45	HSZ/0101	TT 49	Correlated Electrons: Charge Order
15:00	HSZ/0003	TT 50	German-French Focus Session: Superconducting Junctions and Quantum Circuits
15:00	HSZ/0101	TT 51	Correlated Electrons: Method Development II
15:00	HSZ/0103	TT 52	Heavy Fermions
15:00	HSZ/0105	TT 53	Nonequilibrium Quantum Systems II
15:00	HSZ/0204	TT 54	Graphene: Electronic structure, excitations, etc.
15:00	HSZ/0401	TT 55	Topology and symmetry protected materials & Topological insulators
15:00	CHE/0089	TT 56	Superconductivity: Theory I
15:00	CHE/0091	TT 57	Correlated Magnetism Kagome Systems
15:00	POT/0006	TT 58	Quantum Transport and Quantum Hall effects
15:00	POT/0081	TT 59	2D Materials V – Magnetic, spintronic, and topological properties
15:00	POT/0112	TT 60	Spintronics (other effects)
15:00	P4	TT 61	Topology – Poster
15:00	P4	TT 62	Correlated Electrons – Poster II
15:00	P5	TT 63	Quantum Dynamics and Many-body Systems – Poster
16:45	HSZ/0103	TT 64	BKT Physics
18:00	P2	TT 65	2D materials: Stacking and heterostructures – Poster
18:00	P2	TT 66	2D Materials: Electronic structure, excitations, etc. – Poster
18:00	P2	TT 67	2D Materials beyond graphene: Growth, structure and substrate interaction – Poster
18:00	P2	TT 68	Graphene: Electronic structure, excitations, etc. – Poster

DD

Prize Talk

09:30	HÜL/S386	DD 35.1	Die Bonner Physikshow – ein Öffentlichkeitsprojekt mit Studierenden •Herbi Dreiner (Laureate of the Georg-Kerschensteiner-Prize 2026)

Wednesday, March 11, 2026

DD

Sessions

09:30	HÜL/S386	DD 35	Kerschensteiner-Preisvortrag
10:45	SCH/A101	DD 36	Quantenphysik III
10:45	SCH/A252	DD 37	Lehr- und Lernforschung
10:45	SCH/A284	DD 38	Nature of Science
10:45	SCH/A285	DD 39	Interesse II
12:00	SCH/A101	DD 40	Quantenphysik IV
12:00	SCH/A252	DD 41	Lehrkräfteaus- und -fortbildung II
12:00	SCH/A285	DD 42	Neue Konzepte II
13:00	SCH/A101	DD 43	Abschlussplenum

QI

Invited Talk

09:30	BEY/0245	QI 11.1	Nb-trilayer Josephson junction based parametric amplifiers for microwave frequency signals •Lukas Grünhaupt

Sessions

09:30	BEY/0137	QI 10	Quantum Information: Concepts and Methods I
09:30	BEY/0245	QI 11	Implementations IV
15:00	BEY/0137	QI 12	Quantum Foundations
15:00	BEY/0245	QI 13	Quantum Control
18:00	P4	QI 14	Quantum Information Poster Session

UP

Sessions

09:30	MER/0002	UP 6	Upper Atmosphere, Polar Chemistry and Volcanic Aerosols
11:15	MER/0002	UP 7	Aquatic Systems: Limnology, Natural Waters, Wetlands and Soilmoisture
15:00	P1	UP 8	Poster

AKBP

Topical Talk

15:00	SCH/A117	AKBP 10.1	Multiscale longitudinal electron bunch characteristics of LWFA bunches determined by single-shot CTR spectroscopy •Alexander Debus

Sessions

09:30	P4	AKBP 8	Poster AKBP
11:00	SCH/A117	AKBP 9	RF Cavities I
15:00	SCH/A117	AKBP 10	Plasma Accelerators, Diagnostics I
16:30	SCH/A117	AKBP 11	Plasma Accelerators, Diagnostics II

AIW

Invited Talks, Discussions

14:10	BAR/SCHÖ	AIW 1.2	From Particle Physics to Patient Care – The Evolution of Accelerator-Based Tumor Therapy in Germany •Andrea Denker
14:30	BAR/SCHÖ	AIW 1.3	High Energy X-rays: Pioneering Hope and Success in Cancer Therapy •Stefan Scheib
14:50	BAR/SCHÖ	AIW 1.4	A Compact Accelerator Driven Neutron Source for Industry and Medicine •Holger Höltermann
15:10	BAR/SCHÖ	AIW 1.5	Panel discussion: Precision, Particles, Patients – The Future of Accelerator-Based Therapies •Andrea Denker, •Stefan Scheib, •Holger Höltermann, •John Kettler

Wednesday, March 11, 2026

AIW

16:00	BAR/SCHÖ	AIW 2.2	Accelerating Research with Particle Accelerators •Christoph Quitmann
16:20	BAR/SCHÖ	AIW 2.3	Advancements in Superconductor Technology for High-Energy Accelerators and Fusion Applications •Klaus Schlenga
16:40	BAR/SCHÖ	AIW 2.4	Application of Electron Accelerators for the Crosslinking of Polymers in Industry •Andreas Ostrowicki
17:00	BAR/SCHÖ	AIW 2.5	Panel discussion: Accelerating Innovation – Industrial Applications of High-Energy Physics •Christoph Quitmann, •Klaus Schlenga, •Andreas Ostrowicki, •John Kettler
			Sessions
14:00	BAR/SCHÖ	AIW 1	Medical Applications – Accelerators in the Service of Health
15:55	BAR/SCHÖ	AIW 2	Medical Applications – Accelerators in the Service of Health
17:20	BAR/SCHÖ	AIW 3	Ceremony of the DPG Technology Transfer Award & Presentation
18:00	BAR/SCHÖ	AIW 4	Open Reception of the AIW for the winners

JOB

			Invited Talks
11:00	HSZ/0405	JOB 2.1	Data-Analytics in der HUK-COBURG – Wie Physiker den Weg in ein datengetriebenes Versicherungsunternehmen mitgestalten •Jannik Hofestädt, •Andreas Gleixner, •Goran Nakerst
13:00	HSZ/0405	JOB 2.2	Basycon Unternehmensberatung GmbH: Aus der Wissenschaft in die Beratung •Tobias Weisrock, •Katharina Gräßel
15:00	HSZ/0405	JOB 2.3	Pädagogischen Hochschule Karlsruhe: Physik studiert – und jetzt? Dein Weg ins Lehramt. •Kay Burger, •Yvonne Ewen
			Session
11:00	HSZ/0405	JOB 2	Job Market II

09:30	Tents A and C	**Exhibition of Scientific Instruments and Literature** (free entrance)

			Public Evening Talk (free entrance)
19:00	HSZ/AUDI	PSV VIII	Gravitationswellenastronomie – quo vadis? •Michèle Heurs

DPG Industry Day & Technology Transfer Award 2026

High Energy Meets High Impact – Industrial and Medical Applications of Accelerators

The Industry Day will be held as part of the DPG Spring Conference, which usually has over 6,000 participants. Around 250 people (mostly students and doctoral candidates) taking part in the Industry Day, which is organized and carried out by the Industry and Economy Working Group (AIW) of the DPG. The aim of the events is to inspire students and PhD candidates for careers in business and industry. Following the Industry Day the DPG Technology Transfer Award will be conferred.

2.00 p.m.	**Welcome and greeting** Dr. Hans-Georg Grothues / Chairman of the AIW Dr. John Kettler / Moderator
Topic 1	**Medical Applications – Accelerators in the Service of Health**
2.10 p.m.	**From Particle Physics to Patient Care – The Evolution of Accelerator-Based Tumor Therapy in Germany** Prof. Dr. Andrea Denker – Helmholtz-Zentrum für Materialien und Energie
2.30 p.m.	**High Energy X-rays: Pioneering Hope and Success in Cancer Therapy** Dr. Stefan Scheib – Varian Medical Systems Imaging Lab GmbH
2.50 p.m.	**A Compact Accelerator Driven Neutron Source for Industry and Medicine** Holger Höltermann – Bevatech GmbH
3.10 p.m.	**Panel discussion: Precision, Particles, Patients – The Future of Accelerator-Based Therapies**
3.30 p.m.	**Coffee break**
3:55 p.m.	**Find your way: Career orientation and support from the DPG** Gabriele Becker – Advisor to the DPG Board
Topic 2	**Industrial Applications – Accelerators for Safety, Quality, and Innovation**
4.00 p.m.	**Accelerating Research with Particle Accelerators** Dr. Christoph Quitmann – RI Research Instruments
4.20 p.m.	**Advancements in Superconductor Technology for High-Energy Accelerators and Fusion Applications** Dr. Klaus Schlenga – Bruker Energy & Supercon Technologies
4.40 p.m.	**Application of Electron Accelerators for the Crosslinking of Polymers in Industry** Dr. Andreas Ostrowicki – BGS Beta-Gamma-Service
5.00 p.m.	**Panel discussion: Accelerating Innovation – Industrial Applications of High-Energy Physics**
5.20 p.m.	**Ceremony of the DPG Technology Transfer Award & Presentation**
6.00 p.m.	**Open Reception of the AIW for the winners**

As of January 12, 2026, subject to program changes

Technical University of Dresden
Schönfeld-Hörsaal BAR/SCHÖ/E
Georg-Schumann-Straße 13
01069 Dresden

March, 11th 2026
2:00 – 7:30 p.m.

Thursday, March 12, 2026

Plenary Talks

08:30	HSZ/AUDI	PV VIII	Insights into aqueous solution oxide interfaces from ab initio neural network potential molecular dynamics •Annabella Selloni
14:00	HSZ/AUDI	PV IX	On the sunny side – polymer-based organic solar cells •Peter Müller-Buschbaum
14:00	HSZ/0002	PV X	Towards a Science of Cities: A Complex Systems Approach •Marta Gonzalez

Prize Talks

13:00	HSZ/0002	PRV V	Observation of Floquet states in graphene •Marcel Reutzel (Laureate of the Walter-Schottky-Prize 2026)
13:00	HSZ/0003	PRV VI	Knots and Links in Magnetism •Maria Azhar (Laureate of the Hertha-Sponer-Prize 2026)

Lunch Talk

13:00	HSZ/0004	PSV IX	The organic development and growth story of aSpect Systems GmbH •Marcus Verhoeven

SYAI

Invited Talks

09:30	HSZ/AUDI	SYAI 1.1	Data and Experimental Foundations for Reliable Self-Driving Laboratories •Dr. Marcus Tze-Kiat Ng
10:00	HSZ/AUDI	SYAI 1.2	Digital Catalysis – AI for Experiment Planning and Control •Christoph Scheurer
10:30	HSZ/AUDI	SYAI 1.3	Autonomous, Data-Driven Workflows for Materials Acceleration Platforms with pyiron •Jan Janssen
11:15	HSZ/AUDI	SYAI 1.4	Machine Learning for Autonomous Optimization and Discovery of Materials •Pascal Friederich
11:45	HSZ/AUDI	SYAI 1.5	Transforming Our View on Transformers in the Sciences •Kevin Maik Jablonka

Session

09:30	HSZ/AUDI	SYAI 1	AI and Data Challenges behind Emerging Self-Driving Laboratories

SYTP

Invited Talks

15:00	HSZ/AUDI	SYTP 1.1	Social Tipping in Heterogeneous and Polarized Populations •Sara Constantino
15:30	HSZ/AUDI	SYTP 1.2	Tipping points and regime shifts in coupled social-climate systems •Chris Bauch
16:00	HSZ/AUDI	SYTP 1.3	How to tune Earth system models toward tipping? •Sebastian Bathiany
16:45	HSZ/AUDI	SYTP 1.4	Algorithmic amplification and contextual sensitivity in political information exposure •Joana Gonçalves de Sá
17:15	HSZ/AUDI	SYTP 1.5	The complex interplay between democracy and platform power •Philipp Lorenz-Spreen

Session

15:00	HSZ/AUDI	SYTP 1	Tipping Points in Social and Climate Systems

BP

Invited Talks

11:15	BAR/SCHÖ	BP 26.7	Directed evolution of material-producing bacteria •André Studart

Thursday, March 12, 2026

BP

09:30	BAR/0205	BP 27.1	Tissue interplay and the coordination of morphogenesis •Elias Barriga
10:15	BAR/0106	BP 30.1	Mechanogenetics for Cell ImmunoTherapy •Yingxiao Wang
11:30	BAR/0106	BP 30.4	Recent theoretical progress on sound-propelled microsystems •Raphael Wittkowski
15:00	BAR/0205	BP 33.1	Expanding the Bag of Optical Tricks for (Neuro)Biology •Fabian F. Voigt

Sessions

09:30	BAR/SCHÖ	BP 26	Biomaterials and Biopolymers
09:30	BAR/0205	BP 27	Cell Mechanics I
09:30	ZEU/0160	BP 28	Active Matter V
09:30	ZEU/0260	BP 29	Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates I
10:15	BAR/0106	BP 30	Focus Session: Controlling Microparticles and Biological Cells by Ultrasound
11:30	ZEU/0260	BP 31	Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates II
15:00	BAR/SCHÖ	BP 32	Statistical Physics of Biological Systems III
15:00	BAR/0205	BP 33	Bioimaging
15:00	ZEU/0160	BP 34	Focus Session: Emergent Transport in Active Systems
15:15	ZEU/LICH	BP 35	Focus Session: 75 Years Division Polymer Physics: From Curiosity to Smart Materials

CPP

Invited Talk, Topical Talks

09:30	ZEU/LICH	CPP 44.1	Shedding light on wide bandgap perovskites •Michael Saliba
09:30	ZEU/0260	CPP 45.1	Wetting transitions in biomolecular coacervates •Susanne Liese
15:15	ZEU/LICH	CPP 51.1	The Loops of Life •Michael Rubinstein
15:45	ZEU/LICH	CPP 51.2	Polyelectrolytes and Biological Systems: A Charged Relationship •Matthias Ballauff
16:15	ZEU/LICH	CPP 51.3	From block copolymer morphologies to functional polymer membranes •Volker Abetz
16:45	ZEU/LICH	CPP 51.4	Molecular electronic materials and devices for solar energy conversion •Jenny Nelson
17:15	ZEU/LICH	CPP 51.5	Control of cell and tissue stiffness by biopolymer networks and particle inclusions •Paul Janmey

Sessions

09:30	BAR/SCHÖ	CPP 43	Biomaterials and Biopolymers
09:30	ZEU/LICH	CPP 44	Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics V
09:30	ZEU/0260	CPP 45	Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates I
09:30	P5	CPP 46	Poster II
10:15	BAR/0106	CPP 47	Focus Session: Controlling Microparticles and Biological Cells by Ultrasound
11:30	ZEU/LICH	CPP 48	Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics VI
11:30	ZEU/0255	CPP 49	Gels, Polymer Networks and Elastomers I
11:30	ZEU/0260	CPP 50	Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates II
15:15	ZEU/LICH	CPP 51	Focus Session: 75 Years Polymer Physics Division: From Curiosity to Smart Materials
18:00	ZEU/LICH	CPP 52	Members' Assembly

Thursday, March 12, 2026

DS

Invited Talk

17:00	REC/C213	DS 18.8	Insights from Quantum Dynamics Simulations: From Molecules to Organic-Material Interfaces •Frank Ortmann

Sessions

09:30	HSZ/0003	DS 15	Focus Session: Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects II
09:30	REC/C213	DS 16	Thin Film Application
15:00	HSZ/0003	DS 17	Focus Session: High-Temperature Superconductivity in Hydride Materials at High Pressures
15:00	REC/C213	DS 18	Spins in Molecular Systems
17:45	REC/C213	DS 19	Members' Assembly
18:30	P2	DS 20	Poster

DY

Invited Talks

09:30	ZEU/0160	DY 49.1	Active memory and non-reciprocity as pathways to pattern formation in conserved scalar fields •Suropriya Saha
15:00	ZEU/0160	DY 55.1	Out-of-equlibrium synthetic cells: the future of active matter •Laura Alvarez
15:45	ZEU/0160	DY 55.3	Chemotactic like behavior in by active Brownian particles: from single particles to to polymers •Hidde Vuijk
16:45	ZEU/0160	DY 55.5	From non-reciprocal torques towards shape-flexible and res-ponsive prototypic worms •Holger Stark

Sessions

09:30	GÖR/0226	DY 45	Focus Session: Physics of AI – Part I
09:30	HÜL/S186	DY 46	Many-body Quantum Dynamics I
09:30	ZEU/0114	DY 47	Statistical Physics: General I
09:30	ZEU/0118	DY 48	Nonlinear Dynamics and Time-Delay Systems
09:30	ZEU/0160	DY 49	Active Matter V
10:15	BAR/0106	DY 50	Focus Session: Controlling Microparticles and Biological Cells by Ultrasound
11:15	ZEU/0118	DY 51	Networks: From Topology to Dynamics – Part III
15:00	BAR/SCHÖ	DY 52	Statistical Physics of Biological Systems III
15:00	HÜL/S186	DY 53	Many-body Quantum Dynamics II
15:00	ZEU/0114	DY 54	Statistical Physics: General II
15:00	ZEU/0160	DY 55	Focus Session: Emergent Transport in Active Systems
18:00	ZEU/0160	DY 56	Members' Assembly

FM

Invited Talks

09:30	BEY/0138	FM 17.1	Piled higher, probed deeper: X-ray insights into ferroelectric devices •Martina Müller
10:15	BEY/0138	FM 18.1	Stabilizing antiferroelectricity in PbZrO3 thin films using epitaxial tensile strain •Vincent Garcia
10:45	BEY/0138	FM 18.2	Strain effects in free-standing membranes of antiferroelectric Lead Zirconate •Umair Saeed

Sessions

09:30	BEY/0138	FM 17	Highlighted Talk: Piled higher, probed deeper: X-ray insights into ferroelectric devices (Martina Müller)
10:15	BEY/0138	FM 18	German-French Focus Session: (Anti)ferroic states – ferroelectrics, ferroelastics and antiferroelectrics II

Thursday, March 12, 2026

FM

10:15	BEY/0E40	FM 19	Advanced Microscopy and Tomography for Functional Materials
13:30	Infineon	FM 20	Excursion and Network-Event at Infineon Dresden AG
18:00	BEY/0138	FM 21	Members Assembly

HL

Invited Talks

11:15	POT/0006	HL 42.1	Transition Metal Nitride Semiconductors for Photoelectrochemical Energy Conversion •Verena Streibel
15:30	POT/0051	HL 46.3	Antisymmetric vibrations in the excited state dynamics of quadrupolar dyes •Antonietta De Sio
16:15	POT/0081	HL 49.1	Phonon-mediated nonlinearity and defects in hexagonal boron nitride •Nahid Talebi

Sessions

09:30	POT/0006	HL 37	Nitrides II – Designed properties and LED
09:30	POT/0051	HL 38	Materials and Devices for Quantum Technology II
09:30	POT/0081	HL 39	2D semiconductors VII – CrSBr and related heterostructures
09:30	POT/0251	HL 40	Oxide Semiconductors: Transport and Spectroscopy
11:00	HSZ/0101	HL 41	Quantum Dots and Point Contacts
11:15	POT/0006	HL 42	Nitrides III – Emerging thin films and electrochemistry
13:30	Infineon	HL 43	Excursion and Network-Event at Infineon Dresden AG
15:00	HSZ/0204	HL 44	2D Materials: Electronic structure, excitations, etc. III
15:00	POT/0006	HL 45	Perovskite and Photovoltaics: Spectroscopy
15:00	POT/0051	HL 46	Ultra-fast Phenomena II
15:00	POT/0081	HL 47	2D Materials VIII – Quantum emitters and defects
15:00	POT/0251	HL 48	Heterostructures, Interfaces and Surfaces: Fabrication and Structure
16:15	POT/0081	HL 49	Quantum Emitters in 2D Semiconductors
17:45	POT/0051	HL 50	Members' Assembly

MA

Invited Talks

09:30	HSZ/0002	MA 40.1	Magnetic order induced chiral phonons in a ferromagnetic Weyl semimetal •Luyi Yang
11:15	HSZ/0002	MA 40.6	Thermal Hall Effects of Magnons and Phonons •Alexander Mook
09:30	POT/0112	MA 43.1	Defect-Induced Phase Transitions in the 2D Magnetic Semiconductor CrSBr •Shengqiang Zhou
09:30	POT/0151	MA 44.1	2D and 3D racetracks: Interplay of geometric and magnetic chiralities •Stuart Parkin
10:00	POT/0151	MA 44.2	Combined MFM/KPFM at the Ultimate Sensitivity Limit for Probing Curvature-Engineered Micromagnetic States •Emily Darwin
10:30	POT/0151	MA 44.3	Curvilinear magnetism in superconducting spintronics •Sol Jacobsen
11:15	POT/0151	MA 44.4	Advanced Control of Magnetic Nanostructures via Metasurface Engineering and Voltage-Driven Functionalities •Anna Palau
11:45	POT/0151	MA 44.5	Magnetic tomography of noncollinear spin textures in curvilinear geometries •Sandra Ruiz-Gomez

Sessions

09:30	HSZ/0002	MA 40	Focus Session: Chiral phonons and crystals coupled to magnetic order II
09:30	HSZ/0003	MA 41	Focus Session: Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects II
09:30	HSZ/0004	MA 42	Molecular Magnetism and Magnetic Particles / Clusters II
09:30	POT/0112	MA 43	Spin-Dependent Phenomena in 2D

Thursday, March 12, 2026

MA

09:30	POT/0151	MA 44	Focus Session: Curvilinear magnetism: Magnetics with nanoscale curved geometries
09:30	POT/0351	MA 45	Magnetic Relaxation and Gilbert Damping
09:30	POT/0361	MA 46	Magnetic Imaging Techniques II
15:00	HSZ/0002	MA 47	Altermagnets V
15:00	HSZ/0004	MA 48	Magnonics II
15:00	POT/0112	MA 49	Magnetic Imaging, Information Technology, and Sensors
15:00	POT/0151	MA 50	Bulk Materials: Soft and Hard Permanent Magnets
15:00	POT/0361	MA 51	Spin Transport and Orbitronics, Spin-Hall Effects II
15:00	P4	MA 52	Poster Magnetism III
18:00	HSZ/0002	MA 53	Members' Assembly

MM

Invited Talks, Topical Talks

09:30	SCH/A251	MM 29.1	Three dimensional sub-Ångström resolution imaging from 4D-STEM experiments •Philipp Pelz
10:15	SCH/A251	MM 32.1	High-Throughput Nanomechanics and Data-Driven Workflows for Mapping Composition-Microstructure-Property Landscapes •Ruth Schwaiger
11:00	SCH/A251	MM 32.3	Expanding nanoindentation capabilities: Data-driven and novel experimental approaches •Michael Wurmshuber
11:45	SCH/A251	MM 32.4	Additive Manufacturing and Nanomechancics – where is the Link? •Ralph Spolenak
15:00	SCH/A251	MM 33.1	LPBF with Ultrashort Laser Pulses - Additive Manufacturing Beyond Current Limits •Stefan Nolte
15:45	SCH/A251	MM 36.1	High-temperature micropillar compression for understanding dislocation-precipitates interactions in Ni-Based superalloys •Subin Lee

Sessions

09:30	SCH/A251	MM 29	Invited Talk: Philipp Pelz
10:15	SCH/A215	MM 30	Interface Controlled Properties, Nanomaterials, and Microstructure Design II
10:15	SCH/A216	MM 31	Transport in Materials: Diffusion, Charge, or Heat Conduction II
10:15	SCH/A251	MM 32	Topical Session: Advanced Nanomechanics – Accelerating Materials Physics from the Bottom I
15:00	SCH/A251	MM 33	Invited Talk: Stefan Nolte
15:45	SCH/A215	MM 34	Hydrogen in Materials I
15:45	SCH/A216	MM 35	Additive Manufacturing / Transport in Materials III
15:45	SCH/A251	MM 36	Topical Session: Advanced Nanomechanics – Accelerating Materials Physics from the Bottom II
15:45	SCH/A315	MM 37	Development of Calculation Methods I

O

Invited Talks, Topical Talk

09:30	TRE/PHYS	O 75.1	Oxide interfaces as platforms for emergent quantum phenomena •Manuel Bibes
10:30	HSZ/0401	O 78.1	The Wendelstein 7-X plasma vessel vacuum system from a scientific perspective •Georg Schlisio
10:30	WILL/A317	O 82.1	Low-energy inverse photoelectron spectroscopy (LEIPS): probing unoccupied states and conduction band structure in functional materials •Hiroyuki Yoshida
11:00	WILL/A317	O 82.2	Enhanced Sensitivity in Low-Energy Inverse Photoemission Spectroscopy with an Off-Axis Parabolic Mirror for Efficient Light Collection •Yongsup Park

Thursday, March 12, 2026

O

15:00	HSZ/0401	O 85.1	From light to pressure: Laser-based quantum technologies for the realization of high-precision pressure and vaccum standards •Tom Rubin
15:00	HSZ/0403	O 86.1	Ultrafast Dynamics at Surfaces with Machine Learning Surrogates •Reinhard Maurer

Sessions

09:30	TRE/PHYS	O 75	Topical Talk Bibes
10:30	HSZ/0201	O 76	Electronic structure of surfaces: Spectroscopy, surface states II
10:30	HSZ/0204	O 77	Nanostructures at surfaces:1D, 2D, networks II
10:30	HSZ/0401	O 78	Vacuum Science & Technology: Theory and Applications I
10:30	HSZ/0403	O 79	Plasmonics and nanooptics: Light-matter interaction, spectroscopy III
10:30	TRE/PHYS	O 80	Gerhard Ertl Young Investigator Award Competition
10:30	TRE/MATH	O 81	Catalysis and surface reactions II
10:30	WILL/A317	O 82	Focus Session: Unoccupied States by Inverse Photoemission III
15:00	HSZ/0201	O 83	Organic molecules on inorganic substrates: electronic, optical and other properties III
15:00	HSZ/0204	O 84	2D Materials: Electronic structure, excitations, etc. III
15:00	HSZ/0401	O 85	Vacuum Science & Technology: Theory and Applications II
15:00	HSZ/0403	O 86	Surface dynamics
15:00	TRE/PHYS	O 87	Solid-liquid interfaces: Structure, spectroscopy
15:00	TRE/MATH	O 88	Catalysis and surface reactions III
15:00	WILL/A317	O 89	Spins on surfaces at the atomic scale II
17:15	HSZ/0401	O 90	Members' Assembly of the Vacuum Science and Technology Divison (VA)
19:00	HSZ/AUDI	O 91	Members' Assembly
19:30	HSZ/AUDI	O 92	Post-Deadline Session

SOE

Invited Talks

09:30	GÖR/0226	SOE 14.1	Generative AI and diffusion models: a statistical physics approach •Giulio Biroli
11:30	GÖR/0226	SOE 16.1	Tipping in Strongly Perturbed Open Networks •Marc Timme

Sessions

09:30	GÖR/0226	SOE 14	Focus Session: Physics of AI I
11:15	ZEU/0118	SOE 15	Networks: From Topology to Dynamics III
11:30	GÖR/0226	SOE 16	Tipping Points in Social and Climate Systems (accompanying session for SYTP)

TT

Topical Talks

15:00	HSZ/0003	TT 80.1	Computational searches for conventional high temperature superconductivity •Chris Pickard
15:30	HSZ/0003	TT 80.2	High-pressure synthesis of hydrides and their characterisation by single-crystal X-ray diffraction •Natalia Dubrovinskaia
16:00	HSZ/0003	TT 80.3	Electrical Transport Studies in bulk and thin-film hydride high-temperature superconductors •Sven Friedemann
16:45	HSZ/0003	TT 80.4	Near room-temperature conventional superconductivity in hydrogen-rich compounds at high pressures: Experimental evidences •Vasily Minkov
17:15	HSZ/0003	TT 80.5	Predictive Tc Calculations in Hydride Superconductors •Christoph Heil

Sessions

09:30	HSZ/0003	TT 69	Focus Session: Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects II

Thursday, March 12, 2026

TT

09:30	HSZ/0101	TT 70	Correlated Electrons: Method Development III
09:30	HSZ/0103	TT 71	Ultrafast Phenomena
09:30	HSZ/0105	TT 72	Correlated Magnetism – Spin Liquids I
09:30	CHE/0089	TT 73	Superconductivity: Tunneling and Josephson Junctions
09:30	CHE/0091	TT 74	Topological Insulators
09:30	HÜL/S186	TT 75	Many-body Quantum Dynamics I
09:30	POT/0151	TT 76	Focus Session: Curvilinear magnetism: Magnetics with nanoscale curved geometries
09:30	TRE/PHYS	TT 77	Topical Talk Bibes
11:00	HSZ/0101	TT 78	Quantum Dots and Point Contacts
11:30	HSZ/0103	TT 79	Correlated Magnetism – Transport
15:00	HSZ/0003	TT 80	Focus Session: High-Temperature Superconductivity in Hydride Materials at High Pressures
15:00	HSZ/0101	TT 81	Correlated Electrons: Other Materials
15:00	HSZ/0103	TT 82	Cryogenic Detectors and Sensors
15:00	HSZ/0105	TT 83	Topology: Quantum Hall Systems
15:00	HSZ/0204	TT 84	2D Materials: Electronic structure, excitations, etc. III
15:00	CHE/0089	TT 85	Superconductivity: Yu-Shiba-Rusinov and Andreev Physics
15:00	CHE/0091	TT 86	Correlated Magnetism – Spin Liquids II
15:00	HÜL/S186	TT 87	Many-body Quantum Dynamics II
15:00	POT/0361	TT 88	Spin Transport and Orbitronics, Spin-Hall Effects II
16:45	HSZ/0103	TT 89	Cryotechnique: Refrigeration
17:00	CHE/0091	TT 90	Quantum Impurities and Kondo Physics
17:30	HSZ/0101	TT 91	Superconductivity: Theory II
18:00	P4	TT 92	Transport – Poster
18:00	P4	TT 93	Superconductivity – Poster II

QI

Invited Talks

11:30	BEY/0137	QI 15.7	Robust shadow tomography: from quantum simulation to high-energy physics •Hai-Chau Nguyen
09:30	BEY/0245	QI 16.1	Measurement-free universal fault-tolerant quantum computation •Friederike Butt
15:00	BEY/0245	QI 18.1	Multipartite Quantum states from guided-wave structures •Virginia D'Auria

Sessions

09:30	BEY/0137	QI 15	Quantum Information: Concepts and Methods II
09:30	BEY/0245	QI 16	Quantum Software
15:00	BEY/0137	QI 17	Decoherence and Open Systems II
15:00	BEY/0245	QI 18	Quantum Communication
18:00	BEY/0245	QI 19	Members' Assembly

AKBP

Topical Talk

09:30	SCH/A117	AKBP 12.1	Cutting-edge research and technology at KIT's advanced accelerator facilities •Erik Bründermann

Sessions

09:30	SCH/A117	AKBP 12	Novel Accelerators I
11:30	SCH/A117	AKBP 13	Novel Accelerators II
15:00	SCH/A117	AKBP 14	RF Cavities II
16:00	SCH/A117	AKBP 15	AKBP Prize Talks
18:00	SCH/A117	AKBP 16	Members' Assembly

Thursday, March 12, 2026

AKC

Invited Talks

11:15	MER/0002	AKC 1.1	From Taboo to Transformation: Addressing Gender-Based Violence in Academia •Anja Wiede
11:45	MER/0002	AKC 1.2	Leadership, Cooperation and Conflicts in Physics: Research Leaders' Perspectives •Maike Reimer
12:15	MER/0002	AKC 1.3	Die Physikidentität von Schüler:innen stärken: Erkenntnisse zu Theorie und Praxis •Paula Becker

Sessions

11:00	MER/0002	AKC 1	AKC
13:00	MER/0002	AKC 2	Women in Physics Lunch

AKjDPG

Session

09:30	SCH/A101	AKjDPG 1	Hacky Hour

AKPIK

Sessions

15:00	P5	AKPIK 5	Poster
16:45	BEY/0127	AKPIK 6	AI Methods for Physics and Materials Science

09:30	Tents A and C	**Exhibition of Scientific Instruments and Literature** (free entrance)

Friday, March 13, 2026

Plenary Talk

08:30	HSZ/AUDI	PV XI	Phase separation in Cell Physiology and Disease •Anthony Hyman

SYQF

Invited Talks

09:30	HSZ/AUDI	SYQF 1.1	Exciton dressing by extreme nonlinear magnons in a layered semiconductor •Geoffrey M. Diederich
10:00	HSZ/AUDI	SYQF 1.2	A tale of demons and decay in two-dimensional (alter)magnets •Alexander Mook
10:30	HSZ/AUDI	SYQF 1.3	Magnetism, light and matter – Role of excitons in two-dimensional magnets •Florian Dirnberger
11:15	HSZ/AUDI	SYQF 1.4	Advantages and challanges of resonance Raman scattering with infrared excitation energy •Leonetta Baldassarre
11:45	HSZ/AUDI	SYQF 1.5	Shining light on 2D antiferromagnets •Dmytro Afanasiev

Session

09:30	HSZ/AUDI	SYQF 1	Interacting Degrees of Freedom in Ultrathin Quantum Films

BP

Invited Talks

09:30	BAR/SCHÖ	BP 36.1	Swimming in complex environments •Christina Kurzthaler
11:30	BAR/0205	BP 41.1	Probing spatiotemportal electrochemical dynamics on single bacterial cells •Ashley Nord

Sessions

09:30	BAR/SCHÖ	BP 36	Statistical Physics of Biological Systems IV
09:30	BAR/0106	BP 37	Tissue Mechanics II
09:30	ZEU/0160	BP 38	Active Matter VI
09:30	ZEU/0260	BP 39	Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates III
10:00	BAR/0205	BP 40	Cell Mechanics II / Cytoskeleton II
11:30	BAR/0205	BP 41	Franco-German Session: Bacterial Biophysics II
13:15	HSZ/0002	BP 42	Closing Talk

CPP

Invited Talks, Topical Talk

09:30	ZEU/LICH	CPP 53.1	Limits and Prospects of Organic Solar Cells •Dieter Neher
09:30	ZEU/0255	CPP 54.1	NMR-based molecular rheology and structural characterization of model gels •Kay Saalwächter
09:30	ZEU/0260	CPP 55.1	Data-driven modelling of phase-separating intrinsically disordered regions •Giulio Tesei
10:45	HÜL/S386	CPP 56.1	Liquid Dynamics at Interfaces •Michael Vogel
13:15	HSZ/0002	CPP 61.1	Closing Talk: Biololecular Condensates: Callenges for Polymer Physics •Jens-Uwe Sommer

Sessions

09:30	ZEU/LICH	CPP 53	Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics VII
09:30	ZEU/0255	CPP 54	Gels, Polymer Networks and Elastomers II
09:30	ZEU/0260	CPP 55	Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates III

Friday, March 13, 2026

CPP

10:45	HÜL/S386	CPP 56	Molecular and Polymer Dynamics, Friction and Rheology I
11:30	ZEU/LICH	CPP 57	Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics VIII
11:30	ZEU/0255	CPP 58	Gels, Polymer Networks and Elastomers III
11:30	ZEU/0260	CPP 59	Crystallization
12:15	HÜL/S386	CPP 60	Molecular and Polymer Dynamics, Friction and Rheology II
13:15	HSZ/0002	CPP 61	Closing Talk

DS

Session

09:30	REC/C213	DS 21	Optical Analysis of Thin Films

DY

Invited Talks

11:15	HÜL/S186	DY 59.7	Anyon dynamics in driven topologically ordered quantum systems •Francesco Petiziol
09:30	ZEU/0160	DY 62.1	Morphogenesis, transport, and computation in micro-scale swarms •Akira Kakugo

Sessions

09:30	BAR/SCHÖ	DY 57	Statistical Physics of Biological Systems IV
09:30	GÖR/0226	DY 58	Focus Session: Physics of AI – Part II
09:30	HÜL/S186	DY 59	Quantum Chaos and Coherent Dynamics
09:30	ZEU/0114	DY 60	Critical Phenomena and Phase Transitions
09:30	ZEU/0118	DY 61	Brownian Motion and Anomalous Transport
09:30	ZEU/0160	DY 62	Active Matter VI
11:30	ZEU/0118	DY 63	Nonlinear Stochastic Systems
13:15	HSZ/0002	DY 64	Closing Talk

FM

Invited Talks

09:30	BEY/0138	FM 22.1	Topological thermoelectrics for solid state cooling •Yu Pan
09:30	BEY/0E40	FM 23.1	Mapping topological textures in compensated magnets with X-rays •Claire Donnelly

Sessions

09:30	BEY/0138	FM 22	Focus Session: Materials Discovery III – New materials and functionalities by general principles
09:30	BEY/0E40	FM 23	Focus Session: (Anti)ferroic states – Magnetic and magnetoelectric III

HL

Invited Talk

09:30	POT/0051	HL 53.1	Organic semiconductors: Opening new perspectives in sustainable electronics •Karl Leo

Sessions

09:30	HSZ/0401	HL 51	2D Materials: Stacking and heterostructures
09:30	POT/0006	HL 52	THz and MIR Physics in Semiconductors
09:30	POT/0051	HL 53	Organic Semiconductors: Carrier Dynamics
09:30	POT/0081	HL 54	2D Materials IX – Photonic properties and devices
09:30	POT/0251	HL 55	Quantum Dots and Wires: (Single) Photonics
11:15	POT/0006	HL 56	Quantum Emitters in 3D Semiconductors
11:30	POT/0051	HL 57	Nitrides IV – Optical properties

Friday, March 13, 2026

MA

Sessions

09:30	HSZ/0002	MA 54	Altermagnets VI
09:30	HSZ/0004	MA 55	Skyrmions III
09:30	BEY/0E40	MA 56	Focus Session: (Anti)ferroic states – Magnetic and magnetoelectric III
09:30	POT/0112	MA 57	Thin Films: Magnetic Coupling Phenomena / Exchange Bias and Magnetic Anisotropy
09:30	POT/0151	MA 58	Computational Magnetism II
09:30	POT/0361	MA 59	Magnonics III

MM

Invited Talk

09:30	SCH/A251	MM 38.1	Alloy design and deformation behaviour of Mo-based silicide materials •Manja Krueger

Sessions

09:30	SCH/A251	MM 38	Invited Talk: Manja Krüger
10:15	SCH/A215	MM 39	Hydrogen in Materials II
10:15	SCH/A216	MM 40	Transport in Materials: Diffusion, Charge, or Heat Conduction IV
10:15	SCH/A251	MM 41	Development of Calculation Methods II

O

Invited Talks, Topical Talk

09:30	HSZ/0204	O 94.1	Surface Chemistry on Copper Oxides •Dario Stacchiola
09:30	TRE/PHYS	O 97.1	Questions of Selectivity in Electrocatalysis •Vanessa J. Bukas
09:30	TRE/MATH	O 98.1	Electron-phonon interactions in the time domain: from non-equilibrium phonon dynamics to theoretical spectroscopy •Fabio Caruso
13:15	TRE/PHYS	O 100.1	Ionic Liquid Surface Science •Hans-Peter Steinrück

Sessions

09:30	HSZ/0201	O 93	Electronic structure of surfaces: Spectroscopy, surface states III
09:30	HSZ/0204	O 94	Oxides and insulators: Adsorption and reaction of small molecules
09:30	HSZ/0401	O 95	2D Materials: Stacking and heterostructures
09:30	HSZ/0403	O 96	Plasmonics and nanooptics: Fabrication, characterization and applications
09:30	TRE/PHYS	O 97	Solid-liquid interfaces: Reactions and electrochemistry III
09:30	TRE/MATH	O 98	Ultrafast electron dynamics at surface and interfaces IV
09:30	WILL/A317	O 99	Spins on surfaces at the atomic scale III
13:15	TRE/PHYS	O 100	Closing Talk Steinrück

SOE

Invited Talks

09:30	GÖR/0226	SOE 17.1	What can we learn from neural quantum states? •Agnes Valenti
11:15	GÖR/0226	SOE 17.6	Creativity in generative AI •Matthieu Wyart

Session

09:30	GÖR/0226	SOE 17	Focus Session: Physics of AI II

Friday, March 13, 2026

TT

Sessions

09:30	HSZ/0101	TT 94	Correlated Magnetism – Low-Dimensional Systems
09:30	HSZ/0103	TT 95	Fe-based Superconductors
09:30	HSZ/0401	TT 96	2D Materials: Stacking and heterostructures
09:30	CHE/0089	TT 97	Superconducting Diodes and Ratchets
09:30	CHE/0091	TT 98	Altermagnets
09:30	HÜL/S186	TT 99	Quantum Chaos and Coherent Dynamics

QI

Invited Talk

09:30	BEY/0245	QI 21.1	Non-Hermitian topology and directional amplification •Clara Wanjura

Sessions

09:30	BEY/0137	QI 20	Metrology and Sensing
09:30	BEY/0245	QI 21	Quantum Information: Concepts and Methods III

Plenary Talks

Plenary Talk PLV I Mon 8:30 HSZ/AUDI

Cavity-altered superconductivity — •Dmitri Basov — Columbia University, New York, USA

Is it feasible to alter the ground state properties of a material by engineering its electromagnetic environment? Inspired by theoretical predictions, experimental realizations of such cavity-controlled properties without optical excitation are beginning to emerge. A grand aspiration of cavity quantum materials research is to uncover fundamentally new routes for controlling properties of matter by judiciously tailoring the quantum electromagnetic environment. We devised and implemented a novel platform to realize cavity-altered materials. Single crystals of hyperbolic van der Waals (vdW) compounds provide a resonant electromagnetic environment with enhanced density of photonic states and prominent mode confinement. We interfaced hexagonal boron nitride (hBN) with the molecular superconductor κ-(BEDT-TTF)2Cu[N(CN)2]Br (κ-ET). Meissner effect measurements demonstrate a strongly altered superfluid density at the hBN/κ-ET interface. Our work highlights the potential of dark cavities devoid of external photons for engineering electronic ground state properties of complex quantum materials. To appear in Nature in 2026.

Plenary Talk PLV II Mon 14:00 HSZ/AUDI

Towards Intelligent Matter: Energy-Efficient In-Materio Computing — •Karin Everschor-Sitte — Faculty of Physics and Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, Duisburg, Germany

The rapid expansion of artificial intelligence has driven computational demands to unprecedented levels, making power consumption a central bottleneck for state-of-the-art hardware architectures. This presentation addresses how functional materials, including magnetic, ferroelectric, optical, and plasmonic systems, offer a path beyond this limitation by leveraging their intrinsic physical properties to compute and process information directly within matter. Our research centers on magnetic materials, whose nonlinear, complex hysteretic responses make them particularly well-suited for low-energy, efficient unconventional computing paradigms like reservoir computing. Advances in harnessing magnetic and ferroelectric textures for in-materio computation will be presented. These developments outline how coordinated integration of material properties, algorithmic design, and device engineering can enable high-performance, energy-efficient computing technologies and ultimately pave the way toward intelligent matter.

Plenary Talk PLV III Mon 14:00 HSZ/0002

Simulating the Hubbard model with moiré semiconductors — •Jie Shan — Max Planck Institute for the Structure and Dynamics of Matter — Cornell University

The Hubbard model is a simple theoretical model of interacting quantum particles in a lattice. It is believed to capture the essential physics of many strongly correlated phenomena, such as high-temperature superconductivity, magnetism, and metal-insulator transitions, but has proved difficult to solve accurately except in one dimension. Physical realizations of the Hubbard model therefore have a vital role to play in the study of correlation physics. Moiré materials, formed by overlaying two van der Waals materials of slightly different orientations or lattice constants, have recently emerged as a promising Hubbard model simulator. In this talk, I will review the recent experimental progress on the realization of both the triangular and honeycomb lattice Hubbard models, and how the electronic phase diagram evolves with the U/W ratio (where U and W denote the onsite Coulomb repulsion and the moiré bandwidth, respectively).

Plenary Talk PLV IV Tue 8:30 HSZ/AUDI

Spins in Quantum Dots: The Quiet Revolution — •Dorian Gangloff — Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom

Solid-state spins in semiconductors provide a natural interface between stationary qubits and single photons, forming key building blocks for future quantum communication networks. Historically, semiconductor quantum dots (QDs) were considered too noisy for spin physics: strong hyperfine interactions within a mesoscopic system, materials inhomogeneity, and limited control tools once cast doubt on their suitability as coherent spin qubits. In recent years this perception has shifted dramatically. Advances in growth, device engineering, coherent control, and nuclear-spin cooling have ushered in a quiet revolution in III-V QDs. They now exhibit excellent optical coherence, near-unity photon collection when integrated with photonic structures, and spin degrees of freedom with long coherence times.

In this talk I will present three developments that illustrate this transformation: (1) High-fidelity electron-spin control, (2) Quantum memories from nuclear spins, and (3) Deterministic design of QD properties prior to growth.

Together, these advances reveal how the long-standing "noise problem" in III-V quantum dots is being turned into a resource, and underline their emergence as a platform for quantum communication and quantum information processing.

Plenary Talk PLV V Wed 8:30 HSZ/AUDI

Reimagining Physics Education for a Planet in Transformation — •Giulia Tasquier — Department of Physics and Astronomy, ALMA MATER STUDIRUM - University of Bologna, Bologna, Italy

The accelerating climate crisis intensifies the need to interpret complex evidence and act upon it. While physics and climate science offer foundations for understanding global warming, scientific knowledge alone does not suffice to support informed action. This plenary examines how physics education can help bridge this gap. Drawing on research in climate change education, I discuss how modelling, causal reasoning, and the epistemology of complex systems can strengthen students' understanding of climate phenomena and uncertainty in scientific prediction. Insights from futures studies highlight the importance of anticipating alternative scenarios and moving beyond deterministic expectations. Integrating these perspectives supports what we define as agency: a capacity connecting scientific understanding with ethical reflection and imaginative anticipation. Empirical work shows that students engaging with complexity-based explanations expand their imaginative horizons and begin to position themselves as agents within complex climate futures. Activities such as exploring branching scenarios or reframing narratives of the climate crisis help them see the future not as fixed, but as a space of plurality, contingency, and imagination. The talk outlines a three-dimensional framework on agency to integrate these elements into physics education, reimagining it as a practice of freedom that turns complexity into a resource for imagination and solidarity.

Plenary Talk PLV VI Wed 14:00 HSZ/AUDI

Materials selection methods: a compass in the jungle — •Yves Bréchet — Monash University, Materials Science Department, Clayton Campus, Melbourne, Australia

Materials use and development have undergone a profound transformation in the last decades: the "book of specifications" is more and more demanding, more and more multifunctional, and additional requests such as sustainability have progressively strengthened conflicting requirements. At the same time, the variety of materials available to engineers has expanded in such a way that materials selection and materials design is a must for efficient use of materials. To meet this new request, materials and process databases, and materials selection tools have been developed in the last 20 years, allowing both for a better use of materials, and for a guidance of "materials by design". The case of materials associated with a prescribed geometry, so-called "architectured materials", are a striking example of this evolution from "materials by chance", via "materials in competition", to "materials by design". Recent developments in AI to generate new materials open new opportunities and raise new challenges for this general trend toward materials by design.

Plenary Talk PLV VII Wed 14:00 HSZ/0002

Stronger yet weaker: Long-range orientational order in 2D active matter — •Hugues Chaté — CEA - Saclay, France

The Mermin-Wagner-Hohenberg theorem tells us that, in a 2D system in equilibrium, the spontaneous breaking of a continuous symmetry cannot lead to true long-range order. Out of equilibrium, and in particular in active matter systems, it is now well known that 2D true long-range orientational order is possible.

I will first give an updated view of our knowledge of polarly ordered phases in 2D active matter systems. I will then proceed to show that many of these phases are metastable to the nucleation of droplets which, opposite to the Peierls argument at play in equilibrium, grow and eventually destroy order. Order is thus both stronger (truly long-range) and weaker (metastable) in 2D active systems.

Plenary Talk PLV VIII Thu 8:30 HSZ/AUDI

Insights into aqueous solution oxide interfaces from ab initio neural network potential molecular dynamics — •Annabella Selloni — Princeton University, Department of Chemistry, Princeton, NJ, United States

Aqueous solution-oxide interfaces play a critical role in many environmental, biological, and energy-relevant processes. Molecular dynamics (MD) simulations employing ab initio based deep neural network potentials (DPs) have recently emerged as a valuable approach to complement experimental observations and obtain detailed molecular scale insights. In this talk, I shall discuss recent applications of DP-MD to understand the structure and properties of aqueous solution-oxide interfaces. Focusing on titanium dioxide, a prototypical metal oxide with a prominent role in energy applications, specific topics will include characterization of the electrified TiO2-electrolyte interface, and the effects of organic compounds such as formic acid and methanol on the structure and chemistry of water at the interface.

Plenary Talk PLV IX Thu 14:00 HSZ/AUDI

On the sunny side - polymer-based organic solar cells — •Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany

Polymer-based organic solar cells open up new fields of application compared to conventional silicon-based solar cells, as they are flexible, lightweight, color-adjustable, and potentially very cost-effective. In addition, they also function in low-light conditions and have a high power density, which makes them very attractive for space applications, in addition to their classic terrestrial applications. Since 2025, single-junction organic solar cells have surpassed the magic 20% efficiency rate. Moreover, organic solar cells are also successfully combined with other solar technologies in tandem devices as recently demonstrated with an efficient near-infrared harvesting in perovskite-organic tandem solar cells [1]. Current research questions focus on the aging mechanisms of organic solar cells and the feasibility of converting solar cell production to highly scalable manufacturing methods. The Müller-Buschbaum Group is investigating both issues using advanced X-ray and neutron scattering methods in situ and operando during production [2] and solar cell operation [3]. In addition, the Müller-Buschbaum Group has conducted pioneering work in investigating organic solar cells in space, demonstrating that organic solar cells function equally well in space as they do in the laboratory [4]. [1] Nature 643, 104-110 (2025); [2] Adv. Energy Mater. 15, 2404724 (2025); [3] Nano Energy 140, 111043 (2025); [4] Joule 4, 1880-1892 (2020)

Plenary Talk PLV X Thu 14:00 HSZ/0002

Towards a Science of Cities: A Complex Systems Approach — •Marta Gonzalez — UC Berkeley, USA

Cities are complex systems whose dynamics emerge from the interactions of millions of individuals, institutions, and infrastructures. In this talk, I present a framework that applies the principles of complex systems science to urban environments, aiming to uncover unifying patterns and mechanisms that govern urban behavior. Drawing on large-scale mobility, traffic, emissions, and financial transaction data, I show how cities can be studied as living laboratories of collective behavior. First, I examine the macroscopic dynamics of urban traffic, identifying critical thresholds that mark the onset and collapse of mobility systems across different cities, and framing these collapses as nonequilibrium phase transitions. I then explore the environmental consequences of these dynamics, introducing a scalable model that links real-world mobility patterns to vehicular CO* emissions, highlighting the pivotal role of vehicle kilometers traveled. Shifting focus to spatial structure, I illustrate how mobility data reveals the transformation of urban form in response to disruptive events, such as pandemics, and offer novel metrics to quantify home-based travel and structural shifts. Finally, I demonstrate how behavioral regularities in credit card transaction sequences encode individual lifestyles and social structures, showing how economic activity reflects deeper patterns of urban life. Together, these studies underscore the value of a data-driven, systems-oriented approach to understanding and shaping the future of cities.

Plenary Talk PLV XI Fri 8:30 HSZ/AUDI

Phase separation in Cell Physiology and Disease — •Anthony Hyman — Pfotenhauerstraße 108

Cells organize many of their biochemical reactions by formation and dissolution of non-membrane-bound compartments. Recent experiments show that a common mechanism for such biochemical organization is phase separation of unstructured proteins to form liquid-like compartments. These liquid-like compartments can be described by principles elucidated from condensed-matter physics and are therefore termed biomolecular condensates. I will discuss the relationship between the formation of liquid like compartments, quality control mechanisms that preserve the liquid-like state, and the onset of aggregated-protein pathology that is commonly observed in neurodegenerative diseases.

Prize Talks

Prize Talk PRV I Mon 13:00 HSZ/0002

Driven Quantum Materials: Controlling Emergent Phenomena away from Equilibrium — •Andrea Cavalleri — Max Planck Institute for the Structure and Dynamics of Matter — Laureate of the Stern-Gerlach-Medal 2026

I will discuss how coherent electromagnetic radiation, when tuned to collective modes in quantum materials, can be used to induce unexpected dynamical phenomena. The core idea is that when uncoupled normal modes are driven nonlinearly, complex correlations are created that are absent in equilibrium. Emergent dynamical orders, which include superconductivity, magnetism, ferroelectricity and other functional phenomena, are created in this way, with both fundamental and applied ramifications. I will touch on the crucial importance of modern ultrafast X-Ray Free Electron Lasers, and novel THz sources that are matched to these.

Prize Talk PRV II Tue 13:00 HSZ/0002

Polymers / Soft Matter as Model Systems for Physics — •Kurt Kremer — MPI für Polymerforschung, Mainz, Deutschland — Laureate of the Max-Planck-Medal 2026

Polymers, long chain molecules, comprise important materials of our daily life, being it simple commodities with all their advantages and disadvantages or high-tech materials in electronics or medicine, etc. Furthermore, bio-polymers such as cellulose or DNA are central constituents of living organisms. Thus, polymers have been subject of applied physics since their discovery. That, however, changed with de Gennes' n->0 theorem, showing that the inverse chain length 1/N can be mapped onto the distance |T-Tc|/Tc from the critical point in a n-vector spin model. At about the same time computer simulations became powerful tools to study critical phenomena, complemented by experiment, most notably neutron scattering for polymers. All this marked the start of polymers becoming versatile systems to study critical phenomena.

Polymers/Soft Matter are susceptible to small molecular stimuli. Thus, minute shifts in local interactions easily turn into macroscopic property changes. Here generic physical concepts meet chemical details, making polymers so versatile. The talk will review a few examples, where such effects lead to physically interesting phenomena (active systems, glass transition, nanoporous materials). Finally, new challenges imposed by soft matter will shortly be discussed.

Prize Talk PRV III Tue 13:00 HSZ/0004

Optics of single molecules explored with sub-nm precision — •Anna Rosławska — Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — Laureate of the Gaede-Prize 2026

Light-matter interaction is essential for mechanisms such as luminescence, photosynthesis, and energy harvesting, defining the emission characteristics of molecular systems and governing the conversion of energy between photons and electrons. While these processes are intensively studied and employed, little is known about their dependence on atomic-scale properties since reaching such precision in optics is extremely demanding. This challenge is nowadays overcome thanks to the combination of optical spectroscopy approaches with scanning probe microscopy, which profit from the extreme field enhancement provided by the tip that enables atomic-scale optics [1]. In my talk, I will discuss how this approach can be applied to gate fluorescence by individual charges [2], used to induce photochemical reactions with sub-nm precision [3], and enables probing optical properties of individual biological pigments.

[1] A. Rosławska, T. Neuman, B. Doppagne, A. Borisov, M. Romeo, F. Scheurer, J. Aizpurua, G. Schull, Phys. Rev. X, 12, 011012, 2022.

[2] K. Kaiser, S. Jiang, M. Romeo, F. Scheurer, G. Schull, A. Rosławska, Phys. Rev. Lett. 133, 156902, 2024.

[3] A. Rosławska, K. Kaiser, M. Romeo, E. Devaux, F. Scheurer, S. Berciaud, T. Neuman, G. Schull, Nat. Nanotechnol., 19, 738-743, 2024.

Prize Talk PRV IV Wed 13:00 HSZ/0003

Fractionalisation, fractals and strong coupling QED in spin liquids — •Roderich Moessner — MPI-PKS Dresden — Laureate of the Max-Born-Prize 2026

After a long and sustained research effort, the quest for an experimental realisation of a quantum spin liquid shows encouraging signs of nearing conclusion. This talk recalls some basic background on the nature of spin liquids and their place in what has become known as topological condensed matter physics. It then covers particularly notable properties which have been experimentally discovered in the magnetisation dynamics, namely the existence of a dynamical fractal and of disorder-free subdiffusion in three dimensions. It concludes with a discussion of the promise of realising an experimental platform for strong coupling quantum electrodynamics in the present work on pyrochlore materials.

Prize Talk PRV V Thu 13:00 HSZ/0002

Observation of Floquet states in graphene — •Marcel Reutzel — Philipps-Universität Marburg, Fachbereich Physik and mar.quest, Germany — Georg-August-Universität Göttingen, I. Physikalisches Institut, Germany — Laureate of the Walter-Schottky-Prize 2026

Material phases are traditionally controlled by parameters such as temperature or doping. Newer efforts employ ultrashort light pulses and correlated - but incoherent - interactions of the electron-lattice-spin systems to create non-thermal phases. While such on-demand material engineering has been established in the last years, more recent efforts strive for the coherent counterpart: By using time-periodic light fields (a.k.a Floquet engineering), new electronic band structures and correlated or even topological phases can be created. Importantly, these phases can then be coherently controlled by the properties of the light field. Therefore, fundamental research on Floquet engineering promises the realization of emergent material phases without any counterpart in thermal equilibrium.

Here, we will outline how the development of time-resolved momentum microscopy - a new variant of time- and angle-resolved photoelectron spectroscopy - has enabled the direct observation of Floquet states in monolayer graphene [1]. These proof-of-principle experiments on semi-metallic graphene open up a new pathway for testing the many theoretical proposals of light-induced phase transitions that have so far remained elusive.

[1] Merboldt *et al.*, Nature Physics 21, 1093 (2025).

Prize Talk PRV VI Thu 13:00 HSZ/0003

Knots and Links in Magnetism — •Maria Azhar — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany — Laureate of the Hertha-Sponer-Prize 2026

Magnetic materials can host remarkably stable, intertwined structures that behave like knots, links, and braids; discrete objects that can be counted and, in principle, used to store information. This talk explains why such complex patterns can exist, ranging from magnetic whirls (Skyrmions) to knots and links (Hopfions), and three-dimensional objects that have only recently been observed, such as screw dislocations of spiral magnetic order.

In some magnets, the far-field is non-uniform, which fundamentally changes which knots or links are possible. Stability is then no longer described by a single number: new states emerge with fractional character, smoothly connecting configurations that would otherwise appear distinct.

At a deeper level, these phenomena follow a simple yet profound geometric idea: magnetic configurations map one sphere onto another, and their winding determines stability. Understanding the underlying principles turns knots and links into practical building blocks for robust and controllable magnetic matter.

Ceremonial, Lunch, Evening Talks and Discussions

Discussion PSV I Mon 13:00 HSZ/AUDI

Sustainability! And now? – Opportunities for young researchers — •Roxana Scharpegge[1,10,11], Hiroki Sayama[2,3], Thomas Schubatzky[4], Birte Höcker[5], Uwe Riedel[6], John Plane[7], Pauleo Nimtz[8,10], and Stefanie Falk[9,11] — [1]Bielefeld University — [2]Binghampton University, State University NY, USA — [3]The University of Tokyo, Japan — [4]Universität Innsbruck, Austria — [5]University of Bayreuth, Germany — [6]DLR Institute für CO2-arme Industrieprozesse, Cottbus, Germany — [7]University of Leeds — [8]Potsdam University, Germany — [9]Karlsruher Institut für Technologie — [10]Working Group Young DPG (AKjDPG) — [11]Working Group Climate (AGK)

Did you miss learning about sustainability during your studies? Does the flood of news about the climate crisis make you feel hopeless? Are you interested in having a societal impact through your day-to-day work? Your skills and experiences from diverse areas can be valuable in developing innovative solutions to sustainability challenges, as collaboration between different disciplines and sectors is crucial to creating a more sustainable future. In this panel discussion, we want to encourage you to consider a career in this future-shaping field.

Inspired by experiences and insights from experts who were once in the same position as you, we aim to offer you a glimpse into the opportunities available and discuss different career pathways. Feel free to contribute your own questions. We hope this discussion helps you in your decision to transform both your future and ours.

Lunch Talk PSV II Mon 13:00 HSZ/0004

Physics Meets Statistics: Advancing Data Analytics in Semiconductor Manufacturing — •Sarah Fischbach — Robert Bosch Semiconductor Manufacturing Dresden GmbH

After earning her Ph.D. in semiconductor physics, Sarah Fischbach transitioned to an industry career. In 2018, she joined the newly established semiconductor plant of Bosch in Dresden, where she began developing concepts and methodologies for data analytics and exploring applications of machine learning. Since 2022, she has been responsible for analytics and digitalization within the technology department of the 300 mm wafer fab. In this session, she will discuss the exciting challenges the semiconductor industry presents to physicists and share insights on how machine learning can support production processes.

Discussion PSV III Tue 13:00 HSZ/AUDI

Soft Science Skills - Self-branding for Scientists — •Lucas Kreuzer[1], •Christian Kuttner[2], and •Alexander Schlaich[3] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), TUM, Garching, Germany — [2]Nature Communications, Berlin, Germany — [3]Technische Universität Hamburg, Hamburg, Germany

This session explores communication and self-branding strategies designed for scientists, helping them to effectively communicate their expertise and build a recognizable professional identity. Our invited speakers will share insights on how science communication can be used as a tool to position oneself strategically within a research or industry field and how to benefit from the multiple opportunities of digital and social media platforms. Thereby, attendees will obtain a specific action plan on how they can enhance their visibility, credibility, and career opportunities in academia and industry.

Lunch Talk PSV IV Tue 13:00 HSZ/0003

Funding Opportunities for International Collaborations at the German Research Foundation — •Joanna Kowalska, Mario Bomers, Christian Hahn, and Michael Mössle — Deutsche Forschungsgemeinschaft e.V., Bonn; Germany

The German Research Foundation (Deutsche Forschungsgemeinschaft, DFG) is Germany's largest organisation for funding fundamental research. As a self-governing body that supports and promotes research, it offers a wide range of funding opportunities, from individual grants to large coordinated programmes. This talk will focus on the DFG's opportunities for supporting international collaborations. It will cover the ways in which international research partners can be included in individual grants and coordinated programmes, as well as outline dedicated funding opportunities for bi- and multilateral projects. It will also introduce the Walter Benjamin Programme, which supports researchers in their early career phase in gaining experience at a research institution, either abroad or in Germany.

PSV V: Ceremonial Session with Award Ceremony

Time: Tuesday 16:00–18:00 Location: HSZ/AUDI

Ceremonial Talk PSV V HSZ/AUDI

Quantum computers as large research instruments - what can we expect and how do we develop them? — •Frank Wilhelm-Mauch — Institute for Quantum Computing Analytics, Forschungszentrum Jülich, Wilhelm-Johnen-Straße, 52428 Jülich, Germany — Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany

Quantum computing is currently a ubiquitous topic in the science and technology media. This has good reasons: The progress has been remarkable, quantum computers promise enhanced computational reach without relying on Moore's law - on the other hand, some promises are also far beyond what can be seriously justified. This talk will give a review of the status of the field and argue that they curretly should be viewed as large research instruments. This means that they should be developed with open access and leave room for creative uses and solutions. This opens great opportunities for physicist to co-develop, understand, and use these machines.

Discussion PSV VI Wed 13:00 HSZ/AUDI

Career Paths: Academia or Industry? — •Joanna Kowalska[1], •Elisabeth Trommer[2], •Jonas Schubert[3], •Annegret Rössler[4], Pauleo Nimtz[4], Aisha Aqeel[5], Lucas Kreuzer[5], and Hans-Georg Grothues[6] — [1]German Research Foundation (DFG), Bonn — [2]Attocube systems AG, Munich — [3]DermaPurge, Dresden — [4]Working Group Young DPG (AKjDPG) — [5]AG young Leaders in Physics (AG youLeaP) — [6]Working Group on Industry and Business (AIW)

After completing your undergraduate studies, your PhD, or, at the latest, your first postdoc, you may ask yourself: Do I want to stay at a research institution or work in industry? In this panel discussion, we would like to talk about this question with experts from different areas of science and industry representing different career paths and stages.

There will be further time for questions and personal discussions at 15:00 to 16:30 in room BEY/0117.

Lunch Talk PSV VII Wed 13:00 HSZ/0002

The French Research Landscape in Physics — •Elisabeth Giacobino — Laboratoire Kastler Brossel, Sorbonne Université, ENS, CNRS, 75005 Paris, France

France has a strong scientific community in physics, with many centers located in several large cities, especially in Paris and in the Ile de France region (the Paris region). In the past years there was an effort to reinforce activities like higher education and research outside the Paris region. The French research is operated by the Universities and by large organisations like CNRS or CEA. Most of the laboratories and institutes in physics are managed jointly by a university and an organisation like CNRS. The large instruments are also mostly operated by research organisations. There is a long tradition of international cooperation in France, especially with Germany. In particular Germany and France are quite successful in the European projects, and Germany is the most frequent partner of France in these collaborative projects. In this presentation we will show more details on the geographic location and on the organization of the French research institutes and laboratories in physics, and on the international and European collaborations, in particular with Germany.

Evening Talk PSV VIII Wed 19:00 HSZ/AUDI

Gravitationswellenastronomie – quo vadis? — •Michèle Heurs — Leibniz Universität Hannover, Hannover, Germany — Deutsches Zentrum für Astrophysik (DZA), Görlitz, Germany — Deutsches Elektronen-Synchrotron DESY, Zeuthen, Germany

Seit der ersten direkten Detektion von Gravitationswellen (GWn) im Jahr 2015 haben wir ein völlig neues Beobachtungsfenster zum Universum aufgestoßen (komplementär zu elektromagnetischem Spektrum, Neutrinos und kosmischer Strahlung) und damit das Zeitalter der Multi-Messenger-Astronomie mit GWn eingeläutet. Eine Fülle wissenschaftlicher Erkenntnisse wurde bereits gewonnen – aber es gibt noch so viel mehr zu entdecken!

Die Empfindlichkeit aktueller laserinterferometrischer GW-Detektoren ist so aberwitzig hoch, dass das durch die Quantenmechanik gegebene Rauschen des verwendeten ultrastabilen Laserlichts die Messungen limitieren würde. Dies erfordert die Verwendung von nichtklassischem (sog. „gequetschtem") Licht, das bereits routinemäßig in der aktuellen (zweiten) Generation von GW-Detektoren, z. B. aLIGO und AdVirgo, eingesetzt wird. Viele zusätzliche Rauschquellen, wie seismisches und thermisches Rauschen, stellen weitere Herausforderungen für die Detektoren der nächsten (dritten) Generation dar, z. B. für das Einstein-Teleskop, ein geplantes unterirdisches GW-Observatorium in Europa.

Um mehr über unser Universum zu lernen, benötigen wir höhere Detektionsraten für eine aussagekräftige Gravitationswellenastronomie; dafür benötigen wir höhere Detektionsempfindlichkeit und größere Detektionsbandbreite. In meinem Vortrag werde ich das Prinzip der interferometrischen GW-Detektion einführen, einige der fortschrittlichen Technologien (bereits eingesetzt oder in Entwicklung) erläutern und die Pläne für zukünftige interferometrische Gravitationswellenobservatorien wie das Einstein-Teleskop beleuchten.

Lunch Talk PSV IX Thu 13:00 HSZ/0004

The organic development and growth story of aSpect Systems GmbH — •Marcus Verhoeven — aSpect Systems GmbH

The talk will present the organic development and growth story of aSpect Systems GmbH, a Dresden-based technology company at the intersection of semiconductor engineering and applied physics. Starting from a small team dedicated to advancing semiconductor test and automation technologies, aSpect has continuously evolved by leveraging deep technical expertise in hardware, software, mechanics and optics to solve real-world industrial challenges. Today, the company supports development services, supply chain solutions, test and automation equipment for imaging, optoelectronics and semiconductor manufacturing, helping to bridge the gap between cutting-edge research and industrial application.

Invited Talks, Tutorials, and Contributed Talks

TUT 1: Hands-on Tutorial: HyperSpy – Multidimensional data analysis using Python (joint session FM/TUT)

HyperSpy is a community-developed, open-source library providing a framework to facilitate interactive analyses of multidimensional datasets – in particular spectrum images – in an easy and reproducible fashion. It facilitates the application of analytical procedures operating on individual spectra/images to a multi-dimensional dataset and gives easy access to tools that exploit the multi-dimensionality of the dataset. Born out of the electron microscopy scientific community and building on the extensive scientific Python environment, HyperSpy provides tools to efficiently explore, manipulate, and visualize complex datasets of arbitrary dimensionality, including those larger than a system's memory. The HyperSpy ecosystem includes Python packages that provide dedicated routines for many electron microscopy-based measurement techniques, but also for luminescence spectroscopy and other fields. Through the library RosettaSciIO, the reading and writing of a large range of file formats is supported.

Please bring your laptop. There will be limited power outlets in the room, so come with a fully charged battery.

Materials will be made available from 01.03.2026 via a dedicated GitHub repository. Participants are encouraged to download them ahead of time, set-up Python on their computer following the instructions and run the jupyter notebooks presented during the tutorials on their laptops:

https://github.com/LumiSpy/DPG2026-Tutorial

Organized by Jonas Lähnemann (PDI Berlin), Benedikt Haas (HU Berlin), Aidan Campbell (PDI Berlin), Hannah C. Nerl (HU Berlin) and Magnus Nord (NTNU Trondheim).

Time: Sunday 16:00–18:15 Location: HSZ/0002

TUT 1.1 Sun 16:00 HSZ/0002

Introduction to HyperSpy — •Jonas Lähnemann[1], Aidan F. Campbell[1], Hannah C. Nerl[2], Magnus Nord[3], and Benedikt Haas[2] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Department of Physics, Humboldt Universität, Berlin, Germany — [3]Department of Physics, Norwegian University of Science and Technology, Trondheim, Norway

The session begins with a brief introduction to HyperSpy that with its 2.0 release has grown to an ecosystem of Python packages that provide dedicated routines for electron microscopy-based measurement techniques such as EELS, EDX, 4DSTEM, holography, tomography and CL, but also for luminescence spectroscopy. In general, it can be useful for any measurement, where a signal is mapped over multiple dimensions (position, time, angle, ...).

Tutorial TUT 1.2 Sun 16:15 HSZ/0002

Hands-On Session 1: General usage HyperSpy/RosettaSciIO — •Jonas Lähnemann — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

In the initial tutorial, we will show how to easily read in data from a variety of formats and introduce the basic data structure of HyperSpy. General data operations, artefact removal and plotting functionalities as a basis of reproducible data analysis workflows will be covered as well.

Tutorial TUT 1.3 Sun 16:45 HSZ/0002

lumiSpy for luminescence spectroscopy — •Aidan Campbell — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

This session will focus on tools ideal for analysing data recorded with cathodoluminescence, photoluminescence or related spectroscopy techniques. We will demonstrate convenience functions for rapid spectroscopy data analysis, model fitting, and visualisation. Luminescence spectroscopy may also lead to more complicated data sets with spectral, spatial and time dimensions for which we showcase interactive tools for navigating and understanding this data.

Tutorial TUT 1.4 Sun 17:15 HSZ/0002

Hyperspy for Electron Energy-loss Spectroscopy — •Hannah Nerl — Humboldt Universität zu Berlin, Berlin, Germany

This hands-on session demonstrates a complete electron energy-loss spectroscopy (EELS) analysis workflow using HyperSpy and its exSpy extension. Participants will work through practical examples covering essential preprocessing steps including spectral alignment and drift correction, followed by quantitative analysis techniques such as model-based peak fitting and automated peak tracking across multidimensional datasets. The tutorial emphasizes reproducible analysis pipelines, showcasing how to leverage principal component analysis (PCA) for noise reduction in low-signal regimes. All examples use real EELS datasets and focus on practical workflows applicable to both core-loss and low-loss spectroscopy of 2D materials and nanostructures. Participants will gain hands-on experience with Jupyter notebooks that can be directly adapted to their own research data.

Tutorial TUT 1.5 Sun 17:45 HSZ/0002

Using pyXem for magnetic and structural analysis of 4D-STEM data — •Magnus Nord — Norwegian University of Science and Technology, Trondheim, Norway

pyXem is an extension of HyperSpy with a focus on data processing of 4D-STEM data: from crystallographic analysis using Scanning Precession Electron Microscopy (SPED), to magnetic imaging with Scanning Transmission Electron Microscopy - Differential Phase Contrast (STEM-DPC). In this tutorial, we will show how one can study the crystal structure and domain structure in a nanostructured magnetic material.

TUT 2: Tutorial des Fachverbands Didaktik der Physik (joint session DD/TUT)

Physics teaching at universities can be significantly enriched by moving beyond traditional lecture formats and embracing interactive, learner-centered approaches that foster deep and sustainable understanding. Drawing on successful practices from universities in Germany and abroad, this workshop highlights how insights from learning psychology and proven teaching innovations can be translated into effective physics education. It invites participants to explore how evidence-based, interactive methods can transform learning experiences and support lasting learning outcomes in everyday teaching practice.

Time: Sunday 16:00–18:15 Location: BEY/0137

Tutorial TUT 2.1 Sun 16:00 BEY/0137

Rethinking University Teaching: Creating interactive and sustainable learning environments in lectures — •Susanne Heinicke[1], Christian Kautz[2], Peter Riegler[3], Claudia Schäfle[4], Silke Stanzel[4], and Micol Alemani[5] — [1]Institute for Physics Education, University of Muenster — [2]Hamburg University of Technology — [3]Ostfalia University of Applied Sciences — [4]Technische Hochschule Rosenheim — [5]University of Potsdam

The workshop bridges current findings from learning psychology with experience and research findings on practical teaching formats to enhance effective learning in university physics education. We will give an overview of key principles from educational psychology concerning how we learn to provide a foundation for understanding learning effectiveness. Participants will explore and critically reflect on evidence-based interactive methods like peer instruction, interactive formats, and problem-based learning that can be transferred to their own teaching. The workshop concludes with a discussion on implementation strategies and evaluation approaches to support sustainable integration into everyday teaching practice.

TUT 3: Tutorial: Machine Learning Use Cases in Materials Science (joint session AKPIK/TUT)

Artificial intelligence (AI) tools are increasingly shaping research in materials science and physics by enabling advanced data analysis, modeling, and predictive capabilities.

This tutorial presents three practical use cases that demonstrate how machine learning methods can support materials science research.

Time: Sunday 16:00–18:15 Location: HSZ/0003

Tutorial TUT 3.1 Sun 16:00 HSZ/0003

Welcome Remarks Arbeitskreis Physik, moderne Informationstechnologie und Künstliche Intelligenz — DPG AKPIK and •Arash Rahimi-Iman — Deutsche Physikalische Gesellschaft e.V.

Inspired by last year's meeting program in Regensburg, March 2025, our interdisciplinary Working Group on Physics, Modern IT and Artificial Intelligence, the AKPIK, again offers a research-focused "AKPIK Day" on Tuesday during the upcoming conference. Together with the practical use cases of machine learning presented in this tutorial session, as well as the presentations and poster session planned for Thursday, we hope to encourage many conference attendees to engange scientifically in the areas of the AKPIK.

Tutorial TUT 3.2 Sun 16:05 HSZ/0003

A practical machine learning case study in materials science: Stumbling blocks, lucky breaks, and helpful colleagues — •Max Grossmann, •Malte Grunert, and Erich Runge — Institute of Physics and Institute of Micro- and Nanotechnologies, Technische Universität Ilmenau, 98693 Ilmenau, German

Machine learning projects in materials science are often exciting at first, but quickly encounter practical challenges. In this tutorial, we present a hands-on case study from our group and walk through the entire process, from the initial idea to building a dataset to training a working model. Rather than focusing solely on technical details, we highlight the stumbling blocks, unexpected insights, helpful colleagues, and lucky coincidences that shaped the project. We discuss the most important aspects of starting a machine learning project in physics or materials science, such as choosing a meaningful target property, designing a reliable dataset, avoiding common pitfalls, and identifying situations where simple approaches are as effective as advanced ones. Our goal is to provide an honest, accessible, and experience-driven introduction and guidance to researchers considering venturing into machine learning for the first time – the kind of guidance we wish we had when we started.

5 min. break

Tutorial TUT 3.3 Sun 16:50 HSZ/0003

Machine Learning-based Analysis of Electron Microscopy Images: Preprocessing and Synthetic Data Generation — •Amir Omidvarnia — Forschungszentrum Jülich, Jülich, Germany

In this tutorial session, participants will learn how to prepare electron microscopy (EM) images for machine learning (ML) analysis using a series of Jupyter Notebook demonstrations. The tutorial illustrates essential preprocessing steps such as denoising, normalization, and contrast enhancement using Python. The session then transitions to synthetic EM data generation, showing how classical augmentation and modern generative models can create controlled datasets that mimic real data. By observing these live examples, attendees will gain a conceptual understanding of how preprocessing pipelines and synthetic data strategies can be used for ML-based EM analysis.

5 min. break

Tutorial TUT 3.4 Sun 17:35 HSZ/0003

Machine Learning-based Analysis of Electron Microscopy Images: Segmentation — •Amir Omidvarnia — Forschungszentrum Jülich, Jülich, Germany

The second session focuses on segmentation of EM images using modern deep-learning architectures. Through a step-by-step Jupyter Notebook demonstration, the tutorial walks through the training and evaluation of a U-Net style segmentation model. Participants will see real examples of common challenges in EM segmentation, such as low contrast, overlapping nanoscale structures, and label ambiguity. By the end of the session, attendees will have an implementation-oriented understanding of how segmentation pipelines are built and validated in practice.

TUT 4: Tutorium: Physics of Behavior (joint session SOE/TUT/DY)

The emerging field of the physics of behavior seeks to quantitatively characterize complex behavior in biological agents under naturalistic conditions, using tools from dynamical systems theory and statistical physics. Even in simple organisms, behavioral richness demands new methods of measurement and analysis, as well as new theoretical frameworks. In the absence of a first-principles theory, data-driven approaches are essential, and the many interacting degrees of freedom call for descriptions capable of handling high-dimensional systems.

This tutorial introduces how concepts from dynamical systems theory and statistical physics can be applied to quantify behavior across biological scales and to develop simple yet predictive models. It is intended for physicists at all levels, beginning with graduate students, who are interested in computational approaches to modeling animal behavior. The tutorial is accompanied by an openly accessible code repository to support hands-on exploration of selected topics.

Time: Sunday 16:00–18:15 Location: HSZ/0004

Tutorial TUT 4.1 Sun 16:00 HSZ/0004

Physics of Behavior — •Greg Stephens — Vrije Universiteit Amsterdam, Amsterdam NL — OIST Graduate University, Tancha, JP

In these tutorials we view behavior as a complex dynamical system and we incorporate insights from dynamical systems theory and statistical physics to quantitatively capture what animals do. Of course, such theory was not historically developed to understand animal behavior, and there are particular challenges associated with the modeling of living systems. Of these, the most important is a lack of first-principles theory necessitating a data-driven approach.

In the first half of our session we will introduce two primary concepts. (1) Posture Space Analysis via Dimensionality Reduction. We explore posture space analysis by demonstrating how to decompose high-dimensional postural data into a few meaningful eigenpostures using Principal Component Analysis (PCA). The dataset used comes from C. elegans posture tracking. (2) Posture Space Dynamics via State Space Reconstruction. We review the concepts of state space and chaotic systems through a toy model. We then introduce a modern data-driven technique for state space reconstruction.

15 min. break

Tutorial TUT 4.2 Sun 17:15 HSZ/0004

Physics of Behavior — •Antonio Carlos Costa — Paris Brain Institute, Paris, France

Animal behavior is inherently nonlinear and multiscale, spanning millisecond movements to hour-long strategies. In the second half of our session, we will complement first-principles approaches with data-driven methods to identify multiscale dynamics in behavioral data.

We will present three key techniques: (1) state space reconstruction combined with transfer operators to extract long-timescale modes from partial observations, (2) coarse-grained modeling to infer slowly-varying behavioral dynamics and explain heavy-tailed statistics, and (3) a multiscale distance metric for reconstructing behavioral phenotypes from dynamic observations.

We will review the theoretical foundations of slow mode identification using transfer operators (illustrated with stochastic and chaotic toy models), and then demonstrate their applicability to real-world data, including posture dynamics in C. elegans and zebrafish.

TUT 5: Hands-On Tutorial: Magnetic Structure Determination Using Fullprof and SARAh Representation Analysis (joint session MA/TUT)

The functionalities of many materials of contemporary interest are related to complex types of magnetic ordering. Accurate magnetic structure determination is thus crucial for understanding and optimizing such materials.

After an introduction into the subject, participants of the tutorial will gain hands-on experience on the methods for magnetic structure determination.

Time: Sunday 16:00–18:15 Location: TRE/PHYS

Invited Talk TUT 5.1 Sun 16:00 TRE/PHYS

Recent advances and challenges in magnetic structure determination — •Dmytro Inosov — Institut für Festkörper- und Materialphysik, TU Dresden, Germany

In this introductory tutorial talk, I will provide an overview of magnetic structure determination in the context of recent advances in magnetic materials. I will focus on the limitations and challenges of magnetic structure refinement, and explain why it is important to use the full range of complementary experimental methods alongside conventional diffraction in order to develop a consistent understanding of magnetic structures. This is particularly important when dealing with complex types of magnetic order, such as noncollinear and multi-Q spin textures, altermagnets, and systems with multiple magnetic sublattices or very weak and/or fluctuating magnetic moments.

Tutorial TUT 5.2 Sun 16:30 TRE/PHYS

Hands-On Tutorial: Magnetic Structure Determination Using Fullprof and SARAh Representation Analysis — •Matthias Frontzek — Oak Ridge National Laboratory, Neutron Scattering Division, One Bethel Valley Road, 37831 Oak Ridge, TN, USA

The determination of magnetic structures is a crucial aspect of materials science, particularly for understanding the magnetic properties of novel materials. Given the limited availability of neutrons with the closure of smaller sources, competitive access to beam time, and the high hurdles associated with software usage, there is an increasing need for training in the analysis of magnetic structures. This tutorial aims to provide participants with practical skills in magnetic structure determination using SARAh and Fullprof, two powerful tools frequently utilized in this field.

Participants will:

-Gain hands-on experience with the tools and techniques necessary for magnetic structure determination.

-Refine nuclear and magnetic structures using real data sets.

-Understand key concepts in diffraction techniques and steps involved in the magnetic structure determination process.

Important: for Hands-on participation, please bring a laptop with a working installation of Fullprof (https://www.ill.eu/sites/fullprof/).

For links to Fullprof, SARAh stand-alone and tutorial data visit: https://neutrons.ornl.gov/wand/users

TUT 6: Hands on tutorial: Linking large language models with digital workflows for materials science simulations (joint session MM/TUT)

Advanced computational simulations often require chaining several models and software packages together, a process that demands careful workflow management. In this tutorial you can gain hands-on experience with the Python based workflow environment pyiron (www.pyiron.org). Participants in the tutorial will be able to run all the examples shown in the presentation interactively on their own laptops. There is no need to install any code, just a standard web browser to explore the applications interactively.

Time: Sunday 16:00–18:15 Location: TRE/MATH

Tutorial TUT 6.1 Sun 16:00 TRE/MATH

Hands on tutorial: Linking large language models with digital workflows for materials science simulations — •Jörg Neugebauer[1], Tilmann Hickel[1,2], and Ralf Drautz[3] — [1]Max Planck Institute for Sustainable Materials — [2]Bundesanstalt für Materialforschung und -prüfung — [3]ICAMS, Ruhr Universität Bochum

Advanced computational simulations now reliably predict material properties, but they often require chaining several models and software packages together, a process that demands expert knowledge and careful workflow management. Efficient, reproducible research therefore hinges on automated workflow tools that can handle this complexity. In this tutorial we introduce pyiron (www.pyiron.org), a Python based workflow environment for building and executing fully automated simulation pipelines. We show how complex simulations workflows can be constructed programmatically via Python code as well as via a flow-based graphical user interface. We further introduce how large language models (LLMs) can be embedded to streamline the ”human in the loop” tasks. After a brief overview of pyiron’s core concepts, we construct workflows for computing ab initio thermodynamic bulk phase diagrams. The necessary steps, such as density functional theory calculations, training ACE-based machine learning potentials, and exploring phase stability using foundational models like GRACE, are all performed within pyiron workflows. Participants will learn how to develop and integrate such workflows into their own materials science simulations, thereby enabling faster, more transparent, and more reproducible research.

Symposium AI and Data Challenges behind Emerging Self-Driving Laboratories (SYAI)

jointly organised by
the Surface Science Division (O),
the Biological Physics Division (BP),
the Metal and Material Physics Division (MM),
the Environmental Physics Division (UP),
the Working Group "Young DPG" (AKjDPG), and
the Working Group on Physics, Modern IT and Artificial Intelligence (AKPIK)

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So-called Self-driving Laboratories (SDLs) or Materials Acceleration Platforms (MAPs) represent a cutting-edge convergence of artificial intelligence (AI) and machine learning (ML) with lab automation and robotics. SDLs are designed to automate and accelerate experimental processes, addressing inefficiencies and enhancing the precision and safety of lab operations. SDLs operate in active learning loops, in which an ML algorithm selects and plans experiments that are subsequently executed by increasingly automated (robotic) modules. Data from these experiments are fed back into the ML model, refining it and guiding subsequent experiments. This iterative process enhances the efficiency and effectiveness of experimental exploration, and it is the adaptive quality to directly exploit the information gained through the experiments in the past loops that distinguishes modern SDLs from classic approaches in high-throughput experimentation or combinatorial chemistry.

With SDLs emerging in a wide range of application fields from heterogeneous catalysis over optoelectronics to batteries, advances in experiment automation and robotization are obvious drivers for improved throughputs. Complementary to this are, however, multiple IT- and AI/ML- related aspects of SDLs, not least comprising data pipelines and management, workflows, AI- agent platforms, featurization of the experimental data or experiment planning (especially using noisy and multi-fidelity data). This symposium will survey the present state-of-the-art of these aspects and discuss current frontiers.

Overview of Invited Talks and Sessions

(Lecture hall HSZ/AUDI)

Invited Talks

SYAI 1.1	Thu	9:30–10:00	HSZ/AUDI	**Data and Experimental Foundations for Reliable Self-Driving Laboratories** — •Dr. Marcus Tze-Kiat Ng
SYAI 1.2	Thu	10:00–10:30	HSZ/AUDI	**Digital Catalysis - AI for Experiment Planning and Control** — •Christoph Scheurer
SYAI 1.3	Thu	10:30–11:00	HSZ/AUDI	**Autonomous, Data-Driven Workflows for Materials Acceleration Platforms with pyiron** — •Jan Janssen, Joerg Neugebauer
SYAI 1.4	Thu	11:15–11:45	HSZ/AUDI	**Machine Learning for Autonomous Optimization and Discovery of Materials** — •Pascal Friederich
SYAI 1.5	Thu	11:45–12:15	HSZ/AUDI	**Transforming Our View on Transformers in the Sciences** — •Kevin Maik Jablonka

Sessions

SYAI 1.1–1.5	Thu	9:30–12:15	HSZ/AUDI	**AI and Data Challenges behind Emerging Self-Driving Laboratories**

Sessions

– Invited Talks –

SYAI 1: AI and Data Challenges behind Emerging Self-Driving Laboratories

Time: Thursday 9:30–12:15 Location: HSZ/AUDI

Invited Talk SYAI 1.1 Thu 9:30 HSZ/AUDI

Data and Experimental Foundations for Reliable Self-Driving Laboratories — •Dr. Marcus Tze-Kiat Ng — Magnusstr. 11, 12489 Berlin

Self-driving laboratories are increasingly guided by machine learning, yet progress is constrained by the quality, structure, and consistency of experimental data. In this work, autonomous experimental platforms are presented in which high-throughput synthesis, electrochemical testing, and multi-modal characterisation are carried out with high reproducibility. Through these systems, challenges that are rarely captured in benchmark datasets are revealed, including drift, batch effects, measurement noise, and incomplete metadata. Physics-informed representations, uncertainty-aware models, and active-learning strategies are shown to be effective when applied to such real-world data. Case studies in catalyst optimisation and discovery are used to demonstrate how large chemical spaces can be explored once the experimental feedback loop is closed. The experimental and data foundations required for reliable AI-driven materials discovery will be outlined.

Invited Talk SYAI 1.2 Thu 10:00 HSZ/AUDI

Digital Catalysis - AI for Experiment Planning and Control — •Christoph Scheurer — Fritz-Haber-Institut der MPG, Berlin

Self-driving laboratories (SDLs) epitomize a cutting-edge integration of machine learning with laboratory automation. Operating in active learning loops, SDLs use machine learning algorithms to plan experiments that are then executed by increasingly automated (robotic) modules. Here, I will present our perspective on emerging SDLs for accelerated discovery and process optimization in heterogeneous catalysis. Drawing on recent work in catalyst discovery, kinetic modelling, and catalyst degradation studies, I will argue against the paradigm of full automation and the objective of keeping the human out of the loop. Analysis of the associated workflows indicates that crucial advances will stem from establishing fast proxy experiments, re-engineering existing apparatuses and measurement protocols, and developing modelling approaches with real-time capabilities. Industrially relevant use cases will also require humans to remain in the loop for continuous decision-making, mandating explainable AI. In turn, active learning algorithms must be advanced to flexibly accommodate adaptations of the design space and variations in information content and noise in the acquired data.

Invited Talk SYAI 1.3 Thu 10:30 HSZ/AUDI

Autonomous, Data-Driven Workflows for Materials Acceleration Platforms with pyiron — •Jan Janssen and Joerg Neugebauer — Max Planck Institute for Sustainable Materials, Düsseldorf, Germany

The hierarchical nature of materials – spanning electronic, atomistic, microstructural, and macroscopic scales – necessitates an integrated multiscale strategy for accelerating materials discovery. Realizing such a strategy requires close coordination across chemistry, materials science, and physics, and an equally tight coupling of simulation and experiment. Materials Acceleration Platforms (MAPs) address this need by embedding both theoretical and experimental data streams into a unified active-learning loop. A central challenge is ensuring that information can be meaningfully transferred across scales. We approach this by propagating uncertainties throughout the entire multiscale workflow, enabling quantitative comparison from ab-initio predictions to experimental measurements. This uncertainty-aware integration makes it possible to reduce the number of required experiments by several orders of magnitude. The resulting hierarchy of simulations is powered by machine-learning models – including ML interatomic potentials, Bayesian optimization, and large-language-model (LLM) agents – each contributing to decision-making within the MAP. The pyiron workflow framework provides the digital backbone for this integration. By encoding domain expertise into modular, machine-actionable workflows, pyiron enables simulation specialists to formalize their methods in a way that is both reproducible and interoperable.

15 min. break

Invited Talk SYAI 1.4 Thu 11:15 HSZ/AUDI

Machine Learning for Autonomous Optimization and Discovery of Materials — •Pascal Friederich — Karlsruhe Institute of Technology, Karlsruhe, Germany

Machine learning can accelerate the screening, design, and discovery of new molecules and materials in multiple ways, e.g. by virtually predicting properties of molecules and materials, by extracting hidden relations from large amounts of simulated or experimental data, or even by interfacing machine learning algorithms for autonomous decision-making directly with automated high-throughput experiments. In this talk, I will focus on our research activities on the use of machine learning for automated data analysis and autonomous decision-making in self-driving labs [1,2]. I will discuss extensions of Bayesian optimization to extend the autonomous decision-making process to more complex experimental and computational self-driving labs, as well as possibilities to include machine learning based recommendations already in the process of designing the experiments [3].

[1] Wu et al., Science 386, 6727 (2024), Inverse design workflow discovers hole-transport materials tailored for perovskite solar cells

[2] Marwitz et al., arXiv:2506.16824 (2025), Predicting New Research Directions in Materials Science using Large Language Models and Concept Graphs

[3] Jenewein et al., J. Mater. Chem. A 12, 3072-3083 (2024), Navigating the unknown with AI: multiobjective Bayesian optimization of non-noble acidic OER catalysts

Invited Talk SYAI 1.5 Thu 11:45 HSZ/AUDI

Transforming Our View on Transformers in the Sciences — •Kevin Maik Jablonka — Friedrich-Schiller Universität Jena, Jena, Germany — HPOLE Jena, Jena, Germany

The sciences face a fundamental challenge: much of the data we need for building models is not currently reported or usable in any structured form. Large language models (LLMs) have shown promise in addressing this through text-to-data conversion and direct predictive capabilities, attracting tremendous attention across scientific applications. In my contribution, I will present a roadmap based on comprehensive benchmarks of language models, multimodal models, and autonomous agents in chemistry and beyond. We have developed specialized evaluation benchmarks to assess scientific knowledge, reasoning abilities, and autonomous tool use across frontier models. Our results reveal a striking paradox: these models can exceed the performance of experts with decades of experience on certain tasks, while simultaneously failing worse than novices on other seemingly basic problems. I will discuss what these benchmark findings mean for the future of LLMs in scientific research, which applications are ready for deployment, where critical gaps remain, and how the field should prioritize development efforts. Finally, I will present the advances in models, systems, and infrastructure we have developed to enable practical impact across the sciences.

Symposium Fluids with Broken Time-Reversal Symmetry: Odd/Hall Viscosity between Active Matter and Electron Flows (SYBS)

jointly organised by
the Dynamics and Statistical Physics Division (DY),
the Chemical and Polymer Physics Division (CPP),
the Magnetism Division (MA), and
the Low Temperature Physics Division (TT)

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Viscosity is a fundamental property of fluids and an important physical quantity characterizing resistance to flow and energy dissipation. While time-reversal symmetry holds in conventional fluids, its violation can lead to striking phenomena, one of which is the emergence of a dissipationless transport coefficient called odd viscosity. Odd viscosity, also known as Hall viscosity, was originally proposed by Avron et al., as a quantized observable in electron fluids with a magnetic field. Since this seminal work, odd viscosity has been studied in various systems, such as 2D electron fluids, fractional Hall fluids, and ionic crystals. Although odd viscosity was also known in plasma physics, it was largely overlooked in fluid dynamics, mainly due to the technical challenges involved in its experimental realization. In recent years, however experiments in driven colloidal systems led to a surge of interest in odd viscosity in the active matter community. In parallel, our understanding of odd phenomena was advanced by continuum theories with many novel exact solutions. Major open questions in the field include the microscopic mechanisms that lead to odd viscosity, its experimental manifestations, the transition from two- to three-dimensional systems, and the effect of odd viscosity on hydrodynamic phenomena at different length scales, ranging from microrheology to turbulent flows. This Symposium will connect the wider condensed matter and active matter physics communities with recent theoretical advances in odd viscosity.

Overview of Invited Talks and Sessions

(Lecture hall HSZ/AUDI)

Invited Talks

SYBS 1.1	Tue	9:30–10:00	HSZ/AUDI	**Odd viscosity in three-dimensional fluids: flows, wakes, and eddies** — •Tali Khain
SYBS 1.2	Tue	10:00–10:30	HSZ/AUDI	**Odd viscosity in two-dimensional hydrodynamic electron transport** — •Igor Gornyi, Dmitry Polyakov
SYBS 1.3	Tue	10:30–11:00	HSZ/AUDI	**Odd slip on chiral active surfaces** — •Andrej Vilfan, Yuto Hosaka
SYBS 1.4	Tue	11:15–11:30	HSZ/AUDI	**Parity-odd transport in electron fluids** — •Johanna Erdmenger
SYBS 1.5	Tue	11:30–11:45	HSZ/AUDI	**Curved Odd Elasticity** — Lazaros Tsaloukidis, Yuan Zhou, Jack Binysh, Nikta Fakhri, Corentin Coulais, •Piotr Surówka

Sessions

SYBS 1.1–1.5	Tue	9:30–11:45	HSZ/AUDI	**Fluids with broken time-reversal symmetry: Odd/Hall viscosity between active matter and electron flows**

Sessions

– Invited Talks –

SYBS 1: Fluids with broken time-reversal symmetry: Odd/Hall viscosity between active matter and electron flows

Time: Tuesday 9:30–11:45 Location: HSZ/AUDI

Invited Talk SYBS 1.1 Tue 9:30 HSZ/AUDI

Odd viscosity in three-dimensional fluids: flows, wakes, and eddies — •Tali Khain — Harvard University, Cambridge, MA, USA

Systems composed of spinning particles or driven by a magnetic field break mirror symmetry at the microscopic level. These chiral fluids can be described by adding so-called "odd" viscosities, which do not dissipate energy, in the Navier-Stokes equations. In this talk, I will discuss a theoretical fluid mechanics framework to describe the consequences of these broken symmetries on fluid flow [1]. Using a combination of analytical and numerical methods, we show how these odd viscosity coefficients modify flow across a range of Reynolds numbers. In the low Reynolds number limit, sedimenting objects in a chiral fluid generate a rotating flow that is absent in usual fluids; in turn, this flow affects how immersed objects respond to forces and torques [2]. At intermediate Reynolds numbers, odd viscosity reshapes the vortex structure of the wake of a sphere, which affects the onset and nature of the periodic vortex shedding state. At high Reynolds numbers, the non-dissipative nature of odd viscosity disrupts the energy cascade that occurs in fully developed turbulent flows, leading to pattern formation with a tunable scale [3].

[1] Khain, Scheibner, Fruchart, Vitelli, JFM (2022)
[2] Khain, Fruchart, Scheibner, Witten, Vitelli, JFM (2024)
[3] de Wit, Fruchart, Khain, Toschi, Vitelli, Nature (2024)

Invited Talk SYBS 1.2 Tue 10:00 HSZ/AUDI

Odd viscosity in two-dimensional hydrodynamic electron transport — •Igor Gornyi and Dmitry Polyakov — Karlsruhe Institute of Technology, Karlsruhe, Germany

We discuss the role of odd (Hall) viscosity in two-dimensional hydrodynamic electron transport in two spatial dimensions. We formulate a general framework to study the flow of the electron fluid past a random array of impenetrable obstacles in the presence of a magnetic field and derive a linear-response resistivity tensor. For the no-slip boundary condition on the obstacles, the resistivity tensor does not depend on the Hall viscosity. By contrast, for the specular boundary condition, the total electric field is rotated by Hall viscosity, which means the emergence of a Hall-viscosity-induced effective magnetic field that leads to a deviation of the Hall constant from its universal value, as well as to a modification of the longitudinal resistivity. We combine the hydrodynamic and electrostatic perspectives by addressing the distribution of charges that create the flow-induced electric fields around obstacles and provide a connection between the resistivity tensor and the disorder-averaged electric dipole induced by viscosity at the obstacle. This establishes a conceptual link between the resistivity in hydrodynamics and the notion of the Landauer dipole.

Invited Talk SYBS 1.3 Tue 10:30 HSZ/AUDI

Odd slip on chiral active surfaces — •Andrej Vilfan[1] and Yuto Hosaka[2] — [1]Jožef Stefan Institute, Ljubljana, Slovenia — [2]Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Chiral active surfaces are characterized by persistent energy input with a defined sense of chirality, for example by a carpet of symmetrically rotating biological or artificial cilia. We demonstrate that when subjected to a shear flow, such a surface can lead to an effective odd slip velocity, in addition to classical Navier slip. Odd Navier slip represents a novel category of odd responses beyond the established concepts of odd viscosity and elasticity, which occur in bulk fluids or solids, and odd diffusivity of point particles. We show that a suspension of particles with odd slip can exhibit odd viscosity, providing a new mechanism for its emergence.

15 min. break

Invited Talk SYBS 1.4 Tue 11:15 HSZ/AUDI

Parity-odd transport in electron fluids — •Johanna Erdmenger — Institut für Theoretische Physik und Astrophysik, Julius-Maximilians-Universität Würzburg, 97074 Würzburg

Parity-odd transport in two-dimensional electron systems reveals an interplay between geometry, topology, and hydrodynamics. In channel geometries, the Hall viscous force competes with the Lorentz force, leading to nonlinear Hall voltage profiles and, at a critical magnetic field, a complete cancellation of the total Hall response [1,2]. Channel voltage measurements provide a direct experimental probe. Similar effects arise for the hydrodynamic inverse Nernst signal [2].

For hydrodynamic spin transport, non-dissipative parity-breaking transport phenomena are generated by torsion. The torsional Hall viscosity has interesting connections to recent developments in general relativity. We analyse the impact of magnetic fields and quadratic band-structure corrections on the torsional transport coefficient, showing that torsional response can reverse direction relative to conventional Hall viscous forces, while still distinguishing topologically trivial and nontrivial regimes [3].

[1] I. Matthaiakakis, D. Rodríguez, C. Tutschku, J. Erdmenger, E. M. Hankiewicz and R. Meyer, Phys.Rev.B 101 (2020) 4, 045423.
[2] Z.Y. Xian, S. Danz, I. Matthaiakakis, R. L. Klees, J. Erdmenger, R. Meyer, E. M. Hankiewicz et al, Phys.Rev.B 107 (2023) 20, L201403.
[3] I. Matthaiakakis, W.Z. Jia, R. L. Klees, D. Rodríguez Fernández, Z.Y. Xian, R. Meyer, J. Erdmenger and E. M. Hankiewicz, arXiv:2504.13250 [cond-mat.mes-hall].

Invited Talk SYBS 1.5 Tue 11:30 HSZ/AUDI

Curved Odd Elasticity — Lazaros Tsaloukidis[2], Yuan Zhou[3], Jack Binysh[3], Nikta Fakhri[4], Corentin Coulais[3], and •Piotr Surówka[1] — [1]Institute of Theoretical Physics, Wrocław University of Science and Technology, 50-370 Wrocław, Poland — [2]Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, 01187, Dresden, Germany — [3]Institute of Physics, University of Amsterdam, Science Park 904, 1098 XH, Amsterdam, The Netherlands — [4]Department of Physics, Massachusetts Institute of Technology, Cambridge, MA, USA

Living materials such as membranes, cytoskeletal assemblies, cell collective and tissues can often be de- scribed as active solids materials with a elastic response about a well defined reference configuration and energized from within. These materials often live in complex and curved manifolds, yet most descriptions of active solids are flat. Here, we explore the interplay between curvature and non-reciprocal elasticity by a co- variant effective theory on curved manifolds in combination with numerical simulations. We find that curvature spatially patterns activity, gaps the spectrum, modifies exceptional points and introduces non-Hermitian de- fect modes. Together these results establish a foundation for hydrodynamic and rheological models on curved manifolds, with direct implications for living matter and active metamaterials.

Symposium Beyond Transistors: Material-Based Edge Computing Paradigms (SYBT)

jointly organised by
the Magnetism Division (MA) and
the Functional Materials Division (FM)

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The rapid progress of artificial intelligence has led to unprecedented computational capabilities, but also to growing energy and resource demands that challenge edge computing applications such as autonomous systems and smart sensors. These resource limitations are rooted in the conventional von Neumann architectures and silicon-based transistors of the current technology. This symposium explores alternative paradigms in which computation emerges directly from the intrinsic properties and dynamics of materials. Bringing together experts primarily from condensed matter physics and optics, the focus lies on material-based platforms, including spintronics, ferroelectrics, ionic and phase-change materials, as well as photonic and hybrid ligh-matter platforms. These systems enable complementary functionalities, including non-volatile, analog, and high-speed information processing, naturally supporting concepts such as neural networks and physical reservoir computing. By focusing on material-intrinsic physical effects for computing, the symposium aims to highlight conceptually new, energy-efficient pathways toward scalable edge AI beyond traditional transistor-based technologies.

Overview of Invited Talks and Sessions

(Lecture hall HSZ/AUDI)

Invited Talks

SYBT 1.1	Wed	9:30–10:00	HSZ/AUDI	**Finding Neuromorphic Advantage with Magnetism** — •Johan Mentink
SYBT 1.2	Wed	10:00–10:30	HSZ/AUDI	**Accelerating Neural Networks Computation with Ferroelectric Oxides** — •Laura Bégon-Lours, Nikhil Garg, Alexandre Baigol, Anwesha Panda, Nathan Savoia, Alexander Flasby
SYBT 1.3	Wed	10:30–11:00	HSZ/AUDI	**a photonic approach to probabilistic computing** — •Wolfram Pernice
SYBT 1.4	Wed	11:15–11:45	HSZ/AUDI	**Tackling Reliability and Scalability in Neuromorphic Computing via Noise-aware Learning** — •Eleni Vasilaki
SYBT 1.5	Wed	11:45–12:15	HSZ/AUDI	**Bayesian nanodevices for trustworthy artificial intelligence** — •Damien Querlioz

Sessions

SYBT 1.1–1.5	Wed	9:30–12:15	HSZ/AUDI	**Beyond Transistors: Material-Based Edge Computing Paradigms**

Sessions

– Invited Talks –

SYBT 1: Beyond Transistors: Material-Based Edge Computing Paradigms

Time: Wednesday 9:30–12:15 Location: HSZ/AUDI

Invited Talk SYBT 1.1 Wed 9:30 HSZ/AUDI

Finding Neuromorphic Advantage with Magnetism — •Johan Mentink — Radboud University, Nijmegen, Netherlands

Neuromorphic computing promises much faster and much more energy-efficient computations with applications domains spanning the whole compute continuum. Nevertheless, rather little is known about applications of neuromorphic computing in computational physics such as the simulation of magnetic materials. In this talk we present our results on exploring and benchmarking neuromorphic computing for probabilistic simulations of quantum magnetism. Our explorations include hardware paradigms such as in-memory computing [1], probabilistic bits [2,3] and large-scale simulations with spiking-based systems electronic systems. We find that the massively parallel nature of neuromorphic hardware offers important scaling advantages over existing digital hardware and enables orders of magnitude faster and more energy-efficient variational quantum Monte Carlo simulations. Moreover, beyond existing neuromorphic paradigms, we show that even better scaling is in reach by adopting new magnetic device concepts, such as those harnessing Brownian skyrmion dynamics [4]. Our results open a path to find neuromorphic computational advantage in probabilistic quantum simulation and suggest high potential to break existing computational barriers for selected computational problems in general.

[1] D. J. Kösters, et al. APL ML 1, 016101 (2023) [2] R.J.L.F. Berns et al., arXiv:2504.18359 (2025) [3] S. Chowdhury, Nat Commun 16, 9193 (2025) [4] Th. Winkler et al., arXiv:2508.19623 (2025)

Invited Talk SYBT 1.2 Wed 10:00 HSZ/AUDI

Accelerating Neural Networks Computation with Ferroelectric Oxides — •Laura Bégon-Lours, Nikhil Garg, Alexandre Baigol, Anwesha Panda, Nathan Savoia, and Alexander Flasby — Integrated Systems Laboratory, D-ITET, ETH Zürich

On conventional computers, the performance of AI models is limited by the data transfer between the memory and the processor. Compute-in-Memory architectures offer a new paradigm: Vector-Matrix Multiplications may be performed by a voltage drop through a matrix of programmable resistances, the *synaptic weights*. Ferroelectric materials are excellent candidates for their realization: the conductance is programmed by controlling the configuration of the ferroelectric domains. The mechanisms governing the resistive switching in WOx / HZO-SL (5 nm) bilayers are discussed. The effect of the programming pulse duration and amplitude on the polarization switching are investigated, from milliseconds to nanoseconds timescales. Devices of different sizes and shapes are measured down to 500 nm in dimension. For an device size of 1 micrometer square, an On/Off ratio as high as 4 is obtained for 20 ns pulses, a 4-fold improvement compared to 40 um devices. The relatively low crystallization temperature of polycrystalline hafnium oxide / zirconium oxide superlattices (HZO-SL) is compatible with the Back-End-Of-Line (BEOL) of CMOS transistors. These results not only demonstrate the functionalization of the BEOL with synaptic weights, but also pave the way for the integration of ferroelectric field-effect transistors with Beyond CMOS semiconductors.

Invited Talk SYBT 1.3 Wed 10:30 HSZ/AUDI

a photonic approach to probabilistic computing — •Wolfram Pernice — Heidelberg University, Kirchhoff-Institute for Physics, Heidelberg, Germany

Unlike artificial neural networks (ANNs), which focus on maximizing accuracy, biological systems excel at handling uncertainty. This ability is believed to be essential for adaptability and efficiency, yet traditional ANNs, implemented on deterministic hardware, struggle with capturing the full probabilistic nature of inference. To address this limitation, Bayesian neural networks (BNNs) replace deterministic parameters with probability distributions, allowing us to distinguish between epistemic uncertainty (due to limited data) and aleatoric uncertainty (arising from noise). By incorporating Bayesian inference, BNNs enable uncertainty quantification and allow for out-of-distribution detection in cases of incomplete data. However, processing probabilistic models remains a challenge for conventional digital hardware, which relies on deterministic von Neumann architectures that separate memory from computation. In electronic crossbar arrays, memristors exhibit inherent stochasticity, making them suitable for probabilistic inference. Yet, sequential sampling and variability in memristive materials present obstacles. To address these challenges, I will outline recent progress in photonic computing architectures that harness hardware noise as a computational resource rather than a constraint.

15 min break

Invited Talk SYBT 1.4 Wed 11:15 HSZ/AUDI

Tackling Reliability and Scalability in Neuromorphic Computing via Noise-aware Learning — •Eleni Vasilaki — Computer Science, The University of Sheffield, 211 Portobello, Sheffield, S1 4DP, UK

Neuromorphic computing has evolved into a broad label covering technologies ranging from biologically inspired systems to machine-learning-style architectures. Computing with materials is often promoted as a potentially energy-efficient alternative to conventional hardware, but some of these claims lack robust empirical support. In this talk I will outline key challenges in the field, with a focus on variability and scalability. I will present concrete examples from my recent work showing how noise-aware learning in systems with stochastic, device-level behaviour can help mitigate variability and improve robustness. These results suggest that while variability poses real constraints, it can be addressed through appropriate learning strategies.

Invited Talk SYBT 1.5 Wed 11:45 HSZ/AUDI

Bayesian nanodevices for trustworthy artificial intelligence — •Damien Querlioz — Univ Paris-Saclay, CNRS, Palaiseau, France.

Artificial intelligence (AI) increasingly powers safety-critical systems that demand robust, energy-efficient computation, often under conditions of data scarcity and uncertainty. Traditional AI approaches are limited in their ability to quantify confidence, leaving them vulnerable to unreliable predictions. In this talk, we introduce Bayesian electronics, which harnesses the intrinsic randomness of emerging nanodevices for on-device Bayesian computations. By encoding probability distributions at the hardware level, these devices naturally estimate uncertainty and reduce overhead compared with purely deterministic designs. We examine how Bayesian networks and Bayesian neural networks can be implemented in this framework to enhance sensor fusion and out-of-distribution detection. We also describe how hardware training via Markov chain Monte Carlo or Langevin dynamics yields energy-frugal sampling-based learning. Finally, we draw parallels with biological systems that are hypothesized to similarly exploit noise for probabilistic computation. By integrating device physics, algorithmic design and system-level optimization, Bayesian electronics offers a path towards more trustworthy and adaptive AI hardware.

Symposium Designing Quantum Materials with Light: From Floquet to Cavity Engineering (SYFC)

jointly organised by
the Semiconductor Physics Division (HL),
the Surface Science Division (O), and
the Low Temperature Physics Division (TT)

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This symposium focuses on how tailored light fields and optical cavities can be used to design and control novel phases of quantum matter far from thermal equilibrium or even in the dark. Building on rapid progress in ultrafast experiments – including time-resolved momentum microscopy and high-quality 2D/3D materials – Floquet and cavity engineering now enable the creation of engineered band structures, correlated and topological phases, and emergent "polaritonic quantum matter." In parallel, ab initio and advanced many-body theory have matured to the point of providing quantitative guidance and interpretation for these experiments. The symposium will bring together leading international experts from theory and experiment to discuss current breakthroughs and future directions towards optoelectronic and quantum-information devices based on light-designed quantum materials.

Overview of Invited Talks and Sessions

(Lecture hall HSZ/AUDI)

Invited Talks

SYFC 1.1	Mon	9:30–10:00	HSZ/AUDI	**Subcycle videography of strong-field controlled band structures** — •Rupert Huber, Manuel Meierhofer, Ulrich Höfer
SYFC 1.2	Mon	10:00–10:30	HSZ/AUDI	**Engineering Quantum Materials through Structured Cavity Vacuum Fluctuations** — •Angel Rubio
SYFC 1.3	Mon	10:30–11:00	HSZ/AUDI	**Floquet engineering of quantum materials: from semiconductors to semimetals** — •Shuyun Zhou
SYFC 1.4	Mon	11:15–11:45	HSZ/AUDI	**(Quantum) Light Control of Materials** — •Dante Kennes
SYFC 1.5	Mon	11:45–12:15	HSZ/AUDI	**Lightwave-driven electrons in a Floquet topological insulator** — Daniel Lesko, Tobias Weitz, Weizhe Li, Selina Nöcker, Celina Hüttner, Tamara Pröbster, Simon Wittigschlager, Christian Heide, Ofer Neufeld, •Peter Hommelhoff

Sessions

SYFC 1.1–1.5	Mon	9:30–12:15	HSZ/AUDI	**Designing Quantum Materials With Light: from Floquet to Cavity Engineering**

Sessions

– Invited Talks –

SYFC 1: Designing Quantum Materials With Light: from Floquet to Cavity Engineering

Time: Monday 9:30–12:15 Location: HSZ/AUDI

Invited Talk SYFC 1.1 Mon 9:30 HSZ/AUDI

Subcycle videography of strong-field controlled band structures — •Rupert Huber[1], Manuel Meierhofer[1], and Ulrich Höfer[1,2] — [1]Department of Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, Germany — [2]Department of Physics, Marburg University, Germany

In lightwave electronics, the oscillating carrier field of intense light pulses has been utilized as an alternating bias to coherently accelerate electrons through solids [1]. Lightwave-driven closed quantum trajectories can lead to new eigenstates and tailored Floquet-Bloch band structures. We will first report how all-optical measurements can uniquely identify the presence of Floquet-Bloch states using high-order sideband generation [2]. A direct momentum-resolved observation of the formation and decay of Floquet-Bloch band structures on subcycle time scales has become available with ARPES-based band-structure videography [3]. While our lead-off experiments were limited to subcycle dynamics at small electron momenta, a novel approach using momentum microscopy with few-fs XUV pulses affords a panoramic view of strong-field dynamics throughout the first Brillouin zone. We will illustrate how this approach allows us to reveal the anatomy of strong-field light-matter interaction in quantum materials ranging from graphene to novel flat-band materials.

[1] Borsch et al., Nature Reviews Materials 8, 668 (2023); Kira et al., Optics and Photonics News 36, 28 (2025). [2] Freudenstein et al., Nature 610, 290 (2022); Kneller et al., in preparation. [3] Ito et al., Nature 616, 696 (2023); Reimann et al., Nature 562, 396 (2018).

Invited Talk SYFC 1.2 Mon 10:00 HSZ/AUDI

Engineering Quantum Materials through Structured Cavity Vacuum Fluctuations — •Angel Rubio — Max Planck Insttitue for the Structure and Dynamics of Matter

Structuring the photon density of states in optical cavities enables control of material properties through strong light*matter coupling. Quantum Electrodynamical Density Functional Theory (QEDFT) extends TDDFT by incorporating quantized electromagnetic fields into electronic structure theory, providing an ab initio framework for predicting cavity-induced phenomena. Experiments such as photon-mediated superconductivity and optically engineered topological phases show that vacuum fluctuations, rather than classical light, can reshape material ground states and drive new quantum phases.

We present an ab initio approach to study cavity effects in two-dimensional materials. Using QEDFT, we show how vacuum fields modify van der Waals systems, inducing charge localization, tunable band gaps, and interlayer spacing that alter ferroelectric and optical responses. A non-perturbative Hartree*Fock framework further reveals cavity-mediated electron interactions in graphene and dichalcogenides, where anisotropic photon modes open Dirac gaps while isotropic ones renormalize the Fermi velocity. Cavity photons thus emerge as a new control parameter for correlated quantum states.

Invited Talk SYFC 1.3 Mon 10:30 HSZ/AUDI

Floquet engineering of quantum materials: from semiconductors to semimetals — •Shuyun Zhou — Department of Physics, Tsinghua University

Time-periodic light-field can dress the electronic states of quantum materials, providing a fascinating controlling knob for transient modifications of the electronic structure with versatile light-induced emergent phenomena. In this talk, I will present our recent experimental progress on the Floquet engineering of quantum materials using time- and angle-resolved photoemission spectroscopy (TrARPES). In particular, experimental progress on the Floquet engineering of semiconductors and semimetals. Experimental insights on Floquet engineering and light-matter interactions in quantum materials will also be discussed.

15 min. break

Invited Talk SYFC 1.4 Mon 11:15 HSZ/AUDI

(Quantum) Light Control of Materials — •Dante Kennes — RWTH Aachen University, Germany — MPSD Hamburg, Germany

Light offers a versatile handle for tailoring quantum materials. I will outline two complementary examples focusing on their theoretical and computational nonequilibrium quantum many-body descriptions: (i) Ultrafast optical drives can transiently reshape a solid's symmetry and electronic structure, where for the latter Floquet engineering provides the framework for accessing and stabilizing novel non-equilibrium phases [1]. (ii) Embedding a material in an optical cavity couples it to quantized photon modes, unlocking new many-body phenomena in the realm of cavity quantum electrodynamics [2]. I will close with an outlook on merging these strategies with the flexibility of two-dimensional heterostructures to enable on-demand design of quantum functionalities [3].

[1] Rev. Mod. Phys. 93, 041002 (2021)
[2] Appl. Phys. Rev. 9, 011312 (2022)
[3] Nat. Phys. 17, 155 (2021)

Invited Talk SYFC 1.5 Mon 11:45 HSZ/AUDI

Lightwave-driven electrons in a Floquet topological insulator — Daniel Lesko[1,2], Tobias Weitz[1,2], Weizhe Li[1], Selina Nöcker[1,2], Celina Hüttner[1], Tamara Pröbster[1], Simon Wittigschlager[1], Christian Heide[1,3], Ofer Neufeld[4], and •Peter Hommelhoff[1,2] — [1]Department Physik, Friedrich-Alexander-Universität, Erlangen — [2]Fakultät für Physik, Ludwig-Maxilians-Universität, München — [3]University of Central Florida, Orlando, Fl, USA — [4]Technion, Haifa, Israel

Topological insulators enable novel quantum and electronic phenomena but are limited by material constraints. Floquet topological insulators (FTIs), created by time-periodic driving, promise tunable topological properties and petahertz operation. We demonstrate optical control of photocurrents in light-dressed graphene, where circularly polarized pulses induce an FTI state and phase-locked second-harmonic pulses drive electron dynamics. This enables measurement of all-optical anomalous Hall and valley-polarized photocurrents, revealing sub-cycle phase sensitivity and dynamical symmetry selection rules. Supported by ab-initio and analytical theory, our results establish a bridge between Floquet and topological physics, attosecond science, and valleytronics, advancing ultrafast topotronic control beyond static band engineering.

Guest Country Symposium France: Soft, Active and Alive: Emergent Properties in Living Matter (SYGF)

jointly organised by
the Biological Physics Division (BP),
the Chemical and Polymer Physics Division (CPP),
the Dynamics and Statistical Physics Division (DY), and
the Physics of Socio-economic Systems Division (SOE)

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Biological systems are composed of molecular components similar to those found in soft matter, yet they exhibit extraordinary and often extreme material properties that are essential for the robustness of living cells, tissues, and populations. These remarkable properties frequently emerge from the multiple hierarchical levels of organization intrinsic to living matter. This guest country symposium with speakers from France and Germany discusses the active and hierarchical principles that apply across diverse biological scales, from molecular assemblies to cells, tissues and even swarms of animals, and their role in biology's unique emergent properties.

Overview of Invited Talks and Sessions

(Lecture hall HSZ/AUDI)

Invited Talks

SYGF 1.1	Wed	15:00–15:30	HSZ/AUDI	**Liquid crystal geometries in type I collagen-based tissues** — •Nadine Nassif
SYGF 1.2	Wed	15:30–16:00	HSZ/AUDI	**Self-organization of the cytoplasm by physical instabilities** — •Jan Brugues
SYGF 1.3	Wed	16:00–16:30	HSZ/AUDI	**From morphogenesis to space partitioning by microtubules and molecular motors.** — •Manuel Thery
SYGF 1.4	Wed	16:45–17:15	HSZ/AUDI	**More than the sum: how composite interfaces govern function** — •Alba Diz-Muñoz
SYGF 1.5	Wed	17:15–17:45	HSZ/AUDI	**Swimming and Swarming of Intelligent Active Particles** — Segun Goh, Priyanka Iyer, Rajendra Singh Negi, •Gerhard Gompper
SYGF 1.6	Wed	17:45–18:15	HSZ/AUDI	**Perturbing the collective motion of fish with challenging environments** — •Aurélie Dupont

Sessions

SYGF 1.1–1.6	Wed	15:00–18:15	HSZ/AUDI	**Guest Country Symposium France: Soft, Active and Alive: Emergent Properties in Living Matter (SYGF)**

Sessions

– Invited Talks –

SYGF 1: Guest Country Symposium France: Soft, Active and Alive: Emergent Properties in Living Matter (SYGF)

Time: Wednesday 15:00–18:15 Location: HSZ/AUDI

Invited Talk SYGF 1.1 Wed 15:00 HSZ/AUDI

Liquid crystal geometries in type I collagen-based tissues — •Nadine Nassif — Sorbonne Université/CNRS, UMR7574, Paris, France

Many biological tissues exhibit hierarchical fibrillar architectures that resemble the geometry of liquid crystalline phases. Such ordering occurs in matrices composed of collagen, chitin, cellulose, or DNA, and governs essential structure/property relationships. Bone and cornea are two emblematic examples: bone exhibits a twisted-plywood architecture, whereas the cornea displays a highly organized orthogonal plywood arrangement that ensures transparency and mechanical integrity. In bone, collagen confinement creates supersaturation of proteins and ions, with major consequences for mineral formation. Our research aims to reproduce the collagen-based building blocks underlying these tissues to better understand morphogenesis and develop advanced biomaterials. Type I collagen shows lyotropic behavior, forming successive ordered phases and retaining liquid-crystal organization during fibrillogenesis. Using a bioinspired continuous-injection process mimicking cellular secretion, we scale up collagen assemblies from droplets to 3D bulk materials. Their biomimetic mineralization produces collagen/apatite composites with strong structural and functional similarity to bone, as demonstrated by in vitro and in vivo investigations. Overall, our results demonstrate the importance of physico-chemical processes in biomineralization, which are usually discussed from a biological perspective.

Invited Talk SYGF 1.2 Wed 15:30 HSZ/AUDI

Self-organization of the cytoplasm by physical instabilities — •Jan Brugues — Cluster of Excellence Physics of Life, TU-Dresden, Dresden, Germany

Early development across vertebrates and insects critically relies on robustly reorganizing the cytoplasm of fertilized eggs into individualized cells. This intricate process is orchestrated by large microtubule structures that traverse the embryo, partitioning the cytoplasm into physically distinct and stable compartments. Despite the robustness of embryonic development, here we uncover an intrinsic instability in cytoplasmic partitioning driven by the microtubule cytoskeleton. We reveal that embryos circumvent this instability through two distinct mechanisms: either by matching the cell cycle duration to the time needed for the instability to unfold or by limiting microtubule nucleation. These regulatory mechanisms give rise to two possible strategies to fill the cytoplasm, which we experimentally demonstrate in vitro and in zebrafish and Drosophila embryos. Our results indicate that the temporal control of microtubule dynamics could have driven the evolutionary emergence of species-specific mechanisms for effective cytoplasmic organization. Furthermore, our study unveils a fundamental synergy between physical instabilities and biological clocks, uncovering universal strategies for rapid, robust, and efficient spatial ordering in biological systems.

Invited Talk SYGF 1.3 Wed 16:00 HSZ/AUDI

From morphogenesis to space partitioning by microtubules and molecular motors. — •Manuel Thery — ESPCI, Paris, France

Microtubules are not just tracks for transport; they can also be moved by the forces exerted by molecular motors. In this presentation, we will first demonstrate how the interplay between moving microtubules and transported motors can result in the emergence of shapes from random mixtures (morphogenesis). We will explain how these shapes are maintained in dynamic steady-states by active and polar boundaries. Then, we will explore the plasticity and adaptation of these boundaries to geometric constraints, as well as their ability to polarise or bipolarise a confined space (space partitioning). Finally, we will discuss the relevance of this process to various forms of intracellular organisation.

15 min. break

Invited Talk SYGF 1.4 Wed 16:45 HSZ/AUDI

More than the sum: how composite interfaces govern function — •Alba Diz-Muñoz — European Molecular Biology Laboratory, Heidelberg, Germany

The cell surface of animal cells is a composite interface with several layers, the plasma membrane, the actomyosin cortex and a membrane-to-cortex attachment protein layer that binds them together. Biochemically and mechanically each of these layers differs. My group is taking an engineering-inspired approach, combined with traditional cell biology methods, to quantitatively measure and predict how the various mechanical layers at the surface of animal cells govern function. Together, our work identifies membrane-to-cortex attachment as a critical mechanotransducer in cells, and the membrane-to-cortex distance as a key geometrical parameter that regulates protein activity at the cell surface.

Invited Talk SYGF 1.5 Wed 17:15 HSZ/AUDI

Swimming and Swarming of Intelligent Active Particles — Segun Goh[1,2], Priyanka Iyer[1], Rajendra Singh Negi[1], and •Gerhard Gompper[1] — [1]Institute for Advanced Simulation, Forschungszentrum Juelich, Germany — [2]Sejong University, Seoul, South Korea

The collective behavior of motile active matter displays many emergent self-organization, like flocking and swarming [1]. For living systems, as well as microrobotic systems, activity and locomotion is combined with sensing of the environment and adaption of motion. We study such system by considering models of 'intelligent' active particles with visual perception and self-steering in both dry [2,3] and wet systems [4,5].

Here, we focus on wet systems, where hydrodynamic interactions contribute significantly or dominate the self-organization [4,5]. Pusher- and puller-type squirmers display very different emergent behaviors. Pusher-pursuers may not be able to catch up with pusher-targets even at larger pursuer speeds [4]. Also, aligning pushers can form stable pairs only with speed adjustment of the pursuer . In large ensembles, pushers display active turbulence, while pullers form unstable clusters, vortices, and jets [5].

[1] G. Gompper et al.; J. Phys. Condens. Matter 37, 143501 (2025). [2] R.S. Negi et al.; Phys. Rev. Research 6, 013118 (2024) [3] P. Iyer et al.; Commun. Phys. 7, 379 (2024) [4] S. Goh et al.; Commun. Phys. 6, 31 (2023) [5] S. Goh et al.; Phys. Rev. Research 7, 013142 (2025)

Invited Talk SYGF 1.6 Wed 17:45 HSZ/AUDI

Perturbing the collective motion of fish with challenging environments — •Aurélie Dupont — LIPhy, CNRS Univ. Grenoble Alpes, Grenoble France

Collective movements can be observed across species and on various scales: from bacteria to mammals. We are interested in the collective behavior of small fish when confronted with external physical perturbations. When forced to escape through a narrow opening, most animals behave like granular materials and clogging events decrease the efficiency of evacuation. In this emergency exit scenario, we challenged the gregarious behavior of a group of macroscopic aquatic agents, neon fish, by forcing the school to pass through a small opening[Larrieu, Sci. Rep. 2023]. Using a statistical analysis developed for granular material and applied to crowd evacuation, our results clearly show that, unlike human crowds or herds of sheep, no clogging forms at the bottleneck. The fish do not collide and wait by respecting their social distance and a minimum delay between two successive exits. In a second experiment, we perturbed the schooling behavior of a group of zebrafish by adding an array of pillars to the observation tank[Ventejou Phys. Rev. E 2024]. We observed a behavioral transition from a polarized group when the density of pillars is low to independent fish aligned with the array of pillars. The abrupt transition from natural to artificial orientation occurs when the distance between pillars is comparable to the social distance of the fish. We developed a stochastic model of relative orientation between pairs of fish that captures the behavioral transition and provides information on the evolution of cognitive parameters.

Symposium Interacting Degrees of Freedom in Ultrathin Quantum Films (SYQF)

jointly organised by
the Semiconductor Physics Division (HL),
the Thin Films Division (DS),
the Magnetism Division (MA), and
the Low Temperature Physics Division (TT)

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Understanding the interactions between different degrees of freedom and their associated low-energy excitations is crucial for comprehending the physical behavior of condensed matter systems. In atomically thin quantum films, reduced dimensionality and enhanced confinement lead to amplified or modified interactions, resulting in novel physical phenomena. This symposium provides an interdisciplinary platform to discuss recent advances in the field of coupled degrees of freedom in ultrathin materials, with contributions from both experimental and theoretical perspectives. Exploring these effects not only deepens our understanding of quantum nanomaterials but also paves the way for integrating systems with interacting degrees of freedom into next-generation electronic, optoelectronic, and quantum technologies.

Overview of Invited Talks and Sessions

(Lecture hall HSZ/AUDI)

Invited Talks

SYQF 1.1	Fri	9:30–10:00	HSZ/AUDI	**Exciton dressing by extreme nonlinear magnons in a layered semiconductor** — •Geoffrey M. Diederich
SYQF 1.2	Fri	10:00–10:30	HSZ/AUDI	**A tale of demons and decay in two-dimensional (alter)magnets** — •Alexander Mook
SYQF 1.3	Fri	10:30–11:00	HSZ/AUDI	**Magnetism, light and matter - Role of excitons in two-dimensional magnets** — •Florian Dirnberger
SYQF 1.4	Fri	11:15–11:45	HSZ/AUDI	**Advantages and challanges of resonance Raman scattering with infrared excitation energy** — •Leonetta Baldassarre
SYQF 1.5	Fri	11:45–12:15	HSZ/AUDI	**Shining light on 2D antiferromagnets** — •Dmytro Afanasiev

Sessions

SYQF 1.1–1.5	Fri	9:30–12:15	HSZ/AUDI	**Interacting Degrees of Freedom in Ultrathin Quantum Films**

Sessions

– Invited Talks –

SYQF 1: Interacting Degrees of Freedom in Ultrathin Quantum Films

Time: Friday 9:30–12:15 Location: HSZ/AUDI

Invited Talk SYQF 1.1 Fri 9:30 HSZ/AUDI

Exciton dressing by extreme nonlinear magnons in a layered semiconductor — •Geoffrey M. Diederich — University of Maryland Baltimore County, 1000 Hilltop Circle, Baltimore MD, USA

Collective excitations presenting nonlinear dynamics are fundamental phenomena with broad applications. A prime example is nonlinear optics, where diverse frequency-mixing processes are central to communication and attosecond science, and extreme (>sixth-order) harmonic generation provides broad wavelength conversion. Leveraging recent progress in van der Waals magnetic semiconductors, we demonstrate nonlinear optomagnonic coupling. In the layered antiferromagnetic semiconductor CrSBr, we observe exciton states dressed by up to 20 harmonics of magnons, resulting from their extreme nonlinearities. We also create tunable optical sidebands via sum- and difference-frequency generation between two optically bright magnon modes under symmetry-breaking magnetic fields. Moreover, we can tune the observed difference-frequency generation mode into resonance with one of the fundamental magnons, which results in parametric amplification of magnons. Our findings realize the modulation of the optical-frequency exciton with the extreme nonlinearity of magnons at microwave frequencies, which could find applications in magnonics and hybrid quantum systems, and provide a method for optomagnonic neuromorphic computing devices.

Invited Talk SYQF 1.2 Fri 10:00 HSZ/AUDI

A tale of demons and decay in two-dimensional (alter)magnets — •Alexander Mook — Universität Münster

Altermagnets are a newly discovered class of magnetic materials that combine broken time-reversal symmetry with zero net magnetization, offering promising opportunities for spintronics. I will introduce the basic principles of altermagnetism and discuss two recent advances in understanding their collective excitations. First, electron-electron interactions create a new type of low-energy mode: spin-polarized acoustic plasmons ("spin demons"). Second, I will show how the splitting of magnon bands enables spontaneous magnon decay driven purely by quantum many-body fluctuations, setting an intrinsic limit on magnon lifetimes. These findings highlight the unconventional excitation physics of altermagnets and their potential for future functional materials.

Invited Talk SYQF 1.3 Fri 10:30 HSZ/AUDI

Magnetism, light and matter - Role of excitons in two-dimensional magnets — •Florian Dirnberger — Zentrum für QuantumEngineering (ZQE), Technical University of Munich, Garching, Germany — Department of Physics, TUM School of Natural Sciences, Technical University of Munich, Munich, Germany

Studies on van der Waals magnetic materials have recently unveiled a rare type of optical quasiparticle formed by spin-polarized electronic states in magnets. With properties that have no analogue among excitons in conventional semiconductors, these so-called magnetic excitons offer a compelling playground to explore the interplay between magnetism, light and matter.

In this talk, I will review the magneto-optical properties of excitonic van der Waals magnets, with a particular focus on recent work on the antiferromagnetic insulator CrSBr. This archetypal layered magnet provides key insights into how magnetic order alters excitonic responses, and how excitons in turn influence magnetic dynamics. It further enables experiments to probe magnetic excitons in the regime of strong light-matter coupling, bringing concepts from photonics into the picture. Optical spectroscopy reveals pronounced exciton responses to applied magnetic fields, dynamic coupling between excitons and both coherent and incoherent magnons, and magnon-induced excitonic correlations. Together, these results open new directions for magneto-optics and highlight opportunities to control magnetically correlated quantum materials through strong light-matter interactions.

15 min. break

Invited Talk SYQF 1.4 Fri 11:15 HSZ/AUDI

Advantages and challanges of resonance Raman scattering with infrared excitation energy — •Leonetta Baldassarre — Department of Physics, Sapienza University of Rome, I-00185 Rome Italy

Resonance Raman scattering is a valuable spectroscopic technique, providing a probe into the intertwined electronic and vibrational properties of materials. The main strength of resonance Raman lies in its ability to selectively map distinct regions of the electron and phonon dispersion simply by tuning the excitation laser energy.

I will introduce our experimental approach of performing resonance Raman by lowering the excitation energy deep into the Near-Infrared. This frequency shift is strategic, enabling us to probe scattering processes resonant with the bottom of the conduction band in narrow-band semiconductors or close to the Dirac points. I will provide an overview of the custom-built experimental setup and present the results from its application to diverse materials such as layered semiconductors like $MoSe_2$ and $MoTe_2$ or graphene.

Our measurements are compared to *ab-initio* calculations so to identify the phonons involved in the resonant processes and, in the case of graphene, introduce the existence of a momentum-dependent electron-phonon coupling between low-energy carriers and zone-boundary optical phonons. Resonance Raman scattering with infrared excitation can be thus viewed as an indispensable tool for exploring and understanding the essential, often-hidden, charge-carrier and lattice dynamics that define the physics of low-dimensional quantum matter.

Invited Talk SYQF 1.5 Fri 11:45 HSZ/AUDI

Shining light on 2D antiferromagnets — •Dmytro Afanasiev — Radboud University

Ultrafast optical control of antiferromagnetic order is a key goal in spintronics and magnonics. Resonant excitation of local orbital degrees of freedom, such as dd transitions in transition-metal ions, offers a direct route to modify magnetic exchange and anisotropy on femtosecond timescales. However, orbitally driven photomagnetism has been demonstrated in only a few materials, and the factors governing its efficiency remain unclear.

Here, we study ultrafast spin dynamics induced by resonant pumping of dd transitions in layered antiferromagnetic thiophosphates XPS3. We first establish the photomagnetic response in single magnetic-ion compounds, where local orbital excitation triggers coherent spin precession via ultrafast anisotropy modulation. We then extend this approach to binary compounds containing two distinct transition-metal ions, demonstrating that selective excitation of specific orbital resonances strongly enhances the efficiency and controllability of magnon generation.

These results identify general design principles for orbitally driven photomagnetism in collinear antiferromagnets and establish transition-metal substitution as a powerful strategy for achieving efficient ultrafast control of antiferromagnetic spin dynamics.

Symposium The Sustainability Challenge: A Decade of Transformation (SYSC)

jointly organised by
the Environmental Physics Division (UP),
the Biological Physics Division (BP),
the Chemical and Polymer Physics Division (CPP),
the Physics Education Division (DD),
the Thin Films Division (DS),
the Dynamics and Statistical Physics Division (DY),
the Metal and Material Physics Division (MM),
the Physics of Socio-economic Systems Division (SOE),
the Working Group on Industry and Business (AIW),
the Working Group "Young DPG" (AKjDPG), and
the Working Group on Physics, Modern IT and Artificial Intelligence (AKPIK)

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The UN Sustainable Development Goals call for transformative action across all sectors. Physics, as a foundational science, plays a key role - from understanding complex natural and socio-economic systems to developing sustainable technologies, fostering responsible resource use, and advancing sustainability-oriented education and public outreach. This symposium brings together diverse perspectives from within the physics community to explore interdisciplinary contributions to sustainability, including earth system modeling, energy systems, transport, molecular recycling and circularity as well as science education. Through five expert talks from various fields, we aim to highlight the relevance of physics and physics education for future-oriented transformation and inspire early-career researchers to engage with pressing global challenges in meaningful, scientifically grounded ways.

Overview of Invited Talks and Sessions

(Lecture hall HSZ/AUDI)

Invited Talks

SYSC 1.1	Mon	15:00–15:30	HSZ/AUDI	**Open-Endedness and Community-Based Approaches to Sustainability Challenges** — •Hiroki Sayama
SYSC 1.2	Mon	15:30–16:00	HSZ/AUDI	**Education as a Social Tipping Element: Evidence from Climate and Physics Education Research** — •Thomas Schubatzky
SYSC 1.3	Mon	16:00–16:30	HSZ/AUDI	**Mechanistic and Material Perspectives on Enzymatic Hydrolysis of Semicrystalline Polyesters** — •Birte Höcker
SYSC 1.4	Mon	16:45–17:15	HSZ/AUDI	**Decarbonization Options for Industry** — •Uwe Riedel
SYSC 1.5	Mon	17:15–17:45	HSZ/AUDI	**Impacts of Cosmic Dust and Space Debris in the Terrestrial Atmosphere** — •John Plane

Discussion on Sustainability on Monday during Lunch Break

PSV I	Mon	13:00–13:45	HSZ/AUDI	**Sustainability! And now? – Opportunities for young researchers** — •Roxana Scharpegge, Hiroki Sayama, Thomas Schubatzky, Birte Höcker, Uwe Riedel, John Plane, Pauleo Nimtz, Stefanie Falk

Accompanying session in UP

UP 1.1–1.4 Mon 9:30–10:30 MER/0002 **Sustainability: Challenges and Solutions (joint session UP/CPP/SOE)**

Sessions

SYSC 1.1–1.5 Mon 15:00–17:45 HSZ/AUDI **The Sustainability Challenge: A Decade of Transformation**

Sessions

– Invited Talks –

SYSC 1: The Sustainability Challenge: A Decade of Transformation

Time: Monday 15:00–17:45 Location: HSZ/AUDI

Invited Talk SYSC 1.1 Mon 15:00 HSZ/AUDI

Open-Endedness and Community-Based Approaches to Sustainability Challenges — •Hiroki Sayama — Binghamton University, State University of New York, Binghamton, NY, USA — Waseda University, Tokyo, Japan

The sustainability of our natural and social environments is of utmost importance in today's complex world. Achieving this goal is challenging because of: the complexity of interconnected networks involving numerous variables, factors, and stakeholders; the uncertainty and unpredictability in the dynamics of these components and their interactions; the possibility of unexpected outcomes resulting from well-planned solutions; and the fundamental lack of cooperative incentives for stakeholders to participate in actions that are collectively beneficial yet individually detrimental. To address these difficult sustainability challenges, one can benefit from insights into complex systems, especially the open-endedness of complex dynamical/evolutionary systems and the active involvement of community members in participatory solution development. In this talk, I will provide a birds-eye view of the recent open-endedness literature being developed in complexity science, artificial life, and AI, and discuss its relevance to sustainability issues. I will also report on a concrete example of community-based approaches to sustainability implemented in the Greater Binghamton area (called the "Binghamton Two Degrees" project). These approaches are becoming increasingly relevant in our sustainability efforts, as we now face irreversible environmental changes arising in a world that may have already passed the critical transition point.

Invited Talk SYSC 1.2 Mon 15:30 HSZ/AUDI

Education as a Social Tipping Element: Evidence from Climate and Physics Education Research — •Thomas Schubatzky — University of Innsbruck, Innsbruck, Austria

The concept of social tipping elements draws attention to societal leverage points that may accelerate transitions towards sustainability. Education is frequently named as one of these leverage points. In this talk, I outline key findings from recent meta-analyses and review studies in climate and physics education research and discuss the conditions under which educational processes may exert transformative effects. The evidence thereby consistently shows substantial gains in climate-related knowledge, while effects on attitudes and behavioural outcomes are smaller but reliably detectable. The pronounced heterogeneity across studies, however, indicates that the underlying mechanisms of effective climate education are still insufficiently understood. The talk addresses this challenge by drawing on selected empirical studies that illustrate how educational interventions can initiate reinforcing feedbacks at both the individual and collective level. These studies are intended to highlight concrete pathways through which education may operate as a social tipping element, and how micro-level learning processes could scale up to support broader societal transformation.

Invited Talk SYSC 1.3 Mon 16:00 HSZ/AUDI

Mechanistic and Material Perspectives on Enzymatic Hydrolysis of Semicrystalline Polyesters — •Birte Höcker — Biochemie, Universität Bayreuth, Germany

Enzymatic degradation of polyethylene terephthalate (PET) provides a sustainable route for polyester recycling, yet efficiency remains limited by both enzyme diversity and substrate properties. To address this, we developed a tunable degradation platform incorporating realistic substrates and adaptable to various polyesters, enabling parallelized purification and high-throughput characterization of novel enzymes and engineered variants. Using this system, we identified halophilic PETases from the marine Halopseudomonas lineage. High-resolution crystallography of one candidate revealed a unique active-site architecture lacking the canonical π-stacking clamp and exhibiting altered loop conformations, prompting an extension of the PETase classification to include type III enzymes. These enzymes demonstrated remarkable salt tolerance and improved PET hydrolysis at elevated temperatures. Complementary studies on polybutylene terephthalate (PBT) highlight the critical role of semicrystalline morphology: reducing crystallinity and optimizing incubation near the glass transition significantly enhance hydrolysis. By expanding the structural and sequence space of PET-degrading enzymes, combined with material-specific insights, we aim to establish a foundation for efficient enzymatic recycling of semicrystalline polyesters and support the development of next-generation biocatalysts for sustainable plastic management.

15 min break

Invited Talk SYSC 1.4 Mon 16:45 HSZ/AUDI

Decarbonization Options for Industry — •Uwe Riedel — DLR Institut für CO2-arme Industrieprozesse, 03046 Cottbus, Deutschland

Industrial decarbonization is pivotal to achieving emission targets. In 2024, CO2-emissions from the industrial sector amounted to approximately 153 million tons, accounting for around 25% of Germanys total CO2-emissions.

However, decarbonizing this sector is challenging due to the wide variety of processes involved. In some cases, electrification is a viable solution, but often, sector-specific approaches are necessary. The presentation will show examples from various sectors and explain the options available for different process temperatures.

Invited Talk SYSC 1.5 Mon 17:15 HSZ/AUDI

Impacts of Cosmic Dust and Space Debris in the Terrestrial Atmosphere — •John Plane — School of Chemistry, University of Leeds, UK

Cosmic dust particles are produced from sublimating comets and collisions between asteroids. Because the particles enter the atmosphere at hypersonic velocities, collisional heating with air molecules leads to vaporization of their metallic constituents. The injection of these elements causes a wide variety of atmospheric phenomena: global layers of metal atoms between 80 and 105 km; airglow emissions; metallic ions (sporadic E layers) which affect radio communications; and meteoric smoke particles which enable the nucleation of mesospheric ice clouds and the freezing of polar stratospheric clouds. Certain metal atoms can be observed by ground-based lidar and from satellites, providing excellent tracers of dynamics and chemistry at the edge of space.

The global mass input rate of cosmic dust to the atmosphere is estimated to be around 27 tonnes per day. This estimate was obtained using an astronomical dust model to provide the size and velocity distributions of dust in the inner solar system, combined with a chemical ablation model to determine the rates of metal injection and deposition of cosmic spherules in the polar ice-caps. The re-entry of spacecraft from low Earth orbit currently produces influxes of metals such as aluminium and lithium which already exceed natural background levels. The atmospheric implications of the expected significant increase in these anthropogenic fluxes during the next decade will be discussed.

Symposium SKM Dissertation Prize 2026 (SYSD)

jointly organised by
all divisions of the Condensed Matter Section of the DPG

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The divisions belonging to the Condensed Matter Section (SKM) of the DPG annually award the SKM Dissertation Prize. The prize acknowledges outstanding research during the doctoral studies in the research areas of the SKM completed between October 2023 and 2025, and its excellent oral presentation. Based on nominations, a jury consisting of the chair persons of all SKM divisions has selected five finalists to present their work in this symposium. The winner will be selected after the symposium and publicly announced Tuesday, March 10, 2026 in the afternoon during the ceremonial session (Lecture hall HSZ/AUDI starting at 16:00).

Overview of Invited Talks and Sessions

(Lecture hall HSZ/0002)

Invited Talks

SYSD 1.1	Mon	9:30–10:00	HSZ/0002	**Stochastic-Calculus Approach to Non-equilibrium Statistical Physics** — •Cai Dieball
SYSD 1.2	Mon	10:00–10:30	HSZ/0002	**Nonuniform magnetic spin textures for sensing, storage and computing applications** — •Sabri Koraltan
SYSD 1.3	Mon	10:30–11:00	HSZ/0002	**Anomalous Quantum Oscillations beyond Onsager's Fermi Surface Paradigm** — •Valentin Leeb
SYSD 1.4	Mon	11:00–11:30	HSZ/0002	**Coherent Control Schemes for Semiconductor Quantum Systems** — •Eva Schöll
SYSD 1.5	Mon	11:30–12:00	HSZ/0002	**On stochastic thermodynamics under incomplete information: Thermodynamic inference from Markovian events** — •Jann van der Meer

Sessions

– Invited Talks –

SYSD 1: SKM Dissertation Prize Symposium 2026

Time: Monday 9:30–12:00 Location: HSZ/0002

Invited Talk SYSD 1.1 Mon 9:30 HSZ/0002

Stochastic-Calculus Approach to Non-equilibrium Statistical Physics — •Cai Dieball — Max Planck Institute of Multidisciplinary Sciences, Göttingen, Germany

Truly understanding living matter requires understanding physical processes far from thermodynamic equilibrium on the level of individual molecules. While single-molecule experiments can probe individual stochastic trajectories, the strong influence of thermal noise and limited number of repetitions pose significant challenges. Here, we address these challenges using the mathematical framework of stochastic calculus. This approach yields important insights into fluctuations of time-averaged densities and currents, which are central observables in non-equilibrium stochastic thermodynamics [1]. Building on these methodological advances, we provide a new route to derive thermodynamic uncertainty relations that link observed currents to the distance to equilibrium, quantified via entropy production [2]. Strikingly, this new derivation generalizes to trade-off relations beyond thermodynamic uncertainty relations, enabling thermodynamic inequalities for bulk observables and dynamics with inertia [3]. Furthermore, we employ the stochastic framework to theoretically predict and experimentally confirm an asymmetry between heating and cooling dynamics far from equilibrium [4].

[1] C. Dieball, A. Godec, Phys. Rev. Lett. 129, 140601 (2022)
[2] C. Dieball, A. Godec, Phys. Rev. Lett. 130, 087101 (2023)
[3] C. Dieball, A. Godec, Phys. Rev. Lett. 133, 067101 (2024)
[4] M. Ibáñez, C. Dieball, et al., Nat. Phys. 20, 135 (2024)

Invited Talk SYSD 1.2 Mon 10:00 HSZ/0002

Nonuniform magnetic spin textures for sensing, storage and computing applications — •Sabri Koraltan — Insitute of Applied Physics, TU Wien, Vienna, Austria

Spintronic materials underpin many modern technologies, from hard-disk drives to magnetic sensors. While these applications traditionally rely on uniform magnetization states, recent advances focus on nonuniform magnetic textures such as vortices, and skyrmions. In my doctoral thesis, I explored such textures for sensing, storage, and computing applications [1].

The first part of my talk covers the discovery and characterization of spin textures with arbitrary topological charge in ferromagnetic [Co/Ni] multilayers [2]. Using simulations and experiments, we demonstrate coexisting higher-order skyrmions and antiskyrmions and uncover their distinct dynamics under spin-transfer torques.

The second part presents a three-dimensional magnetic-field sensor with a wide linear range and intrinsic offset cancellation, enabled by spin-orbit torque symmetry in a [W/CoFeB/MgO]*10 multilayer that stabilizes stripe domains and skyrmions [3]. I will show, through experiment and micromagnetics, how spin-orbit torques reshape the magnetic state at high current densities to achieve full 3D sensing, with topological transitions detected electrically via the anomalous Hall effect.

[1]SK (2025), PhD Thesis, doi:10.25365/THESIS.77909;[2] MH, SK et al., Nat. Phys. 20 (2024) 615*622;[3] SK et al., arXiv:2403.16725 (2024).

Invited Talk SYSD 1.3 Mon 10:30 HSZ/0002

Anomalous Quantum Oscillations beyond Onsager's Fermi Surface Paradigm — •Valentin Leeb — University of Zurich — Technical University of Munich

Quantum oscillation measurements are the most precise method for determining Fermi surface properties in bulk three-dimensional metals, owing to Onsager's relation, which connects the oscillation frequency to an extremal cross-section of the Fermi surface. This canonical, semiclassical theory of quantum oscillations has been remarkably successful in unearthing electronic properties of metals for over 75 years. However, with the emergence of modern quantum materials and advancements in experimental sensitivity, breakdowns of the semiclassical theory have recently come to light. In this talk, I demonstrate that additional quantum oscillation frequencies - breaking Onsager's relation - emerge generically in multiband metals. These anomalous frequencies, referred to as non-Onsager oscillations, are induced by impurities, scattering from fluctuations, or weak and strong electronic interactions. Using a combination of analytic theory, numeric modeling, and experimental verification, I establish them as fundamental features of quantum oscillation spectra. Properly identifying non-Onsager oscillations is essential for accurately reconstructing the Fermi surface. Moreover, these frequencies encode rich information about underlying material properties beyond the scope of the semiclassical theory. The results, presented here, refine our understanding of quantum oscillations in complex materials and open new avenues for probing electronic correlations, emergent phenomena, and unconventional metallic states.

Invited Talk SYSD 1.4 Mon 11:00 HSZ/0002

Coherent Control Schemes for Semiconductor Quantum Systems — •Eva Schöll — PhoQS Institute, CeOPP, and Department of Physics, Paderborn University, Paderborn, Germany — Institute of Semiconductor and Solid State Physics, Johannes Kepler University, Linz, Austria — Institute for Integrated Circuits and Quantum Computing, Johannes Kepler University, Linz, Austria

Single photons are fundamental building blocks for advancing quantum technologies. Therefore, quantum light sources that simultaneously exhibit properties such as high single-photon purity, indistinguishability, and entanglement fidelity are essential. Semiconductor quantum dots (QDs) are promising candidates that already meet many of these requirements. In this talk, I will provide a deeper understanding of the underlying quantum-level schemes and reveal an intrinsic limit on indistinguishability for photons arising from a radiative cascade. To address this, we studied QDs under s-shell resonant excitation and two-photon excitation (TPE), and introduced a novel excitation technique combining TPE with stimulation of the first transition. This method can overcome the previously mentioned limit on indistinguishability.

Invited Talk SYSD 1.5 Mon 11:30 HSZ/0002

On stochastic thermodynamics under incomplete information: Thermodynamic inference from Markovian events — •Jann van der Meer — Department of Physics No. 1, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan

Stochastic thermodynamics provides the framework for analyzing thermodynamic quantities along individual trajectories of small but fully observable systems. If, however, the observable dynamics is coarse-grained, i.e., does not capture all relevant degrees of freedom, the principles of stochastic thermodynamics generally cannot be applied directly. With access to some observables, preeminent results in the field (e.g. the thermodynamic uncertainty relation) often establish lower bounds on the average entropy production in terms of such observables.

However, there is no reason why attention should be limited to bounds on the averaged entropy production only. In my talk, I present the concept of a fluctuating entropy production on the coarse-grained level, which contains more information than about averages only, thereby allowing us to, e.g., estimate the strength of driving forces and localize entropy production spatially and temporally. From a theoretical point of view, these results rely on the identification of Markovian events, a systematic way of describing the dynamics and thermodynamics of a variety of possible coarse-grained dynamics in terms of semi-Markov processes.

Symposium Tipping Points in Social and Climate Systems (SYTP)

jointly organised by
the Physics of Socio-economic Systems Division (SOE),
the Dynamics and Statistical Physics Division (DY),
the Environmental Physics Division (UP),
the Thin Films Division (DS), and
the Working Group "Young DPG" (AKjDPG).

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The concept of tipping points has become central to understanding both climate dynamics and social transformations. This symposium brings together physicists and interdisciplinary researchers to explore the mechanisms underpinning tipping behavior in complex systems. Topics include nonlinear dynamics of the Earth system, early warning signals of climate tipping points, and the emergence of social tipping cascades in response to policy, technology, and behavioral shifts.

Overview of Invited Talks and Sessions

(Lecture hall HSZ/AUDI)

Invited Talks

SYTP 1.1	Thu	15:00–15:30	HSZ/AUDI	**Social Tipping in Heterogeneous and Polarized Populations** — •Sara Constantino, Sonke Ehret, Elke Weber, Sonja Vogt, Charles Efferson
SYTP 1.2	Thu	15:30–16:00	HSZ/AUDI	**Tipping points and regime shifts in coupled social-climate systems** — •Chris Bauch
SYTP 1.3	Thu	16:00–16:30	HSZ/AUDI	**How to tune Earth system models toward tipping?** — •Sebastian Bathiany, Niklas Boers
SYTP 1.4	Thu	16:45–17:15	HSZ/AUDI	**Algorithmic amplification and contextual sensitivity in political information exposure** — Iris Damião, Ana Vranic, Paulo Almeida, Lília Perfeito, •Joana Gonçalves de Sá
SYTP 1.5	Thu	17:15–17:45	HSZ/AUDI	**The complex interplay between democracy and platform power** — •Philipp Lorenz-Spreen

Sessions

SYTP 1.1–1.5	Thu	15:00–17:45	HSZ/AUDI	**Tipping Points in Social and Climate Systems**
SOE 16.1–16.4	Thu	11:30–12:45	GÖR/0226	**Tipping Points in Social and Climate Systems (accompanying session for SYTP)**

Sessions

– Invited Talks –

SYTP 1: Tipping Points in Social and Climate Systems

Time: Thursday 15:00–17:45 Location: HSZ/AUDI

Invited Talk SYTP 1.1 Thu 15:00 HSZ/AUDI

Social Tipping in Heterogeneous and Polarized Populations — •Sara Constantino[1], Sonke Ehret[2], Elke Weber[3], Sonja Vogt[2], and Charles Efferson[2] — [1]Stanford University, Stanford, USA — [2]University of Lausanne — [3]Princeton University

Leveraging social norms to create widespread social change through circumscribed interventions has been hailed as an effective mechanism for addressing climate change. Lab experiments find that a small fraction of a population - a committed minority - can tip a population to an alternative stable state. However, the feasibility of social tipping interventions to incite widespread change depend on specific conditions. In two online experiments, we test (1) the role of group identities in facilitating and interrupting the emergence of social norms, and (2) how heterogeneous preferences impact whether an intervention is effective or not. In the first study, we ran an online experiment in which participants faced consistent incentives to coordinate their choices. We found that while the control groups developed norms slowly before intervention, they transitioned to new norms rapidly after intervention. In contrast, the identity groups developed norms rapidly before intervention but persisted in a state of costly disagreement after an intervention. In a second study, we ran a group experiment where we tested the effects of prior preferences and the magnitude and targeting of tipping interventions. Our results show that pre-intervention heterogeneity significantly moderated the effects of tipping interventions. These findings suggest social tipping success depends on mundane features of the environment.

Invited Talk SYTP 1.2 Thu 15:30 HSZ/AUDI

Tipping points and regime shifts in coupled social-climate systems — •Chris Bauch — Department of Applied Mathematics, University of Waterloo, Canada

Coupled social-climate interactions are important, yet the modelling of such systems is in its infancy, including the study of their tipping points. In this talk, I will touch briefly on two coupled social-climate models*a simpler model intended to study potential interactions between climate and social tipping points, and a more realistic model with regional structure that is parametrised with geophysical, economic, demographic and social data. Among other findings, I will highlight some unexpected predictions that emerge from the nonlinear interactions in the models. I will also touch upon data-driven dynamical systems approaches to predicting tipping points in climate and social-climate systems.

Invited Talk SYTP 1.3 Thu 16:00 HSZ/AUDI

How to tune Earth system models toward tipping? — •Sebastian Bathiany[1,2] and Niklas Boers[1,2] — [1]Technical University of Munich — [2]Potsdam Institute for Climate Impact Research

Models of complex dynamical systems like the Earth's climate often involve large numbers of uncertain parameters. Comprehensive exploration of the parameter space is typically prohibitive due to excessive computational costs. Systematic gradient-based parameter optimization is not feasible because such models are typically not differentiable. This is especially problematic in cases where the models describe highly nonlinear and possibly abrupt dynamics, where sensitivity to parameter changes is high. Components of Earth's climate system, such as the North Atlantic Overturning Circulation or the polar ice sheets, are at risk of undergoing critical transitions in response to anthropogenic climate change. Concerns have been raised that these Earth system components are too stable in state-of-the-art models. In my presentation, we will see examples how new scenario simulations allow studying the possibility and the consequences of tipping events in Earth system models. Also, we will discuss a method for efficient, systematic, and objective calibration of dynamical complex system models, targeted at adjusting system stability. Given a number of physical or observational constraints, the method can efficiently adjust stability biases in a range of complex system models and help reveal potentially hidden instabilities, with important implications for Earth system modelling.

15 min. break

Invited Talk SYTP 1.4 Thu 16:45 HSZ/AUDI

Algorithmic amplification and contextual sensitivity in political information exposure — Iris Damião, Ana Vranic, Paulo Almeida, Lília Perfeito, and •Joana Gonçalves de Sá — LIP, Lisbon, Portugal

Understanding criticality and tipping points is key to analyzing how small changes can cascade into large-scale effects. In information ecosystems, these dynamics emerge in both social media and algorithmically mediated platforms, where recommendation systems interact with user behavior to produce disproportionate societal impacts.

Misinformation on platforms like Twitter (X) is often assumed to spread faster than the truth. Yet, empirical evidence varies. Analyzing three large datasets - Vosoughi News, Global Claims, and Truth Seeker- we find that cascade size distributions are very dependent on sampling choices and this sensitivity can lead to opposite results when studying information diffusion.

Beyond social media, search engines (SEs) and large language models (LLMs) increasingly shape access to information. Using a privacy-preserving bot system, we conducted synchronized searches prior to the 2024 European Parliament. Results varied by location and query type; however, SEs and LLMs consistently emphasized right-leaning entities, revealing systematic algorithmic bias.

Together, these findings illustrate that algorithmically driven platforms can reflect and amplify political biases, creating fragmented informational realities.

Invited Talk SYTP 1.5 Thu 17:15 HSZ/AUDI

The complex interplay between democracy and platform power — •Philipp Lorenz-Spreen — Center Synergy of Systems, TU Dresden, Germany

Information and communication technology has undergone dramatic developments over the last two decades. Increasing interconnectedness has led to more self-organized public debates, platforms and their algorithms have gained new power over discourse, and generative AI has made content fabrication easier than ever. But it has also given research new tools to quantify precisely these systemic changes. Detailed data from social media allows us to measure and model their network structures and dynamics. Against this background, we ask: What is really changing, what does science know about the connection between the crises of democracy and the worldwide use of digital and social media? A number of political behaviors appear to be influenced by the use of digital media, such as increasing polarization or declining trust in institutions. Our findings show that while there is agreement in the literature on some of the relationships, these vary across the world and, above all, the underlying mechanisms by which these dimensions are linked are still unknown. A better understanding of these systems is critical for civil society in democracies worldwide, and I will conclude with a methodological outlook on how we are currently trying to explore these missing puzzle pieces.

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Overview of Invited Talks and Sessions

(Lecture halls BAR/SCHÖ, BAR/0205, and BAR/0106; Poster P2 and P5)

Invited Talks

BP 1.7	Mon	11:15–11:45	BAR/SCHÖ	**Modeling and inference of magnetotactic motility in complex environments** — •Stefan Klumpp
BP 3.1	Mon	9:30–10:00	BAR/0205	**The unreasonable effectiveness of computational models in biological patterning and morphogenesis** — •Michel Milinkovitch
BP 4.1	Mon	15:00–15:30	BAR/SCHÖ	**The Multi-faceted Role of Cholesterol in Cellular Membranes and Lipid Nanoparticles** — •Rainer Böckmann
BP 8.3	Mon	17:15–17:45	BAR/0106	**Constructing synthetic life-like vesicle systems by integration of artificial metabolic reaction networks** — •Laura Heinen
BP 9.1	Mon	16:45–17:15	BAR/0205	**Breaking the photobleaching limit in single-molecule FRET with nanophotonic DyeCycling.** — Benjamin Vermeer, Dong Hoon Shin, Alexander Vogel, Fabian Zundel, Sabina Caneva, •Sonja Schmid
BP 11.7	Tue	11:15–11:45	BAR/0106	**Physics of bacterial adhesion: heterogeneity, patchiness, and surface interactions** — •Karin Jacobs
BP 12.1	Tue	9:30–10:00	BAR/0205	**Tuning the Tracks: Functional Diversity Encoded in Microtubule Lattice States** — •Lukas Kapitein
BP 16.1	Wed	9:30–10:00	BAR/0205	**Illuminating mitochondrial permeabilisation in apoptosis** — •Ana J. Garcia Saez
BP 18.1	Wed	10:30–11:00	BAR/0106	**Protein complex structure prediction, state-of-the-art and challenges** — •Ezgi Karaca
BP 18.4	Wed	11:45–12:15	BAR/0106	**From Sparse Restraints to All-Atom Models: Integrative Reconstruction of Hidden GPCR Conformations** — •Matthias Elgeti
BP 20.4	Wed	15:45–16:15	BAR/0106	**Solution scattering and MD simulation as quantitative probes of protein-specific and temperature-dependent hydration** — •Jochen S Hub
BP 21.1	Wed	15:00–15:30	HÜL/S386	**Microbial Behavior in Context** — •Fernanda Pinheiro
BP 21.4	Wed	16:15–16:45	HÜL/S386	**The navigability of fitness landscapes shaped by global and universal epistasis** — •Joachim Krug
BP 26.7	Thu	11:15–11:45	BAR/SCHÖ	**Directed evolution of material-producing bacteria** — •André Studart
BP 27.1	Thu	9:30–10:00	BAR/0205	**Tissue interplay and the coordination of morphogenesis** — •Elias Barriga
BP 30.1	Thu	10:15–10:45	BAR/0106	**Mechanogenetics for Cell ImmunoTherapy** — •Yingxiao Wang
BP 30.4	Thu	11:30–12:00	BAR/0106	**Recent theoretical progress on sound-propelled microsystems** — •Raphael Wittkowski
BP 33.1	Thu	15:00–15:30	BAR/0205	**Expanding the Bag of Optical Tricks for (Neuro)Biology** — •Fabian F. Voigt
BP 36.1	Fri	9:30–10:00	BAR/SCHÖ	**Swimming in complex environments** — •Christina Kurzthaler
BP 41.1	Fri	11:30–12:00	BAR/0205	**Probing spatiotemportal electrochemical dynamics on single bacterial cells** — Anaïs Biquet-Bisquert, Baptiste Carrio, Nathan Meyer, Thales Fernandes, Manouk Abkarian, Farida Seduk, Axel Magalon, •Ashley Nord, Francesco Pedaci

Invited Talks of the joint Symposium SKM Dissertation Prize 2026 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	HSZ/0002	**Stochastic-Calculus Approach to Non-equilibrium Statistical Physics** — •Cai Dieball
SYSD 1.2	Mon	10:00–10:30	HSZ/0002	**Nonuniform magnetic spin textures for sensing, storage and computing applications** — •Sabri Koraltan
SYSD 1.3	Mon	10:30–11:00	HSZ/0002	**Anomalous Quantum Oscillations beyond Onsager's Fermi Surface Paradigm** — •Valentin Leeb
SYSD 1.4	Mon	11:00–11:30	HSZ/0002	**Coherent Control Schemes for Semiconductor Quantum Systems** — •Eva Schöll
SYSD 1.5	Mon	11:30–12:00	HSZ/0002	**On stochastic thermodynamics under incomplete information: Thermodynamic inference from Markovian events** — •Jann van der Meer

Invited Talks of the joint Symposium The Sustainability Challenge: A Decade of Transformation (SYSC)

See SYSC for the full program of the symposium.

SYSC 1.1	Mon	15:00–15:30	HSZ/AUDI	**Open-Endedness and Community-Based Approaches to Sustainability Challenges** — •Hiroki Sayama
SYSC 1.2	Mon	15:30–16:00	HSZ/AUDI	**Education as a Social Tipping Element: Evidence from Climate and Physics Education Research** — •Thomas Schubatzky
SYSC 1.3	Mon	16:00–16:30	HSZ/AUDI	**Mechanistic and Material Perspectives on Enzymatic Hydrolysis of Semicrystalline Polyesters** — •Birte Höcker
SYSC 1.4	Mon	16:45–17:15	HSZ/AUDI	**Decarbonization Options for Industry** — •Uwe Riedel
SYSC 1.5	Mon	17:15–17:45	HSZ/AUDI	**Impacts of Cosmic Dust and Space Debris in the Terrestrial Atmosphere** — •John Plane

Invited Talks of the joint Symposium France: Soft, Active and Alive: Emergent Properties in Living Matter (SYGF)

See SYGF for the full program of the symposium.

SYGF 1.1	Wed	15:00–15:30	HSZ/AUDI	**Liquid crystal geometries in type I collagen-based tissues** — •Nadine Nassif
SYGF 1.2	Wed	15:30–16:00	HSZ/AUDI	**Self-organization of the cytoplasm by physical instabilities** — •Jan Brugues
SYGF 1.3	Wed	16:00–16:30	HSZ/AUDI	**From morphogenesis to space partitioning by microtubules and molecular motors.** — •Manuel Thery
SYGF 1.4	Wed	16:45–17:15	HSZ/AUDI	**More than the sum: how composite interfaces govern function** — •Alba Diz-Muñoz
SYGF 1.5	Wed	17:15–17:45	HSZ/AUDI	**Swimming and Swarming of Intelligent Active Particles** — Segun Goh, Priyanka Iyer, Rajendra Singh Negi, •Gerhard Gompper
SYGF 1.6	Wed	17:45–18:15	HSZ/AUDI	**Perturbing the collective motion of fish with challenging environments** — •Aurélie Dupont

Invited Talks of the joint Symposium AI and Data Challenges behind Emerging Self-Driving Laboratories (SYAI)

See SYAI for the full program of the symposium.

SYAI 1.1	Thu	9:30–10:00	HSZ/AUDI	**Data and Experimental Foundations for Reliable Self-Driving Laboratories** — •Dr. Marcus Tze-Kiat Ng
SYAI 1.2	Thu	10:00–10:30	HSZ/AUDI	**Digital Catalysis - AI for Experiment Planning and Control** — •Christoph Scheurer
SYAI 1.3	Thu	10:30–11:00	HSZ/AUDI	**Autonomous, Data-Driven Workflows for Materials Acceleration Platforms with pyiron** — •Jan Janssen, Joerg Neugebauer
SYAI 1.4	Thu	11:15–11:45	HSZ/AUDI	**Machine Learning for Autonomous Optimization and Discovery of Materials** — •Pascal Friederich
SYAI 1.5	Thu	11:45–12:15	HSZ/AUDI	**Transforming Our View on Transformers in the Sciences** — •Kevin Maik Jablonka

Sessions

BP 1.1–1.11	Mon	9:30–12:45	BAR/SCHÖ	**Active Matter I (joint session BP/CPP/DY)**
BP 2.1–2.12	Mon	9:30–12:45	BAR/0106	**Computational Biophysics I**
BP 3.1–3.11	Mon	9:30–12:45	BAR/0205	**Tissue Mechanics I**
BP 4.1–4.5	Mon	15:00–16:30	BAR/SCHÖ	**Computational Biophysics II**
BP 5.1–5.6	Mon	15:00–16:30	BAR/0205	**Membranes, Vesicles and Synthetic Life-like Systems I**
BP 6.1–6.12	Mon	15:00–18:30	ZEU/0160	**Active Matter II (joint session DY/BP/CPP)**
BP 7.1–7.56	Mon	15:00–17:00	P5	**Poster Session I**
BP 8.1–8.6	Mon	16:45–18:30	BAR/0106	**Systems and Networks Biophysics**
BP 9.1–9.6	Mon	16:45–18:30	BAR/0205	**Single Molecule Biophysics**
BP 10.1–10.12	Tue	9:30–12:45	BAR/SCHÖ	**Active Matter III (joint session BP/CPP/DY)**
BP 11.1–11.11	Tue	9:30–12:45	BAR/0106	**Franco-German Session: Bacterial Biophysics I**
BP 12.1–12.11	Tue	9:30–12:45	BAR/0205	**Cytoskeleton I**
BP 13.1–13.5	Tue	14:00–15:30	ZEU/0160	**Active Matter IV (joint session DY/BP/CPP)**
BP 14.1–14.96	Tue	18:00–21:00	P2	**Poster Session II**
BP 15.1–15.11	Wed	9:30–12:45	BAR/SCHÖ	**Computational Biophysics III**
BP 16.1–16.11	Wed	9:30–12:45	BAR/0205	**Membranes, Vesicles and Synthetic Life-like Systems II**
BP 17.1–17.12	Wed	9:30–12:45	ZEU/0114	**Statistical Physics of Biological Systems I (joint session DY/BP)**
BP 18.1–18.6	Wed	10:30–12:45	BAR/0106	**Focus session: Integrative Structural Modeling**
BP 19.1–19.1	Wed	11:45–12:45	ZEU/LICH	**Round Table Discussion: The Future of Neutrons in France and Germany (joint session CPP/BP)**
BP 20.1–20.9	Wed	15:00–17:45	BAR/0106	**Protein Structure and Dynamics**
BP 21.1–21.7	Wed	15:00–17:30	HÜL/S386	**Focus Session: Sequence Spaces, Populations and Evolution**
BP 22.1–22.5	Wed	15:00–16:30	ZEU/0114	**Statistical Physics of Biological Systems II (joint session DY/BP)**
BP 23.1–23.6	Wed	15:00–16:45	ZEU/0255	**Biopolymers, Biomaterials and Bioinspired Functional Materials I (joint session CPP/BP)**
BP 24.1–24.7	Wed	17:00–18:45	ZEU/0255	**Biopolymers, Biomaterials and Bioinspired Functional Materials II (joint session CPP/BP)**
BP 25	Wed	18:30–20:00	BAR/0205	**Members' Assembly**
BP 26.1–26.11	Thu	9:30–12:45	BAR/SCHÖ	**Biomaterials and Biopolymers (joint session BP/CPP)**
BP 27.1–27.11	Thu	9:30–12:45	BAR/0205	**Cell Mechanics I**
BP 28.1–28.11	Thu	9:30–12:45	ZEU/0160	**Active Matter V (joint session DY/BP)**
BP 29.1–29.6	Thu	9:30–11:15	ZEU/0260	**Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates I (joint session CPP/BP)**
BP 30.1–30.7	Thu	10:15–12:45	BAR/0106	**Focus Session: Controlling Microparticles and Biological Cells by Ultrasound (joint session BP/CPP/DY)**
BP 31.1–31.5	Thu	11:30–12:45	ZEU/0260	**Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates II (joint session CPP/BP)**
BP 32.1–32.12	Thu	15:00–18:15	BAR/SCHÖ	**Statistical Physics of Biological Systems III (joint session BP/DY)**
BP 33.1–33.12	Thu	15:00–18:30	BAR/0205	**Bioimaging**
BP 34.1–34.8	Thu	15:00–18:00	ZEU/0160	**Focus Session: Emergent Transport in Active Systems (joint session DY/BP)**
BP 35.1–35.5	Thu	15:15–17:45	ZEU/LICH	**Focus Session: 75 Years Division Polymer Physics: From Curiosity to Smart Materials (joint session CPP/BP)**
BP 36.1–36.11	Fri	9:30–12:45	BAR/SCHÖ	**Statistical Physics of Biological Systems IV (joint session BP/DY)**
BP 37.1–37.12	Fri	9:30–12:45	BAR/0106	**Tissue Mechanics II**
BP 38.1–38.9	Fri	9:30–12:15	ZEU/0160	**Active Matter VI (joint session DY/BP)**
BP 39.1–39.6	Fri	9:30–11:15	ZEU/0260	**Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates III (joint session CPP/BP)**
BP 40.1–40.5	Fri	10:00–11:15	BAR/0205	**Cell Mechanics II / Cytoskeleton II**
BP 41.1–41.4	Fri	11:30–12:45	BAR/0205	**Franco-German Session: Bacterial Biophysics II**
BP 42.1–42.1	Fri	13:15–14:00	HSZ/0002	**Closing Talk (joint session CPP/BP/DY)**

Members' Assembly of the Biological Physics Division

Wednesday 18:30–20:00 BAR/0205

- Report
- Elections
- Miscellaneous

Sessions

– Invited, Topical, Contributed Talks, Discussions, and Posters –

BP 1: Active Matter I (joint session BP/CPP/DY)

Time: Monday 9:30–12:45 Location: BAR/SCHÖ

BP 1.1 Mon 9:30 BAR/SCHÖ

Bayesian inference of magnetosensing in a magnetotactic bacterium — •Sascha Lambert[1], Emilie Gachon[2], Damien Faivre[2], and Stefan Klumpp[1] — [1]University of Göttingen, Institute for the Dynamics of Complex Systems, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany. — [2]Aix Marseille Université, CEA, CNRS, BIAM, 13115 Saint-Paul-Lez-Durance, France.

Magnetotactic bacteria are often assumed to align only passively with external magnetic fields, yet recent observations of the magnetotactic bacterium SS-5 reveal a pronounced increase in swimming speed under geomagnetic conditions. Because flagellated microorganisms typically follow helical paths, magnetic torques could, in principle, straighten their trajectories and create an apparent increase in speed, offering a purely mechanical explanation. We test this hypothesis using a physical swimming model based on Active Brownian Particles that incorporates magnetic torques, rotational propulsion, and helical motion, and we explore the relevant parameter space using Bayesian inference constrained by three-dimensional trajectory data. Posterior predictive simulations demonstrate that the mechanically induced increase in apparent speed is far too small to account for the experimental observations, even under extreme parameter choices. The results quantitatively rule out swaying as a sufficient explanation for the behaviour of SS-5 and instead support the presence of an active magnetic sensing mechanism.

BP 1.2 Mon 9:45 BAR/SCHÖ

Vorticity-induced surfing and trapping in porous media — •Pallabi Das[1], Mirko Residori[1], Axel Voigt[2,3,4], Suvendu Mandal[5], and Christina Kurzthaler[1,3,4] — [1]Max Planck Institute for the Physics of Complex Systems, Germany — [2]Institute of Scientific Computing, TU Dresden, Germany — [3]Center for Systems Biology Dresden, Germany — [4]Cluster of Excellence, Physics of Life, TU Dresden, Germany — [5]TU Darmstadt, Germany

Microorganisms often encounter strong confinement and complex hydrodynamic flows while navigating their habitats. Combining finite-element methods and stochastic simulations, we study the interplay of active transport and heterogeneous flows in dense porous channels. We find that swimming always slows down the traversal of agents across the channel, giving rise to robust power-law tails of their exit-time distributions. These exit-time distributions collapse onto a universal master curve with a scaling exponent of $\approx 3/2$ across a wide range of packing fractions and motility parameters, which can be rationalized by a scaling relation. We further identify a new motility pattern where agents alternate between *trapping* along fast streams and extended *surfing* phases, the latter determining the power-law exponent. Unexpectedly, trapping occurs in the flow backbone itself – not only at obstacle boundaries – due to vorticity-induced reorientation in the highly-heterogeneous flow environment. These findings provide a fundamentally new active transport mechanism with direct implications for biofilm clogging and the design of novel microrobots capable of operating in heterogeneous media.

BP 1.3 Mon 10:00 BAR/SCHÖ

Adhesion Patterns in Gliding Filamentous Cyanobacteria — •Elias Fischer[1], Paul Nieschwitz[2], Stefan Karpitschka[2], and Holger Stark[1] — [1]Institute of Physics and Astronomy, TU Berlin, Germany — [2]Department of Physics, Universität Konstanz, Germany

Filamentous cyanobacteria play an important role in many ecosystems and the carbon cycle of our planet. They exhibit gliding motility when in contact with solid surfaces or each other. Despite their ecological relevance and increased use in biotech applications, the exact nature of the force-generating process remains not fully understood.

Our recent measurements of filamentous cyanobacteria gliding across flat surfaces and visualized in kymographs show spatio-temporal adhesion regions along the filament, indicating an intrinsic helical shape. Based on our a novel approach for modeling the mechanical aspects of individual cyanobacteria filaments, we are able to interpret the complex kymograph patterns. Each filament is modeled as a helical chain of thin cylindrical segments in 3D with bending and twisting elasticity. The filaments interact with nearby surfaces and filaments via a hard-core repulsion and an exponentially decaying adhesion force. Importantly, the propulsion forces that push the filament forward are only applied locally at surface-contacting segments.

Our simulated kymographs reveal how both the helical shape and the adhesion strength strongly influence the filament's gliding speed and the dynamics of the surface-attachment regions. Thereby, we crucially contribute to the understanding of how real filamentous cyanobacteria generate their propulsion forces.

BP 1.4 Mon 10:15 BAR/SCHÖ

The 3D chirality of malaria parasites determines their motion patterns in 2D and originates at the apical pole — •Leon Lettermann[1], Mirko Singer[2], Smilla Steinbrück[2,3], Falko Ziebert[1], Sachie Kanatani[3], Photini Sinnis[3], Friedrich Frischknecht[2], and Ulrich Schwarz[1] — [1]Institute for Theoretical Physics & BioQuant, Heidelberg University — [2]Parasitology, Center for Infectious Diseases, Heidelberg University — [3]School of Public Health and Malaria Research Institute, Johns Hopkins University

Plasmodium sporozoites, the slender forms of the malaria parasite injected by mosquitoes into the skins of their vertebrate hosts, provide a medically highly relevant model system for active chiral particles. Using 3D tracking in synthetic hydrogels, we show that sporozoites consistently move on right-handed helical trajectories. When they encounter a two-dimensional substrate, they switch to clockwise circular motion, whereas circling on glass in medium occurs with the opposite sense of rotation, suggesting on glass they try to invade the medium above. Using a sandwich assay, we demonstrate that chirality also determines the reverse transition from two-dimensional to three-dimensional motion. Combining these measurements with a theory for gliding motility allows us to identify the likely origin of chirality, namely an asymmetric distribution of adhesins. After confirming this via two-sided traction force microscopy, we finally use STED super-resolution microscopy to reveal a corresponding tilt in the apical ring complex. In summary, our analysis thus uncovers both the biological relevance and the molecular basis of chirality in the movement of malaria parasites.

BP 1.5 Mon 10:30 BAR/SCHÖ

Squirmer dynamics in porous environments — •Mirko Residori[1], Christina Kurzthaler[1], and Sebastian Aland[2] — [1]Max Planck Institute for the Physics of Complex Systems — [2]TU Freiberg

We introduce a computational framework for simulating the dynamics of microswimmers in complex porous environments. Specifically, we adopt a diffusive domain approach to represent the surface of a micro-swimmer, modeled as a squirmer. This method ensures accurate and stable finite-element simulations, even in highly confined geometries. Validation against analytical and numerical benchmarks confirms the model*s accuracy and robustness. We then apply it to explore squirmer motion in heterogeneous porous media, revealing how hydrodynamic interactions lead to behaviors such as dynamic trapping due to hydro-dynamically induced re-orientations. Moreover, we demonstrate that the squirmer parameter and the repulsive potential critically influence a squirmer's ability to navigate and escape confinement. The proposed framework offers a versatile and efficient tool for studying active motion in complex fluids and provides new insights into micro-swimmer transport and control in natural and engineered systems.

BP 1.6 Mon 10:45 BAR/SCHÖ

Dynamics of passive tracers in active dumbbell suspension — •Chandranshu Tiwari and Sunil P. Singh — Department of Physics, Indian Institute of Science Education and Research, Bhopal 462066, India.

The transport of passive tracers in active fluids exhibits rich dynamics arising from persistent interactions between active agents and the tracer. In our work, we employ Brownian dynamics simulations to investigate the dynamical behaviour of both isotropic(circular) and anisotropic(elliptical) tracers in active dumbbell suspension, considering only steric interactions. For circular tracers, we find that the speed shows a crossover from monotonically decreasing to increasing with tracer size as the dumbbells' speed is increased. The tracer's effective diffusion also displays a non-monotonic dependence on area fraction: the diffusivity first increases and then decreases at higher area fractions.

For anisotropic tracers, the characteristic non-monotonic trend persists. Moreover, their motion along the major and minor axes differs significantly. Anisotropic accumulation of active particles around the tracer generates direction-dependent forces and fluctuations, favouring motion along the major axis. Consequently, both the speed and diffusivity along the major axis exceed those along the minor axis.

15 min. break

Invited Talk BP 1.7 Mon 11:15 BAR/SCHÖ

Modeling and inference of magnetotactic motility in complex environments — •Stefan Klumpp — Institute for the Dynamics of Complex Systems, University of Göttingen, Göttingen, Germany

Magnetotactic bacteria orient themselves and swim along field lines of the geomagnetic field. Their magnetically directed self-propelled motion makes them an instance of dipolar active matter. Here we focus on the interaction of these bacteria with walls or obstacles. Experiments in microfluidic systems show that interactions with walls result in (possibly transient) alignment parallel to the wall, which may compete with the alignment with the magnetic field. The dynamic behavior arising from the competition of the two alignments includes U-turn trajectories in circular chambers and trapping and escape dynamics in channels with overlapping cylindrical obstacles. In a phenomenological picture, the resulting motion can be described in an Active Brownian Particle model by introducing a wall torque that competes with the magnetic torque, which results in good agreement with experimental observations. Systematic Bayesian inference of the wall torque from observations shows that only a part of the torque function (dependence on incident angle) can be learned reliably from the data.

BP 1.8 Mon 11:45 BAR/SCHÖ

Quantifying aggregation behaviour of filamentous cyanobacteria — •Elias Illing and Stefan Karpitschka — Fachbereich Physik, Universität Konstanz

Cyanobacteria are ubiquitous in nature, frequently causing ecological and economic harm by explosive growth, so called blooms.

We investigate the collective dynamics of entangled filamentous cyanobacteria in open liquid media, reminiscent of their aggregates found during later stages of blooms. We investigate the impact of illumination on the clustering and spreading of the bacteria and quantify the morphology of the bacterial aggregates by image analysis. We determine the critical density necessary for initial clustering and track the evolution of the subsequent stages, ranging from stable clusters to spreading mats. These states can be modulated by light intensity variations, potentially allowing for control of the morphological evolution of cyanobacterial aggregates.

BP 1.9 Mon 12:00 BAR/SCHÖ

Dynamically Induced Spatial Segregation in Multi-Species Bacterial Bioconvection — •Mingqi Yan[1,2], Chenxi Wang[3], Oscar Gallardo-Navarro[4], Rinat Arbel-Goren[4], Joel Stavans[4], and Erwin Frey[1,2] — [1]Department of Physics, Ludwig-Maximilians-Universität München, Theresienstraße 37, 80333 München, Germany — [2]Max Planck School Matter to Life, Hofgartenstraße 8, 80539, München, Germany — [3]School of Science, Harbin Institute of Technology, 518055, Shenzhen, China — [4]Department of Physics of Complex Systems, Weizmann Institute of Science, 7610001, Rehovot, Israel

Bacterial bioconvection is a classic example of collective behavior in active matter, where upward-swimming bacteria create density instabilities leading to large-scale fluid flows. While this phenomenon is well-studied in single-species suspensions, natural environments are typically inhabited by diverse microbial communities. Here, we investigate the collective dynamics of multi-species bacterial suspensions. Combining experiments with a continum model, we show that different bacterial species can spontaneously segregate into stable, spatially interlocked domains. Our theoretical analysis reveals that this segregation is not driven by biochemical antagonism but rather by the interplay between species-specific motility characteristics and the self-generated hydrodynamic flows. This work provides new insights into how physical interactions alone can drive the spatial organization of complex microbial communities.

BP 1.10 Mon 12:15 BAR/SCHÖ

Light-switchable microbial rafts at air-liquid interfaces — •Gustav F. Nolte, Alexandros A. Fragkopoulos, Timo Völkl, Mechthild Rappold, and Oliver Bäumchen — University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany

In biological active matter, clustering occurs across a wide range of time and length scales, from molecular assemblies such as actomyosin networks to macroscopic systems like fire ant rafts. Here, we report on a fast, light-switchable, and fully reversible clustering phenotype on the microscale, observed at air-liquid interfaces: the raft formation of the biciliated microalga *Chlamydomonas noctigama*.

C. noctigama is a relative of the model organism *Chlamydomonas reinhardtii*, which exhibits light-switchable adhesion and subsequent clustering at solid-liquid interfaces [1,2]. We show how the cluster morphology depends on cell density and discuss potential growth mechanisms by analyzing dynamics of individual clusters. Furthermore, we characterize the dependence of raft formation on the light spectrum and interfacial free energy. Using micropipette force spectroscopy [3], we show that single cells exploit capillary forces for light-switchable ciliary adhesion to the air-liquid interface, enabling raft formation. In their natural habitats, reversible clustering may provide an advantage by allowing cells to accumulate in locations optimal for photosynthesis while increasing resilience to environmental stress.

[1] C. T. Kreis, et al., *Nat. Phys.* **14**, 45 (2018).
[2] S. Till, et al., *Phy. Rev. Res.* **4**, L042046 (2022).
[3] M. Backholm and O. Bäumchen, *Nat. Protoc.* **14**, 594-615 (2019).

BP 1.11 Mon 12:30 BAR/SCHÖ

Circadian gravitaxis: Photosynthetic microswimmers remodel local pH to actively tune vertical migration — Arkajyoti Ghoshal[1], Soumitree Mishra[1], Jayabrata Dhar[2], Hans-Peter Grossart[3,4], and •Anupam Sengupta[1,5] — [1]Physics of Living Matter, Department of Physics and Materials Science, University of Luxembourg, Luxembourg — [2]Department of Mechanical Engineering, National Institute of Technology Durgapur, India — [3]Department of Plankton and Microbial Ecology, Leibniz Institute of Freshwater Ecology and Inland Fisheries, Stechlin, Germany — [4]Institute of Biochemistry and Biology, Potsdam University, Germany — [5]Institute for Advanced Studies, University of Luxembourg, Luxembourg

Motile phytoplankton shuttle between bright surface waters and deeper nutrient rich layers, usually controlled by internal circadian clocks. Yet many species show irregular movements, defying the expected circadian rhythm. Studying a bloom forming photosynthetic species, we found that cells adjust their vertical migration by altering local pH, mediated by a shift in their gravitactic behavior. This self-modulation of pH generates sub-populations which are physiologically similar but swim differently, remaining vertically separated even under uniform conditions. Supported by a cell-level analysis and mathematical model, we confirm that the pH-mediated circadian shift is underpinned by morphological adjustments. Our results support a circadian gravitactic model in which diurnal pH control drives diversified migration, enhancing fitness particularly in acidifying oceans.

BP 2: Computational Biophysics I

Time: Monday 9:30–12:45 Location: BAR/0106

BP 2.1 Mon 9:30 BAR/0106

Topology driven spatial organization of DNA-polymers in geometric confinement — •Debarshi Mitra[1], Shreerang Pande[2], and Apratim Chatterji[2] — [1]Leibniz Institute of Polymer Research Dresden, Hohe Strasse 6, 01069 Dresden, Germany — [2]Dept. of Physics, Indian Institute of Science, Education and Research-Pune (IISER-Pune), India-411008

The mechanism of chromosome segregation and organization in the bacterial cell cycle is one of its least understood aspects. The bacterial chromosome is often modeled as a bead spring ring polymer. We introduce cross-links in the DNA-ring polymer, resulting in the formation of loops within each replicating bacterial chromosome. We use simulations to show that the chosen polymer-topology ensures its self-organization along the cell long-axis, such that various chromosomal loci get spatially localized as seen in-vivo, in various growth conditions [1,2]. The organization arises only due to entropic repulsion between polymer loops of each daughter chromosome. We also reconcile observations from complementary experimental techniques probing the organization of the chromosome [1]. We further establish organizational principles for topologically modified polymers in various kinds of geometric confinement and discuss possible relevance to eukaryotic chromosomes.

[1] Debarshi Mitra Shreerang Pande, Apratim Chatterji. Soft Matter, 2022.
[2] Shreerang Pande, Debarshi Mitra, and Apratim Chatterji. Phys. Rev. E, 110(5), November 2024.

BP 2.2 Mon 9:45 BAR/0106

An extended boundary integral method for viscoelastic cells — •Thomas Mayr and Stephan Gekle — University Bayreuth, Bayreuth, Germany

The boundary integral method is a powerful method for modeling soft objects such as capsules, vesicles or red blood cells in flows at low Reynolds numbers. The beauty of this method lies in its effective two-dimensional description of the boundaries making fluid-structure interaction simple in comparison to other methods. So far, the boundary integral method is restricted to cells with a viscoelastic membrane and a purely viscous interior, whereas most biological cells contain a complex cytoskeleton and a nucleus in addition to their membrane. Here, we develop an extended three-dimensional boundary integral method, that can handle such cells, which are treated as a homogeneous viscoelastic material surrounded by a viscoelastic membrane. We use our method to study systematically the influence of bulk and membrane viscoelasticity on the dynamics of a cell in shear flow closely corresponding to recent experiments [1].

[1] Gerum et al., Elife 11, e78823 (2022)

BP 2.3 Mon 10:00 BAR/0106

Synchronization of both microtubule ends facilitates robust spindle length control — •Shane Fiorenza[1], Sheba Cheeran[2], Elena Doria[2], Iva Tolić[3], Patrick Meraldi[2], and Nenad Pavin[1] — [1]Faculty of Science, University of

Zagreb — [2]Faculty of Medicine, University of Geneva — [3]Rudjer Bošković Institute, Zagreb

The mitotic spindle is a biomechanical structure that relies on a well-controlled geometry to accurately segregate genetic material, and so the mechanisms responsible for setting spindle length have been extensively studied both in vivo and in vitro. One of these myriad mechanisms, microtubule poleward flux, has proven difficult to characterize, with experiments showing that decreasing poleward flux can lead to spindle length increasing, decreasing, or remaining constant. How the spindle regulates its length and the role of poleward flux in this process remains unclear. Here we show that length-dependent regulation at both microtubule ends constitutes a fundamental mechanism of spindle length control through poleward flux. Our model demonstrates that length-dependent mechanisms at both microtubule ends allow plus- and minus-end dynamics to synchronize with one another, resulting in perturbations at either end having opposite effects on poleward flux for increasing spindle size. We predict that spindle length and poleward flux can be uncoupled via simultaneous perturbations, which we confirm with in vivo depletion experiments of KIF18A, KIF2A, and KATNB1 proteins. Our results provide a new way of understanding spindle length control and resolve a long-standing paradox of how poleward flux relates to spindle length.

BP 2.4 Mon 10:15 BAR/0106

A coarse-grained model for investigating the ejection of dsDNA from a viral capsid — •Adrian John Pinto[1], Klara Strobl[2], Carmen San Martin[3], Mar Alcazar Hutardo[2], Paul van der Schoot[4], Pedro J. de Pablo[2], Horacio V. Guzman[5], and Peter Virnau[1] — [1]Institute of Physics, JGU, Mainz, Germany — [2]Autonomous University of Madrid, Madrid, Spain — [3]Spanish National Center for Biotechnology, Madrid, Spain — [4]Eindhoven University of Technology, Eindhoven, Netherlands — [5]Institute of Material Science of Barcelona, Barcelona, Spain

Viruses are microscopic infectious agents that hijack the metabolic machinery of their hosts to replicate. They consist of genetic material, DNA for adenovirus, enclosed within a protein shell called a capsid. Adenoviruses are associated with respiratory diseases, gastroenteritis, conjunctivitis, and urinary tract infections. In this work, we investigate the denaturation of the viral capsid in the presence of urea as a chemical denaturant and analyze how increasing urea concentration affects capsid stability. To model the experimental system in simulations, we propose a coarse-grained representation of viral DNA based on a Kratky-Porod chain, which allows us to incorporate solvent conditions and obtain realistic length scales. Additionally, we model the capsid as a spherical confinement composed of discrete beads and introduce openings of various sizes to map changes in urea concentration to the simulation environment. Our findings indicate that the lag time observed in intensity curves can be explained by differences between partial and complete capsid opening.

BP 2.5 Mon 10:30 BAR/0106

Multi-Scale Computational Framework for Modeling Metabolic Pathways — •Miljan Dašić, Ashwathi Poolamanna, Mehrnoosh Khodam Hazrati, and Štěpán Timr — J. Heyrovský Institute of Physical Chemistry of the Czech Academy of Sciences, Dolejškova 2155/3, 182 00 Prague 8, Czech Republic

Spatial organization of enzymes (clustering, assemblies, and substrate channeling) has been increasingly recognized as a key determinant of metabolic efficiency. Recent studies suggest that non-specific enzyme-substrate interactions and molecular crowding can further impact the performance of metabolic pathways. However, the combined effect of these factors remains insufficiently quantified.

To address this gap, we developed a multi-scale computational framework connecting molecular-level enzyme-substrate interactions with emergent pathway-level kinetics. We first perform extensive coarse-grained Molecular Dynamics (MD) simulations with LAMMPS to quantify substrate transition kinetics at varying crowding levels. Resulting trajectories are analyzed using Markov State Models (MSMs) to extract the relevant states and transition rates. These kinetic parameters are then used to parameterize stochastic Reaction-Diffusion (RD) simulations in Smoldyn, enabling the study of large enzyme assemblies, different reaction orders, and multi-step metabolic pathways.

Our results reveal how molecular interaction strengths, crowding conditions as well as enzyme spatial organization impact pathway efficiency across scales: from nanometers and nanoseconds (MD) to micrometers and seconds (RD).

BP 2.6 Mon 10:45 BAR/0106

Coexistence in competition for shared resources with fluctuating fitness — •Angelique Burdinski and Dirk Brockmann — Center Synergy of Systems (Synosys), TUD Dresden University of Technology, 01069, Dresden, Germany

Understanding how species coexist in competitive scenarios has long been a central question in ecology and evolution. The contradiction between the competitive exclusion principle and the observed diversity of species has puzzled researchers for decades. Fluctuating environmental factors that selectively change species fitness have been proposed to stabilize coexistence, but theoretical results remain inconclusive. How competitive forces and temporal variability shape evolutionary outcomes remains debated, with model-specific results and few universal insights. We compare species dynamics under two generic but qualitatively different mechanisms. One model captures direct competition via the standard replicator equation; the other represents a consumer-resource system, yielding the adjusted replicator model. Under uniform fitness, both show identical asymptotics, diverging sharply when fitness fluctuates. The standard replicator leads to quasi-fixation of a single species, whereas the adjusted replicator exhibits stable coexistence below a critical timescale. We derive coexistence bounds based on the mean and variance of fitness, showing that higher mean and lower variability favor fixation, while coexistence may persist even in disadvantaged situations. This contrast reflects direct versus indirect competition and supports coexistence as a generic outcome of shared-resource interactions in temporally varying environments.

15 min. break

BP 2.7 Mon 11:15 BAR/0106

Dielectric response of graphene and MoS_2 nanopores in the detection of single amino acids — •Longlong Li and Maria Fyta — Computational Biotechnology, RWTH Aachen University, Germany

Recent advances in two-dimensional (2D) material nanopores have opened new opportunities for biosensing with single-molecule precision. In this work, we investigate the interaction of single amino acids with graphene and MoS_2 nanopores using density-functional theory (DFT), combined with dielectric response calculations and non-equilibrium Green's function (NEGF) transport simulations. After identifying the most stable conformations of selected amino acids residing inside the nanopores, we calculate both the electronic transport and optical response of the nanopores in the absence and presence of these biomolecules. While electronic current-voltage characteristics reveal only modest amino-acid-dependent variations, the optical response, characterized by frequency-dependent dielectric functions and optical absorption spectra, exhibits distinct material-specific signatures. In particular, MoS_2 nanopores exhibit strong and broadband optical sensitivities, which are significantly larger than those of graphene and thus enable more distinct discrimination of single amino acids across multiple photon energies. Our simulations reveal an enhancement in the optical read-out of nanopores and an even stronger signals in the case of MoS_2 nanopores highlighting the possibility of a broadband optical detection for protein detection platforms and biosensors.

BP 2.8 Mon 11:30 BAR/0106

From Bioanalytics to Neuromorphic Computing: Graphite-Based Nanopores for Protein Sequencing and Iontronic Memristors — •Chandan K. Das and Maria Fyta — Computational Biotechnology, RWTH Aachen University, Worringerweg 3, 52074 Aachen, Germany

Protein sequencing with single amino acid resolution using ionic current signatures is a rapidly advancing technique, yet challenges persist in maintaining protein linearity and controlling their translocation through solid state nanopores. We introduce a graphite-based nanopore featuring a constriction inspired by alpha-hemolysin. All atom MD simulations show that the positively charged pore lumen promotes strong anion selectivity and drives electro-osmotic flow (EOF), which generates hydrodynamic drag opposing the electrophoretic force (EPF). Balancing these forces straightens proteins during translocation and increases their residence time within the constriction, substantially improving sequencing accuracy. This design enables detection of all 20 proteinogenic amino acids and their post-translational modifications. Beyond sequencing, the graphite-based architecture supports diverse iontronic applications. In a graphite-hydrogel-graphite nanofluidic memristor, a neutral hydrogel selectively traps cations, inducing ion concentration polarization. Simulations reveal characteristic memristive behavior, including a hysteretic current-voltage response. Overall, graphite nanopores offer a versatile platform for sequencing and neuromorphic computing.

BP 2.9 Mon 11:45 BAR/0106

Protein Translocation in Two Dimensional Nanopores from Molecular Dynamics and Free Energy Calculations — •Peijia Wei, Mayukh Kansari, Santiago López Páramo, and Maria Fyta — Computational Biotechnology, RWTH Aachen University, Worringerweg 3, 52074 Aachen, Germany

Nanopores, nanometer scale openings in materials, offer strong potential for ultra fast, cost effective and real time next generation sequencing technologies. These pores can electrophoretically drive charged biomolecules through and detect them. Using computer simulations, we compare two dimensional nanopores, graphene and MoS_2, to evaluate their effectiveness in protein detection. Protein translocation and dynamics are being controlled by varying the surrounding solvent, using both a typical monovalent salt solution and a molecular solution. Atomistic simulations assess the ability of each nanopore to thread proteins, on the basis of the ionic current signals through the pore. We also perform free energy calculations to quantify the thermodynamic factors that influence protein entry and passage through the pores. Our results show that graphene nanopores interact strongly with proteins, which hinders transloca-

tion under physiological conditions. This can be overcome by adding a denaturant that forms a hydrophilic and cation rich layer on the surface and enables linearized threading. In contrast, MoS_2 nanopores allow protein passage even in physiological solutions and offer inherent control of the translocation. By combining molecular dynamics with free energy analysis, we reveal how the complex interactions among all components shape translocation behavior.

BP 2.10 Mon 12:00 BAR/0106

Extending quantum-mechanical benchmark accuracy to biological ligand-pocket interactions — •Mirela Puleva[1], Leonardo Medrano Sandonas[2], Balázs D. Lorincz[3], Jorge Charry[4], David M. Rogers[5], Péter R. Nagy[3], and Alexandre Tkatchenko[1] — [1]University of Luxembourg, Luxembourg — [2]TUD Dresden University of Technology, Germany — [3]Budapest University of Technology and Economics, Hungary — [4]Luxembourg Researchers Hub asbl, Luxembourg — [5]Oak Ridge National Laboratory, USA

Predicting the binding affinity of ligands to protein pockets is key in the drug design pipeline, yet accurate capture of interactions in the flex- ible ligand-pocket motifs requires robust quantum-mechanical (QM) benchmarks, which are scarce. Disagreement between "gold standard" Coupled Cluster (CC) and Quantum Monte Carlo (QMC) methods further challenges large non-covalent benchmarks. We introduce the QUantum Interacting Dimer (QUID) benchmark framework modeling diverse ligand-pocket motifs. CC and QMC agree within 0.5 kcal/mol for QUID, which spans key non-covalent binding motifs and energetic contributions from symmetry-adapted perturbation theory. Benchmark results shows several dispersion-inclusive density functional ap- proximations predict energies accurately but differ in atomic van der Waals forces, while semiempirical and empirical methods need im- provements for non-covalent interactions (NCIs) in out-of-equilibrium geometries. With a wide span of NCIs, highly accurate interaction en- ergies, and further molecular properties, QUID goes beyond the "gold benchmark" QM benchmark of ligand-protein systems.

BP 2.11 Mon 12:15 BAR/0106

Insights into Quantum Decoherence in Biological Light Harvesting from First-Principles Simulations — Thomas Trepl, •Ingo Schelter, Johannes M. Foerster, and Stephan Kümmel — University of Bayreuth, Bayreuth, Germany

Photosynthesis is a fascinating process of outstanding importance since it provides the energy for most life on Earth. Considering the remarkable quantum efficiency with which the energy of absorbed photons is transferred in the initial light-harvesting step, there exists a long-standing speculation about the role of quantum coherence.

In this talk, I show the decoherence and localization of excitation energy that evolves from the coupled electron and nuclear dynamics in the B850 ring at room temperature after an initial Laser excitation as typically used in an experiment. The electron dynamics of the whole multichromophoric system is described by the real-time formulation of time-dependent density functional theory. The nuclear dynamics is treated by Ehrenfest dynamics, allowing for a non-adiabatic coupling between electrons and nuclei. The simulations show that nuclear dynamics starts to trigger quantum decoherence after only a few tens of femtoseconds.

BP 2.12 Mon 12:30 BAR/0106

Human breathing pattern dominates the effective diffusivity of droplets emitted while speaking — •Lars Natusch and Roland Netz — Fachbereich Physik, Forschungsgruppe Roland Netz, Freie Universität Berlin, Berlin, Germany

For understanding airborne viral infection pathways, the prediction of the effective diffusivity of saliva droplets emitted from a person while speaking and breathing is crucial.

In enclosed non-ventilated indoor spaces the diffusivity of tracer particles or molecules emitted by a person is governed by the complex interplay of various physical transport mechanisms. By comparison of lattice-based simulations of the three-dimensional compressible Navier-Stokes equation with experiments measuring the spreading of carbon-dioxide emitted from a person, we demonstrate that molecular diffusion and convection due to body heat and temperature gradients at walls and windows are present, but that the main spreading mechanism is related to the periodic breathing pattern of a person, which induces long-range advection.

Our results identify breathing as the dominant mechanism for particle transport in stagnant indoor air.

BP 3: Tissue Mechanics I

Time: Monday 9:30–12:45 Location: BAR/0205

Invited Talk BP 3.1 Mon 9:30 BAR/0205

The unreasonable effectiveness of computational models in biological patterning and morphogenesis — •Michel Milinkovitch — Dept. of Genetics & Evolution, University of Geneva, Geneva, Switzerland

I will discuss how vertebrate skin colours and skin appendages (scales, feathers, hairs) are spatially patterned through Turing and mechanical instabilities. First, I will show that Reaction-diffusion (RD) models are particularly effective for understanding skin colour patterning at the macroscopic scale, without the need to parametrise the profusion of variables at the microscopic scales. I suggest that the efficiency of RD is due to its intrinsic ability to exploit continuous colour states and the relations among growth, skin-scale geometries, and the (Turing) pattern intrinsic length scale. Second, I will show how drug treatments can permanently trigger transitions between scale appendage types or even between chemical and mechanical self-organisation. Third, I will show that a three-dimensional mechanical model, integrating growth and material properties of embryonic skin layers, captures most of the dynamics and steady-state pattern of head scales in crocodiles and tortoises. Fourth, I will show that the spectacular morphogenesis of the strongly overlapping snake scales can be recapitulated with a mechanical model integrating tissue plasticity and active material properties. These studies indicate that Biology, despite its 'messy' nature (with its unmanageable profusion of cellular and molecular variables) can be efficiently and quantitatively investigated mathematically, including with simple phenomenological models.

BP 3.2 Mon 10:00 BAR/0205

Mechano-chemical stabilisation of topological defects in an elasto-nematic sheet — •Suganthan Senthilkumar[1], Kinneret Keren[2], and Marko Popović[1,3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Technion-Israel Institute of Technology, Haifa, Israel — [3]Ruder Bošković Institute, Zagreb, Croatia

Self-organisation of patterns during animal development involves a complex interplay of various biophysical and biochemical mechanisms. A striking example is *Hydra*, where ordered arrays of nematic actin fibers give rise to orientational order on animal-scale with +1 topological defects at the head and foot of an adult animal. To study the nematic patterns observed during *Hydra* regeneration we recently proposed a mechano-chemical feedback loop that involves orientational order, tissue strain and morphogen gradients[1]. Here we develop a continuum formulation of the same feedback loop in 2d and show that it can stabilise aster shaped +1 topological defects in a self organised manner. We obtain a phase diagram for +1 defect stability using analytical calculations and compare it with vertex model simulations that employ the feedback loop. Finally, we calculate the correction to the mobility coefficient of the +1 defect due to the morphogen field associated with it.

1. Maroudas-Sacks *et al* Development, (February 2025) 152; doi: https://doi.org/10.1242/dev.204514

BP 3.3 Mon 10:15 BAR/0205

What jellyfish teach us about tissue mechanics and shape programming — •Anne Materne[1,2], Zhiqi Shen[1,2,3], Daniel Font-Martín[4], Vladislav Koren[5], Ulyana Shimanovich[5], Chiara Sinigaglia[4], and Carl D. Modes[1,2] — [1]MPI of Molecular Cell Biology and Genetics, Dresden, Germany — [2]Center for Systems Biology Dresden, Germany — [3]Southern University of Science and Technilogy, Shenzhen, China — [4]CNRS Languedoc-Roussillon, France — [5]Weizmann Institute of Science, Israel

Jellyfish are little-studied marine organisms with astounding regenerative capacities. Their rapid wound closure has been implicated to rely, at least partially, on the mechanical properties of the individual tissues in the jellyfish umbrella. In particular, this includes the mesoglea, a thick extracellular matrix structure essential for jellyfish shape and body function. Here, we model the mesoglea's role in wound closure using a coarse-grained spring lattice approach. In this way, we can capture essential material processes without knowledge of all molecular- and cellular-scale underpinnings. Our work shows that simple mesoglea pre-strain is sufficient to initiate closure in a broad spectrum of wound shapes. This finding is in line with previous experimental work in the hydrozoan jellyfish *Clytia hemisphaerica* and confirms the essential role of tissue mechanics in the life history of marine invertebrates. It will be interesting to explore this role more systematically in the future. Furthermore, our results presented here also provide unexpected insights for the field of 3D shape-programmable materials.

BP 3.4 Mon 10:30 BAR/0205

Apical extracellular matrix regulates fold morphogenesis in the Drosophila wing disc — •Vincenzo Maria Schimmenti[1], Jana F. Fuhrmann[2], Natalie A. Dye[3,4], and Marko Popovic[1] — [1]Max Planck Institute for Physics of Complex Systems, Dresden, Germany — [2]Aix Marseille Univ, CNRS, IBDM, Marseille, France — [3]Mechanobiology Institute, National University of Singapore,

Singapore — [4]Biomedical Engineering Department, National University of Singapore, Singapore

Tissue folding is a fundamental process in animal organ development. We investigate how fold shape and mechanics change during Drosophila wing disc morphogenesis, from larval stages (when folds deepen and grow) to early pupa, when the tissue unfolds into a bilayer. Using 3D apical surface segmentation, we introduce quantitative metrics for fold depth and width on a curved surface. We also identify a fibrous apical extracellular matrix (aECM) that physically links the two sides of each fold. A lateral vertex model with an adhesive aECM layer predicts that unfolding requires aECM removal. Genetic perturbations confirm that aECM adhesion stabilizes folds: its loss distorts fold shape and dynamics, while failure to remove it prevents unfolding. These perturbations produce adult wing defects, demonstrating that larval fold morphology influences adult wing shape. Together, our work highlights a central mechanical role for aECM in stabilizing epithelial folds during animal development.

BP 3.5 Mon 10:45 BAR/0205

Elastic coupling between nucleus and cell shape drives a mechanical transition in epithelial architecture — •Ian D. Estabrook[1], Anne Rosfelter[2], Yu-Chiun Wang[2], and Anna Erzberger[1] — [1]European Molecular Biology Laboratory (EMBL), Heidelberg, Germany — [2]RIKEN Center for Biosystems Dynamics Research, Kobe, Japan

As the largest organelle, the cell nucleus can affect the shape, spatial organisation and mechanics of cells in a variety of tissue contexts. Despite extensive studies on the molecular mechanisms underlying nuclear positioning and mechanics, it remains unclear whether the nucleus actively controls tissue architecture.

Here, we combine elasticity theory and the Drosophila blastoderm stage embryo as a generic experimental model to investigate the mechanical role of nuclei on epithelial organisation.

By developing a general method that integrates mechanical and geometrical properties extracted from imaging data, we show that from elastic coupling between nuclei and the cell surface, a mechanically driven phase transition emerges between simple columnar and pseudostratified tissue architectures. Genetic and optogenetic experimental perturbations provide evidence supporting such coupling and confirm the predicted transitions following changes in mechanical and geometric parameters.

Our work identifies a novel mechanical role of nuclear elasticity, independent of specialised machineries and may represent a general, generic mechanism controlling emergence of tissue level structures.

15 min. break

BP 3.6 Mon 11:15 BAR/0205

Mechanical regulation of neuroepithelial development — •Niklas Gampl[1,2], Alex Kingston[3], Caren Norden[4], and Kristian Franze[1,2,5] — [1]Max-Planck-Zentrum für Physik und Medizin, Erlangen, DE — [2]Medical Institute of Biophysics, FAU Erlangen-Nürnberg, DE — [3]Cambridge Stem Cell Institute, University of Cambridge, UK — [4]Gulbenkian Institute for Molecular Medicine, Oeiras, PT — [5]Department of PDN, University of Cambridge, UK

During embryonic development, initially flat neuroepithelial tissues remodel themselves into complex 3D structures such as the brain or retina. This process is driven by intrinsically generated forces that depend on the cells' mechanical environment. However, how accumulated tension in the tissue feeds back on individual cells to influence their fate or migration patterns is not well understood. To address this, we downregulated the cellular force sensor Piezo1 in zebrafish and *Xenopus laevis* embryos, thereby reducing local mechanosensing capabilities. Piezo1 downregulation led to impaired retinal lamination, deformed retinae and nuclear rounding. Additionally, live imaging of Piezo1-deficient zebrafish eye primordia revealed defects in retinal progenitor migration during optic cup morphogenesis. These finding suggest that Piezo1 activity contributes to coordinating force generation and tissue level tension in the developing neuroepithelium, thus leading to nuclear and tissue shape changes. Combining laser ablation to locally perturb force propagation with direct measurement of tissue tension will clarify how Piezo1-dependent mechanical feedback links nuclear shape, cell fate decisions and tissue morphogenesis.

BP 3.7 Mon 11:30 BAR/0205

Emergence of hyperuniform tiling in the developing retina — •Mehmet Can Ucar[1] and Sandra Siegert[2] — [1]University of Sheffield, Sheffield, UK — [2]Institute of Science and Technology Austria, Klosterneuburg, Austria

Efficient tiling and space-filling are fundamental design principles of living systems: from neurons and immune cells to vascular networks, these structures must optimize spatial coverage for proper function. Yet how cells collectively achieve non-redundant coverage during growth remains largely unexplored. Here, we combine a theoretical model of growing, branched cells with tunable local interactions and experimental analysis of developing retinal microglia. Our model shows that simple neighbor repulsion during growth is sufficient to drive non-redundant tiling, yielding a substantial increase in coverage with minimal territory overlap. Strikingly, this mechanism also leads to the emergence of a hyperuniform organization, where density fluctuations are progressively suppressed. Consistent with these predictions, microglia in the developing retina exhibit both efficient tiling and suppressed fluctuations, supporting the proposed mechanism for retinal patterning. Together, these findings reveal how local interactions can generate both efficient tiling and hyperuniform order, suggesting a general principle for tissue-wide optimization.

BP 3.8 Mon 11:45 BAR/0205

Reshaping morphogen gradients through porous tissue architecture — •Diana Khoromskaia[1,2], Mohit Dalwadi[4], and Zena Hadjivasiliou[2,3] — [1]Universität Münster, Germany — [2]Francis Crick Institute, London, UK — [3]University College London, UK — [4]University of Oxford, UK

The morphogenesis of tissues during embryonic development is controlled by concentration gradients of morphogens – signalling molecules whose readout determines cell fate decisions. How the spread of morphogens is affected in tissues with complex geometry and spatially heterogeneous architecture is not well understood. To address this question, we introduce a porous vertex model, by explicitly considering the network of extracellular spaces between the cells. Morphogens produced by source cells disperse through the tissue via three modes of transport: extracellular diffusion, membrane-bound diffusion, and cell-based transport through recycling. With this model we investigate how cell-scale geometry, such as cell size, cell shape anisotropy, and cell distance, influences effective diffusion and degradation of morphogens at tissue-scale, employing numerical and semi-analytical upscaling methods. A non-linear coupling between cell packing and morphogen concentration renders the morphogen gradient robust to perturbations by locally buffering fluctuations in the production. Our characterisation of tissues as active porous materials provides new insights into how morphogenesis and cell fate determination may interact during embryonic development.

BP 3.9 Mon 12:00 BAR/0205

Mechanics and hydraulics of the *C. elegans* germ line — •Chandraniva Guha Ray[1,2,3], Jonathan Jackson[2], Jonas Neipel[1,2,3], Julia Pfanzelter[2], Stephan W. Grill[2,3,4], and Pierre A. Haas[1,2,3] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Max Planck Institute of Molecular Cell Biology and Genetics — [3]Center for Systems Biology Dresden — [4]Cluster of Excellence Physics of Life, TU Dresden

In the cylindrical germ line of the nematode *Caenorhabditis elegans*, germ cells surround a tube called the rachis, to which all germ cells are connected via openings in the cells called rachis bridges. These rachis bridges allow exchange of cytoplasm between the rachis and the germ cells, which mature as they move towards the proximal end of the germ line where a hydraulic instability decides germ cell fate [1]. However, cortical contractility would collapse static germ cells by releasing their cytoplasm into the rachis through the rachis bridges. Here, we explain how the hydraulic flows in the germ line prevent this collapse and thus stabilise the germ line mechanically: We present a coarse-grained vertex model of a steady-state germ line that couples these hydraulic effects to cell mechanics. We compare the model to experimental observations and thus show how the interplay of fluid pumping and cell contractility can build a dynamically stable germ line.

[1] N. T. Chartier *et al.*, Nat. Phys. **17**, 920 (2021)

BP 3.10 Mon 12:15 BAR/0205

Hydrodynamic theory of two-dimensional human gastruloid development — •Oliver M. Drozdowski[1], Chloé Roffay[2], Sarah Jay[2], Diana Pinheiro[2], and Edouard Hannezo[1] — [1]Institute of Science and Technology Austria, Klosterneuburg, Austria — [2]Research Institute of Molecular Pathology, Vienna, Austria

Gastrulation is a crucial stage of embryonic development, as it entails the formation of the three germ layers. Two-dimensional in-vitro systems derived from human embryonic stem cells, so-called gastruloid discs, recapitulate the underlying patterning mechanisms, resulting in the formation of concentric rings of extraembryonic amnion-like cells at the edge and the three germ layers. Starting from experimental data of flattening amnion-like cells at the gastruloid edge, we developed a cross-sectional bubbly vertex model to describe the observed columnar to squamous transition. In agreement with experimentally measured morphometrics and mechanical properties, cell flattening is shown to be driven by local active wetting. Since gastruloids display fluid-like tissue properties, we developed a hydrodynamic description of the tissue-scale dynamics derived from the vertex model. This model predicts a gastruloid morphology consistent with experimental observations, suggesting that local cellular mechanics contribute to human gastruloid shape dynamics.

BP 3.11 Mon 12:30 BAR/0205

A mechanical origin for implantation defects in embryos from aged females — Kate E. Cavanaugh[1,2], •Maria-Jose Franco-Oñate[3,4], Diana J. Laird[5], Patrick W. Oakes[6], Ricard Alert[3,4,7], and Orion D. Weiner[1,2] — [1]Cardiovascular Research Institute, University of California, San Francisco, USA — [2]Department of Biochemistry and Biophysics, University of California, San Francisco, USA — [3]Max Planck Institute for the Physics of Complex Sys-

tems, Dresden, Germany — [4]Center for Systems Biology Dresden, Germany — [5]Department of Obstetrics, Gynecology, and Reproductive Sciences, University of California, San Francisco, USA — [6]Department of Cell and Molecular Physiology, Loyola University Chicago Stritch School of Medicine, IL USA — [7]Cluster of Excellence Physics of Life, TU Dresden, Germany

Women over 35 experience reduced fertility, linked to impaired embryo implantation. In mouse embryos from aged mothers, we observe defective spreading of the extra-embryonic tissue. To uncover the mechanism, we use a continuum model that treats the tissue as a droplet of active polar fluid. Fitting the model to experimental data shows that increased tissue surface tension and viscosity in aged embryos account for the impaired spreading. Experimental measurements of forces and spreading dynamics confirm that these mechanical changes are sufficient to explain the implantation defect. This work shows how physical modeling of embryo mechanics can quantitatively predict implantation success and guide embryo selection in Assisted Reproductive Technologies.

BP 4: Computational Biophysics II

Time: Monday 15:00–16:30 Location: BAR/SCHÖ

Invited Talk BP 4.1 Mon 15:00 BAR/SCHÖ

The Multi-faceted Role of Cholesterol in Cellular Membranes and Lipid Nanoparticles — •Rainer Böckmann — Computational Biology - Theoretical & Computational Membrane Biophysics, Friedrich-Alexander-Universität Erlangen-Nürnberg

Cellular membranes serve as dynamic interfaces regulating numerous biological processes, with cholesterol playing a central role in shaping their structure, dynamics, and function. Likewise, cholesterol is crucial for stabilizing lipid nanoparticles (LNPs) in pharmaceutical applications and for enhancing their therapeutic efficacy. Here, we elucidate the multifaceted functions of cholesterol in both biological membranes and LNPs using atomistic molecular dynamics simulations, including constant-pH approaches.

Our findings challenge conventional views of membrane organization by revealing that thermal membrane bending and local cholesterol distribution can collaborate to soften membranes [1], even though cholesterol is widely associated with membrane thickening and reduced permeability. Turning to lipid nanoparticles, we demonstrate that cholesterol is significantly enriched in the LNP shell [2], resulting in shifts of the pK_a of aminolipids by 2-4 units, contingent on the specific lipid composition [3]. This insight underscores the importance of cholesterol-lipid interactions in modulating the physicochemical properties of LNPs, with direct implications for the design and optimization of cholesterol-containing nanocarriers in drug delivery. [1] Pöhnl et al. Nat.Commun. 14, 8038 (2023) [2] Trollmann, Böckmann. Biophys.J. 121, 3927 (2022) [3] Trollmann, Böckmann. Small (2026)

BP 4.2 Mon 15:30 BAR/SCHÖ

Transient interactions between cationic ionizable lipids and anionic lipids foster lamellar to hexagonal phase transition — •David Noel Zimmer[1,2], Friederike Schmid[1], and Giovanni Settanni[1,2] — [1]Physics Department Johannes-Gutenberg University Mainz — [2]Faculty of Physics and Astronomy Ruhr University Bochum

RNA-based therapeutics have demonstrated remarkable efficacy and hold great promise for future applications. The most common delivery systems for these drugs are lipid-based nanoparticles (LNPs), which incorporate ionizable cationic lipids (ICLs) as key components. ICLs are believed to facilitate endosomal escape of the cargo by interacting with anionic lipids in the endosomal membrane, although the underlying molecular mechanism remains unclear. One proposed model suggests that the membrane is destabilized by cone-shaped complexes formed between ICLs and endosomal anionic lipids; clear evidence of stable complexes is still missing. Here[1], we re-examine the problem through equilibrium and nonequilibrium simulations of model membrane systems containing DODMA (ICL), DOPS (anionic lipid) and DOPE (helper lipid). Our results confirm absence of co-localization at equilibrium, but reveal a transient formation of cone-shaped complexes during lamellar-to-inverted-hexagonal phase transitions, which considerably accelerates the transition process. These findings may open new ways for controlling endosomal escape through the rational design of ICLs optimized to interact with cell- or stage-specific endosomal anionic lipids. [1] Zimmer DN, Schmid F, Settanni G. ChemRxiv. 2025; doi:10.26434/chemrxiv-2025-rwb18

BP 4.3 Mon 15:45 BAR/SCHÖ

Osmolyte Effects on Protein Stability: Charge-Regulation is Essential — •Julia Keil and Nico F. A. van der Vegt — Technische Universität Darmstadt, Germany

Osmolytes such as glycine modulate protein stability through differences in their preferential interactions with folded and unfolded states. In this work, we revisit glycine's influence on protein stability by explicitly incorporating charge-regulation effects - protonation and deprotonation of titratable groups - into our study of glycine-protein interactions. Using constant-pH molecular dynamics simulations[1], we develop a titratable glycine model. This pH-dependent model predicts that at pH 7 glycine is depleted from nonpolar elastin-like polypeptides (ELPs) but enriched near acidic and basic ELP residues. It also shows a pH-dependent accumulation of glycine around ELPs and the mini-proteins Trp-cage and GB1, both consistent with prior experimental and computational observations[2-4]. Notably, charge regulation produces systematically stronger preferential binding of glycine to ELPs and mini-proteins at neutral pH than predicted by fixed-charge models. Although glycine is zwitterionic in bulk solution at pH 7, acid-base interactions with NH_3^+ and COO^- protein groups alter its protonation state within biomolecular hydration shells. The corresponding shifts in apparent pKa values promote electrostatically favorable combinations of protonation states, providing a mechanistic explanation for the enhanced preferential binding. [1] J. Chem. Theory Comput. 2022, 18, 10,6148-6160 [2] PNAS 2017, 114, 10, 2479-2484 [3] J. Phys. Chem. B 2020, 124, 30, 6565-6574 [4] Biochem. 1987, 26, 16, 5147-5153

BP 4.4 Mon 16:00 BAR/SCHÖ

Is helicity cooperative? Mechanistic insights from IM30 folding-unfolding dynamics — •Tika Ram Bhandari[1,2], Kurt Kremer[1], Friederike Schmid[2], and Martin Girard[1] — [1]Polymer Theory, Max Planck Institute for Polymer Research, Mainz, Germany — [2]Institute of Physics, Johannes Gutenberg University, Mainz, Germany

Helical transitions help regulate protein behavior, but how different chain segments influence each other's helicity is not well understood. Using coarse-grained molecular dynamics with Hamiltonian Replica Exchange, we examine the disordered-to-helical transition of IM30, the bacterial homolog of ESCRT-III. By tuning hydrogen-bond strengths, we show that the coiled-coil region is more helical than other domains, while overall helicity stays stable due to secondary-structure interactions. Fragments behave differently inside the full chain, revealing cooperative coupling without changing total helicity. Analysis shows both positive and negative links between helicity and chain extension, and identifies four main conformational states. These results clarify how segment interactions control helical transitions and maintain global helicity stability.

BP 4.5 Mon 16:15 BAR/SCHÖ

Grand canonical simulations of micellization in intrinsically disordered proteins — •Rodrigo F. Dillenburg[1,2], Martin Girard[1,5], Friederike Schmid[2], and Edward A. Lemke[3,4] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Institute of Physics, Johannes Gutenberg University, Mainz, Germany — [3]Biocenter, Johannes Gutenberg University, Mainz, Germany — [4]Institute of Molecular Biology, Mainz, Germany — [5]Institute for quantitative and computational biosciences, Mainz, Germany

Molecular dynamics (MD) simulations with coarse-grained force fields have been the gold standard in the computational modeling of liquid-liquid phase separation (LLPS) and biomolecular condensates. While much attention has been focused on large droplets, very little is known about the formation of microphases, such as micelles, in such systems. There is evidence that such assemblies arise from intrinsically disordered proteins (IDPs) with a block co-polymer architecture. However, due to their finite size they are highly sensitive to the periodic boundary conditions of the simulation box. The commonly implemented slab geometry is thus unfit to tackle such systems. To overcome this we have implemented a semi-grand canonical monte carlo (SGCMC) algorithm that significantly speeds-up MD simulations. Our implementation is compatible with implicit solvent 1-bead-per-amino acid force fields such as Calvados and HPS. We show that such approach allows one to run simulations efficiently in a cubic box, at very low densities typical of biological systems. We also highlight the advantages of SGCMC in simulating micelles compared to regular MD.

BP 5: Membranes, Vesicles and Synthetic Life-like Systems I

Time: Monday 15:00–16:30 Location: BAR/0205

BP 5.1 Mon 15:00 BAR/0205

Toward programmable microrobots: DNA-based molecular communication between hydrogel microbeads — •Alexandra Bienau, Alexander Wietfeld, Wolfgang Kellerer, and Friedrich C. Simmel — Technical University Munich, Germany

Emerging applications in biomonitoring and smart therapeutics require materials that can sense biochemical cues, process and transfer information, and respond accordingly. In nature, such capabilities are often achieved through chemical communication, for example in bacterial quorum sensing or immune-cell signaling, where diffusing molecules enable coordinated behavior across many units.

DNA-based hydrogels offer a programmable platform for engineering similar functions, supporting sensing, logic operations, and responsive cargo release. Their porous structure enables molecular diffusion and biochemical exchange. Here, we establish DNA-based molecular communication between hydrogel microbeads. Using emulsion-based droplet microfluidics, we fabricate uniformly sized microbeads that can be modularly loaded with molecular cargo. We immobilize photo-initiated transmitter (TX) and fluorescence-based receiver (RX) systems within them. Communication occurs through diffusing DNA strands, and we characterize signal propagation using experiments and a comprehensive modeling framework.

Looking ahead, this platform enables the design of more sophisticated communication protocols and provides a step toward programmable hydrogel microrobots capable of collective information processing and dynamic interaction with biological environments.

BP 5.2 Mon 15:15 BAR/0205

Microfluidic Micropipettes: A Chip-Based Platform for Membrane Mechanics at Scale — •Sebastian W. Krauss[1], Megan Wong[2], Sepideh Razavi[3], Lorenzo Di Michele[1], and Pietro Cicuta[2] — [1]Department of Chemical Engineering and Biotechnology, University of Cambridge, UK — [2]Cavendish Laboratory, University of Cambridge, UK — [3]School of Sustainable Chemical, Biological and Materials Engineering, University of Oklahoma, USA

The mechanical properties of lipid membranes play an important role in diverse processes, from cell interactions to diseases. Established techniques, however, often suffer from low throughput or provide only bulk mechanical readouts, such as overall stiffness, making it challenging to obtain statistically robust measurements of membrane mechanics. Here, we present a microfluidic platform incorporating hundreds of micropipette like confinements on a single chip, enabling parallel mechanical characterisation of giant unilamellar vesicles (GUVs) in a single experiment. The forces acting on the membrane can be precisely tuned via the applied flow rates and the custom channel geometries, allowing well-defined, controllable mechanical testing. The platform also enables in situ exposure of GUVs to membrane-active compounds, such as surfactants, facilitating direct observation of their impact on membrane mechanics, including the dynamics and reversibility of these effects. This high-throughput approach opens the possibility for systematic screening of compound libraries, providing a quantitative framework to study the interactions between solutes and their impact on membranes.

BP 5.3 Mon 15:30 BAR/0205

Supported DPPC/DPPG Bilayers on Oxide Substrates as a Versatile Platform for Protein*Membrane Studies and Future FRET-Based Sensing — •Daniel Saavedra[1], Benjamin Ruz[1], Marcelo Cisternas[2], Susana Rojas[2], and Ulrich Volkmann[1] — [1]Institute of Physics, Pontificia Universidad Católica de Chile, Santiago, Chile — [2]School of Industrial Engineering, University of Valparaíso, Santiago, Chile

We develop a dry-processed supported lipid platform to study how membrane composition and substrate chemistry modulate protein-lipid interactions. Following the dry two-step self-assembly method for DPPC on silicon [1], we prepare DPPC bilayers with gramicidin A on SiO2 and characterize them by temperature ramps using very-high-resolution ellipsometry, AFM, FTIR, and SERS. Ellipsometry resolves DPPC pre- and main-phase transitions and peptide-induced shifts in thermal stability, which correlate with AFM domain morphology and FTIR amide I changes. In parallel, DPPC/DPPG bilayers are deposited on SiO2 and TiO2 and probed by AFM, FTIR, and ellipsometry to disentangle the influence of lipid charge and oxide surface on bilayer continuity and phase behavior, consistent with previous studies on lipid oxide interfaces [2]. Together, these results establish a solvent-free, thermally robust lipid architecture compatible with multimodal read-out and future integration of carbon quantum dots for FRET-based sensing. Acknowledgements: ANID Fellowship (DS) References 1.Cisternas MA et al. Int J Mol Sci. 2020;21:6819. 2.Tero R et al. Proc SPIE. 2007;6769:67690J.

BP 5.4 Mon 15:45 BAR/0205

Hexagonal and Lamellar Superstructure in DSPE-PEG1000 Monolayers at the Air/Water Interface — •Issam Assi, Heiko Aherns, and Christiane A. Helm — Institute of Physics, University of Greifswald, Germany

Inspired by diblock copolymer self-assembly, we investigate lipopolymer monolayers at the air/water interface. We studied DSPE-PEG1000 monolayers with alkyl chains in the liquid-condensed phase in dependence of the molecular area. Due to its conformational entropy, the moderately hydrophilic PEG has a larger area requirement than the alkyl chains in all-trans conformation. Small-angle grazing incidence X-ray diffraction (GID) measurements identified a hexagonal superstructure. The ordered alkyl chains form hydrophobic domains that are embedded in dissolved PEG. These domains consist of the alkyl chains of ca. 200 PEGylated lipid molecules. During monolayer compression, the number of alkyl chains in a domain remains constant, while their area fraction increases. At an area fraction of 50%, a transition to a lamellar superstructure occurs. During this transition, the alkyl chain domains merge. This transition is attributed to the entropy loss of the laterally compressed PEG chains. Wide-angle GID reveals that the alkyl chains in the liquid-condensed phase possess the same small cross-sectional area, as those in DSPE monolayers, indicating that PEG has little influence on the liquid-condensed phase. The hexagonal superstructure was confirmed with AFM images.

BP 5.5 Mon 16:00 BAR/0205

Numerical simulation of wetting of biomembranes — •Mokbel Marcel and Aland Sebastian — TU Bergakademie Freiberg

Biological cells utilize membranes and liquid-like droplets, known as biomolecular condensates, to structure their interior. The interaction of droplets and membranes, despite being involved in several key biological processes, is so far little understood. Here, we present a first numerical method to simulate the continuum dynamics of droplets interacting with deformable membranes via wetting. The method combines the advantages of the phase-field method for multiphase flow simulation and the arbitrary Lagrangian-Eulerian method for an explicit description of the elastic surface. The model is thermodynamically consistent, coupling bulk hydrodynamics with capillary forces, as well as bending, tension, and stretching of a thin membrane. Its capabilities are illustrated in several two- and three-dimensional axisymmetric scenarios.

BP 5.6 Mon 16:15 BAR/0205

Theory of Michaelis-Menten kinetics in phase-separated systems — •Gaetano Granatelli[1], Samuel S. Gomez[1], Sudarshana Laha[2], and Christoph A. Weber[1] — [1]Faculty of Mathematics, Natural Science, and Materials Engineering, Institute of Physics, University of Augsburg, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Phase-separated systems can regulate chemical reactions through spatial organization. Motivated by their biological relevance, we develop a mean-field theoretical framework for enzymatic kinetics within liquid condensates formed by phase separation. Building on a model that decouples the phase separation dynamics of scaffold components from the chemical kinetics of dilute clients, we generalize the classical Michaelis-Menten theory of enzyme kinetics to spatially heterogeneous systems with coexisting phases. In our framework, the dynamics of client concentrations are governed by scaffold-controlled parameters such as condensate size, partitioning, relative kinetic coefficients, and diffusion. We explore how they modulate the initial reaction rate across regimes set by the interplay of diffusive and reactive timescales, and we derive explicit expressions for the local reaction rate constants in each phase, allowing direct experimental measurement of how condensates modulate reaction kinetics. We find that, compared to homogeneous conditions, phase-separated liquid condensates can mediate either optimal enhancement or suppression of the initial rate. Our results provide experimentally testable predictions to quantify how phase separation modulates enzymatic activity in living and synthetic systems.

BP 6: Active Matter II (joint session DY/BP/CPP)

Time: Monday 15:00–18:30 Location: ZEU/0160

See DY 17 for details of this session.

BP 7: Poster Session I

Biomaterials and biopolymers, cytoskeleton, cell mechanics and tissue mechanics; FS controlling biological cells by ultrasound

Time: Monday 15:00–17:00 Location: P5

BP 7.1 Mon 15:00 P5

Eco-Friendly PEGylated Iron Oxide Nanoparticles for In Vitro Targeted Delivery and Controlled Release of Docetaxel in SK-OV-3 Ovarian Cancer Cells — •Romesa Soomro[1], Che Azurahanim Che Abdullah[1,2], and Halima Alem Marchand[3] — [1]1Biophysics Lab, Department of Physics, Faculty of Science, Universiti Putra Malaysia, 43300, Selangor, Malaysia — [2]2Cancer Research Lab, Institute of Bioscience, Universiti Putra Malaysia, 43300, Selangor, Malaysia — [3]3Department of Matériaux, Métallurgie, Nanosciences, Université de Lorraine, Nancy, France

Iron oxide nanoparticles were green-synthesized using oolong tea extract as a natural reducing and stabilizing agent. A Taguchi L9 design was applied to optimize reaction parameters and obtain stable nanoparticles with reduced hydrodynamic size. The optimized particles were PEG-coated to improve biocompatibility and subsequently loaded with docetaxel for targeted cancer therapy. Characterization using spectroscopy, diffraction, magnetic measurements, and electron microscopy confirmed successful synthesis and coating, with superparamagnetic behavior and particle sizes below twenty nanometers. Drug release studies showed sustained, pH-responsive release under acidic conditions. Cytotoxicity evaluation using SK-OV-3 ovarian cancer cells demonstrated high biocompatibility of PEG-coated nanoparticles and strong anticancer activity of the docetaxel-loaded system. The results indicate that green-synthesized PEGylated iron oxide nanoparticles provide a promising and sustainable platform for controlled anticancer drug delivery.

BP 7.2 Mon 15:00 P5

The Potential Impact of a Novel Chitosan-Titanium dioxide Nanoparticles against Hepatocellular Carcinoma in Rat Model — Omnia Ahmed Mohamed Elbakary[1], Eman Ibrahim Kandil[1], Sawsan Mohamed Elsonbaty[2], Shaimaa El-saied Mohamed[1], and •Nermeen Mohamed Elbakary[3] — [1]Faculty of Science, Biochemistry department, Ain Shams University, Cairo, Egypt — [2]Radiation microbiology department, National center for radiation research and technology, Egyptian Atomic Energy Authority, Cairo, Egypt — [3]Radiation biology department, National center for radiation research and technology, Egyptian Atomic Energy Authority, Cairo, Egypt

Hepatocellular carcinoma (HCC) the most common type of liver cancer, is the fifth most common malignant tumor type worldwide and the second leading cause of cancer-related death. This study investigates the potential therapeutic effects of novel chitosan-titanium dioxide nanoparticles (Cs-Ti NPs) against hepatocellular carcinoma (HCC) in a rat model. The experimental design included five groups: a healthy control group, a group administered with diethylnitrosamine (DEN) to induce liver carcinogenesis, a group treated with Cs-Ti NPs, a DEN group subsequently treated with 5-Fluorouracil (5-FU), and a DEN group treated with Cs-Ti NPs. DEN was administered orally at 20 mg/kg body weight five times weekly for six weeks to induce tumor formation. Therapeutic interventions with Cs-Ti NPs and 5-FU were applied post-induction. The study evaluated apoptotic markers (Bcl-2, Bax, p53, Caspase-3, Cytochrome C), signaling pathways (MAPK, ULK1, mTOR), and serum tumor markers (AFP, NF-κB, COX-2) via ELISA. Results are expected to elucidate the molecular mechanisms involved and assess the efficacy of Cs-Ti NPs in mitigating HCC progression, potentially offering a new nanotherapeutic avenue for liver cancer treatment.

BP 7.3 Mon 15:00 P5

Viscous and Plastic Energy Dissipation Processes of Native Collagen Fibrils in AFM-based Nanoindentation Measurements under Controlled Humidity — •Martin Dehnert, Paul Zech, Mario Zerson, and Robert Magerle — Fakultät für Naturwissenschaften, Technische Universität Chemnitz, Germany

Collagens, lipids, and water are among the major molecular components of connective tissue, yet surprisingly little is known about their interactions in vivo. Here, we use AFM-based nanoindentation experiments to measure the mechanical response of collagen fibrils to deformation under constant strain (relaxation) or constant stress (creep) at different humidity levels and at different deformation speeds. The measured data are evaluated using a power-law analysis, in which the detailed indentation history, including the different indentation velocities, is taken into account. An in-depth analysis reveals that the phenomena of stress relaxation and creep compliance can be described by a time-scaled power law. Furthermore, we show that energy dissipation is primarily caused by plastic deformation during tip indentation and can be quantified with the ductility index. This parameter can also be used for high-resolution imaging of connective tissues. The ductility index provides additional information about the nanomechanical changes in collagen fibrils during development, aging, and disease.

BP 7.4 Mon 15:00 P5

Cyanobacteria as biological actuators — •Paul Nieschwitz and Stefan Karpitschka — Department of Physics, Universität Konstanz, Germany

Filamentous cyanobacteria are highly resilient, light-responsive organisms whose robustness and availability makes them ideal candidates for building engineered living materials (ELMs), that can adapt to or be controlled by external cues.

Here, we present a simple actuator composed of entangled filament assemblies wrapped around elastic PDMS-pillars. Contraction of the network generates a net resultant force that deflects the pillars. By calibrating the compliance of the pillars, we quantify this force. Varying the actuator geometry, filament density and illumination conditions, allows us to characterize the force output and dynamic response of the actuator.

Without requiring the need for genetic modification or sophisticated culture conditions, this platform offers a simple and robust approach to create light-controlled biological machines.

BP 7.5 Mon 15:00 P5

LactiFilm: Hydrogel supported co-culture biofilms of lactobacilli and phytoplankton for sustainable production of lactic acid — •Carina Schneider and Regine von Klitzing — TU Darmstadt, 64289 Darmstadt, Germany

Lactic acid is an essential bulk chemical used across the food, pharma, and cosmetics industry. Recently, its demand has been rising as the monomer for synthesizing polylactic acid, a major biodegradable alternative to conventional plastic. Hence, biological synthesis of lactic acid offers a greener production option. In this work, we develop a biofilm-inspired strategy by immobilizing lactobacilli and algae in smart hydrogels.

The algae immobilization matrix is formed from cross-linkable PNIPAM (Poly N-Isopropylacrylamide) microgels containing the UV-sensitive comonomer HMABP (2-Hydroxy-4-(methacryloyloxy)benzophenone), enabling microgel crosslinking into a stable hydrogel film. Due to the volume phase transition temperature of PNIPAM, the matrix exhibits controllable swelling and deswelling behavior. This responsiveness allows for regulated partial lysis of the algae to release nutrients that support lactic-acid production. To assess the mechanical strength of the hydrogel, we perform atomic force microscopy (AFM) indentation measurements.

BP 7.6 Mon 15:00 P5

Multi-phase coexistence of charged condensates — •Chengjie Luo, Yicheng Qiang, and David Zwicker — MPI-DS, Göttingen, Germany

Biomolecular condensates are complex droplets whose formation is believed to be primarily driven by short-range attractive interactions between diverse molecules. However, charges that mediate long-range interactions can also strongly affect phase separation. Using a mean-field theory, we demonstrate that electrostatic interactions can drive rich phase separation behavior. In a simple system of three charged components, these interactions can lead to the coexistence of multiple phases, including homogeneous phases with different compositions and patterned phases with finite-sized droplets. Furthermore, applying an external electric field can dramatically alter these coexistence states: weak fields cause charged droplets to move like colloidal particles, while stronger fields stretch droplets, leading to the formation of striped patterns. Our work establishes electrostatics and electric fields as potent controllers of phase coexistence, with implications for understanding biological condensates and designing synthetic patterned materials.

BP 7.7 Mon 15:00 P5

Density and viscosity Measurements of the cytosol of human red blood cells — •Thomas John, Karin Kretsch, and Christian Wagner — Experimental Physics, Saarland University

We present a method to determine the viscosity of the intracellular liquid - the cytosol - of human red blood cells (RBCs). Our method combines the measurement of the mass density distribution of RBCs and the viscosity of the cytosol as a function of the water content. The density distribution is measured through buoyant density centrifugation combined with cell counting. By correlating this distribution of cell population densities with the viscosity-density relation of the cytosol, we obtain a log-normal distribution of the cytosol viscosity of healthy RBCs. The viscosity contrast λ, defined as the ratio of viscosities between the RBC cytosol and the blood plasma under physiological conditions, is determined to have a log-normal distribution with a mean value of $\bar{\lambda} = 10$. This value is significantly larger than those used in the literature for numerical simulations. The wide distribution of the viscosity values results from the loss of a small amount

of water from the RBCs over their 120-day lifespan. We find that the viscosity of the cytosol in older cells is more than twice as high as in younger cells, a fact that should be taken into account in future theoretical investigations.

BP 7.8 Mon 15:00 P5

Model particles to study interaction of microplastic particles — •Kai Gossen, Andreas Fery, and Günter Auernhammer — IPF Dresden, Dresden, Germany

Microplastic in the environment is typically coated by natural organic matter forming an ecocorona. We present an approach to model ecocorona on particles with well-defined polymers, synthetic and derived from natural polymers. Polystyrene particles were coated with fluorescent polyelectrolyte multilayer systems, PS(Chitosan/Hyaluronic acid) and PS(Poly(dimethyldiallylammonium chloride) /Polystyrene sulfonate) by the layer-by-layer method. Systems with 2, 4 and 6 bilayers were synthesized. The second layers were fluorescently labelled with SNARF conjugated dextran. It was found that zeta potentials of the PS(Chi/HS)2/4/6 systems assume val- ues (-20 mV to -35 mV) that are similar to those of PS-ecocorona particles (-40 mV to -5 mV). The pH-dependent fluorescence of particle suspensions and indi- vidual particles were measured at pH values between pH 3 and pH 8. A well mea- surable pH dependence between pH 4.5 and 8 for the PS(Chi/HS) systems and the PS(PDADMAC/PSS) system could be measured. Automating particle synthesis via cross-flow filtration produces particle batches of up to 5 g. The system could serve to selectively study effects of surface properties of ecocorona coated particles such as surface stiffness or zeta potential.

BP 7.9 Mon 15:00 P5

Controlled Spray coating of Bacterial Nanocellulose Thin films revealed by Surface-Sensitive X-ray Scattering — •Joanne Neumann[1], LI Li[2], Edina Klein[1,3], Jan Rubeck[1], Ute Römling[2], Holger Sonderrmann[1,3], and Matthias Schwartzkopf[1] — [1]DESY, Photon Science, Notkestr. 85, D-22607 Hamburg — [2]Department of Microbiology, Tumor and Cell Biology, Biomedicum, KI, Karolinska Institutet, Nobels väg 6, S-17177 Stockholm — [3]CSSB, Center for Structural Systems Biology, Notkestr. 85, D-22607 Hamburg

Bacterial nanocellulose (BNC) is a sustainable biomaterial valued for its purity, nanoscale fibrillar structure, and biocompatibility. Its properties can be tailored through genetic engineering, growth conditions, and processing. Here, we fabricate thin films from BNC produced by *S. typhimurium*, *Komagataeibacter*, and *Klebsiella* using airbrush spray deposition of aqueous dispersions as a green, reproducible method. We examine how different extraction procedures (acidic, alkaline, surfactant-based) affect nanoscale organization and film adaptability. High-resolution X-ray scattering (μGIUSAXS/μGIWAXS) is used to probe fibril orientation, aggregation, and hierarchical ordering. Our results show extraction-dependent structural variations that influence film homogeneity and functional performance. By refining spray-coating and scattering protocols, this work links chemical treatment history to structural adaptability and supports sustainable strategies for controlled BNC thin-film fabrication in materials science and bioengineering.

BP 7.10 Mon 15:00 P5

Engineering Shear-Thinning Hydrogels: A Dynamic Scaffold for 3D Tissue Culture — •Bruno Schmelz[1], Fen Li[2], Kai Zhang[2], and Timo Betz[1] — [1]Third Institute of Physics, University Göttingen — [2]Sustainable Materials and Chemistry, University Göttingen

Extracellular matrix scaffolds are essential for advanced 3D cell culture systems, providing structures for cell movement as well as physical and chemical cues that promote migration, proliferation, and differentiation. Hence, the extracellular matrix is crucial for functional tissue formation. However, natural extracellular matrix materials used in vitro, such as collagen and elastin, are difficult to control regarding elastic properties, polymer mesh size, and homogeneity. Our objective is to design a dynamic hydrogel, tailored to meet the specific requirements of 3D tissue culture, such as viscoelastic properties and cell-binding sites, that initially supports tissue formation but can be dissolved and replaced by cell-generated extracellular matrix. We propose a hydrogel with dynamic cross-links that allows for reorganization by embedded cells, resembling processes in physiological tissues. We present the rheological properties of the hydrogel and the initial findings of cellular migration and reorganization of cell-gel systems. When subjected to stress, the hydrogel exhibits a transition to a more liquid-like state, with the potential to solidify again upon stress relaxation. This behavior allows cells to remodel their surrounding matrix and shape their environment, as evidenced by experiments with cells cultured in the hydrogels.

BP 7.11 Mon 15:00 P5

Atomic-Scale Probing of Aluminum Distribution in Catalysts and Peptide COM Fidelity — •Sakshi Sinha — Department of Materials Physics, Institute of Material Science, University of Stuttgart, Heisenbergstr. 3, 70569 Stuttgart

Atom Probe Tomography (APT) enables three-dimensional, atomic-scale mapping of inorganic and biomolecular materials. Using conventional lift-out specimen preparation, we study aluminum distribution in microporous aluminosilicate catalysts with varying Al content. The frequency distribution with considering different sphere sizes N in order to investigate size-dependent effects for segregating or clustering behavior of the Al atoms. APT reveals atomic-scale clustering and uniformity of Al, providing direct insight into acid site density and strength, and complements bulk techniques such as ICP-OES by resolving localized compositional variations. For biomaterials, cryogenic quench-freezing is used to prepare aqueous specimens. Mass spectra indicate that fragmentation behavior is concentration-dependent and influenced by hydration shell disruption during field evaporation. Experimental interfragment distances closely match theoretical center-of-mass distances within 1 Å, demonstrating that APT can preserve biomolecular subunit spatial relationships with sub-angstrom fidelity. These studies demonstrate the versatility of APT in probing both inorganic and biomolecular systems with unprecedented atomic precision, opening pathways for understanding structure*function relationships across material classes.

BP 7.12 Mon 15:00 P5

Decoupling Crosslink Stability and Network Connectivity in Coiled Coil Crosslinked Hydrogels — Stefanie Lenzeder[1], Geonho Song[1,2], Isabell Tunn[2], Alberto Sanz de Leon[2], Tanja D. Singewald[1], and •Kerstin G. Blank[1,2] — [1]Johannes Kepler University, Linz, Austria — [2]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

Biomimetic hydrogels serve as a powerful platform for investigating how cells sense and respond to the mechanical cues in their environment. Despite significant progress, the precise mechanisms how cells evaluate the elastic and viscoelastic properties of their surroundings remain incompletely understood. While hydrogels are typically characterized based on their bulk material properties, cells probe these materials on the molecular scale through receptor-ligand interactions. Bridging the gap between molecular-scale interactions and macroscopic material behavior is thus essential for advancing our understanding of cell-material interactions. Inspired by proteins found in the extracellular matrix, we are investigating biomimetic hydrogels crosslinked with coiled coil forming peptides. These modular building blocks enable precise control over their molecular characteristics, such as thermodynamic, kinetic and mechanical stability as well as oligomerization state. Our findings show that the bulk material properties are governed more strongly by network connectivity than crosslink stability. These insights deepen our understanding of how molecular design impacts the macroscopic behavior of hydrogels, opening new avenues for tailoring materials for specific biological applications.

BP 7.13 Mon 15:00 P5

Development and investigation of coarse-grained particle models for alginates. — •Hensi Gandhi, Rudolf Weeber, and Christian Holm — Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany

Alginates form ion-mediated gel networks whose mesoscale structure and mechanical properties depend on monomer sequence, charge distribution, and environmental conditions. We aim to develop coarse-grained models that capture these molecular features while remaining computationally efficient. Our ongoing work combines all-atom molecular dynamics with systematic coarse-graining to derive bonded interactions, electrostatics, and ion-mediated cross-linking rules. The models will be implemented in ESPResSo [1] using implicit solvent, with extensions for multivalent ions and shear via Lees Edwards or lattice Boltzmann coupling. We will study how monomer sequence, salt concentration, and pH influence chain flexibility, persistence length, gelation kinetics, and network topology, and compare structural and mechanical observables with experiments to assess model transferability. This framework is intended to support mesoscale predictions within the GRK SusGel program [https://www.susgel.kit.edu/24.php] and link molecular design to macroscopic gel properties.

[1] F. Weik, R. Weeber, K. Szuttor, K. Breitsprecher, J. de Graaf, M. Kuron, J. Landsgesell, H. Menke, D. Sean, C. Holm, ESPResSo 4.0 - An extensible software package for simulating soft matter systems, European Physical Journal-Special Topics, 227 (2019), 1789-1816, DOI: 10.1140/epjst/e2019-800186-9.

BP 7.14 Mon 15:00 P5

Cytoskeletal Networks in 3D Cysts Under Strain — •Greta Höhndorf[1], Ruth Meyer[1], Ruben Haag[1], Ulrike Rölleke[1], Ulla Unkelbach[2], Nicole Schwarz[3], Andreas Janshoff[2], and Sarah Köster[1] — [1]Institute for X-Ray Physics, University of Göttingen — [2]Institute of Physical Chemistry, University of Göttingen — [3]Institute of Molecular and Cellular Anatomy RWTH Aachen University

The cytoskeleton of eukaryotic cells mainly consists of actin filaments, microtubules and intermediate filaments (IFs). Unlike actin and microtubules, IFs are cell-type specific. Epithelial cells express keratin IFs, which form a layer close to the membrane in certain cell types. This layer is referred to as the "IF-cortex" and is hypothesized to adopt a "rim-and-spokes" structure with radial spokes supporting mechanotransduction properties of the cell. This structure raises questions about how the actin and IF cortices complement each other and how the mechanical properties of keratin influence force transmission in cells under high strain. To address these questions, we show a 3D approach where epithelial cells form polarized cysts and are stretched by injecting mineral oil into the

lumen. When comparing wild-type (WT) and keratin knock-out (KO) cysts, we find that KO cysts deform more easily at low strains and respond more sensitively at high strains than WT cysts, indicating a stabilizing role of keratin under increased mechanical load. Furthermore, by staining actin, keratin, and the nuclei and performing fluorescence imaging pre and post stretching, we investigate strain dependent network changes and deformations.

BP 7.15 Mon 15:00 P5

Interactions between single actin and vimentin filaments — •Pallavi Kumari[1], Kristian Pajanonot[1,2], Komal Bhattacharyya[2], Stefan Klumpp[2], and Sarah Köster[1] — [1]Institute for X-Ray Physics, University of Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, University of Göttingen, Germany

The cytoskeleton plays a crucial role in maintaining cellular structure, mechanics, and function. Recent advances suggest that the diverse tasks of the eukaryotic cytoskeleton depend on the interactions between its filamentous components–microtubules, actin filaments, and intermediate filaments. Despite a growing number of studies aimed at a better understanding of these interactions, it remains unclear whether actin and intermediate filaments interact directly in the absence of an auxiliary protein. Previous *in vitro* studies on reconstituted mixed filament networks have reported inconclusive results. To clearly resolve this inconclusiveness, it is essential to further simplify the system down to the single filament level. Here, we present a study on the direct interactions between actin and vimentin intermediate filaments at the single filament level. Using quadruple optical tweezers combined with confocal microscopy and microfluidics, we precisely control the interaction conditions, visualize the interactions in real time, and measure the forces involved. Our research provides direct evidence of actin-vimentin interactions, together with a quantification of the interaction forces they exert on each other.

BP 7.16 Mon 15:00 P5

Mechanical Properties of Intermediate Filament Networks — •Jonas Penning, Komal Bhattacharyya, and Stefan Klumpp — Institut für Dynamik komplexer Systeme, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The mechanical strength and dynamics of cells are essential for sustaining life. For instance, during simple activities such as breathing or walking, cells experience significant tensile stresses as they are stretched, sheared, or compressed. The cytoskeleton - a cross-linked composite network of actin, microtubules, and intermediate filaments - plays a central role in determining the cells' mechanical properties. This work focuses primarily on intermediate filaments, with particular emphasis on vimentin. Compared to actin, intermediate filaments exhibit much smaller persistence lengths, but are much more stretchable with highly nonlinear elasticity. A simplified, lattice-based model of fibrous networks with variable connectivity has been developed to investigate the mechanical and physical properties of such vimentin filament networks, as the model allows for the corresponding nonlinear behavior of individual vimentin filaments under strain. Analogous to experimental approaches, the mechanical properties of the model are tested by applying normal and shear strains or stresses and analyzing the resulting responses. Stretching the networks isotropically and comparing linear and nonlinear strain-behavior of individual filaments, the model shows an internal energy decrease for nonlinear elasticity and a strain-softening quantified by a turning point in the bulk modulus with increasing network-strain.

BP 7.17 Mon 15:00 P5

Phosphorylation-induced softening of vimentin networks revealed by optical tweezers microrheology — •Yuzhen Feng, Shanay Zafari, and Sarah Köster — Institute for X-Ray Physics, University of Göttingen, Germany

Phosphorylation is a key post-translational modification regulating intermediate filament (IF) organization and cell mechanics. While phosphorylation-induced softening of single vimentin filaments has been reported, its impact on network-level mechanics remains unclear. Here, we employ optical tweezers-based active microrheology to quantify the mechanical properties of vimentin IF networks containing defined fractions of the phosphomimetic vimentin mutant S72E. Both unmodified and phosphomimetic vimentin networks exhibit a viscoelastic response with partial stress relaxation after deformation. Increasing the phosphomimetic content reduces the overall stiffness, indicating phosphorylation-induced softening at the network level. These findings extend the understanding of how biochemical regulation at the molecular level translates into mechanical remodeling of IF across scales from the single-filament to the network level.

BP 7.18 Mon 15:00 P5

Microtubule networks exhibit amorphous material behavior — •Claudia Marcelli[1], Raffaele Mendozza[2], Shanay Zafari[1], Ruben Haag[1], Peter Sollich[2], and Sarah Köster[1] — [1]Institute for X-Ray Physics, University of Göttingen, Germany — [2]Institute for Theoretical Physics, University of Göttingen, Germany

Microtubules (MTs), together with intermediate filaments and actin, are the main components of the cytoskeleton. Among these filaments, MTs are the stiffest. They can form a rigid cellular scaffold and transmit forces across the cell while remaining extremely dynamic and able to assemble into specific cell structures (e.g. mitotic spindles). While MTs have been extensively characterized at the single-filament level, it is still not fully resolved how they collectively behave at the network-scale level. Here, we present a comprehensive characterization of the linear and nonlinear mechanical responses of stabilized MT networks at the microscale by using optical tweezers. To this aim, we employ both strain-ramp and large-amplitude oscillatory strain protocols, applying a range of deformations that allows us to probe both regimes. Our results show that MTs can withstand high stress and behave as an amorphous material, exhibiting a yielding transition from an elastic response at small strains to a viscous response at large strains. These findings provide us with a deeper understanding of the mechanics of MT networks while setting the stage for future studies in which dynamic or active elements can be incorporated into the network to understand how activity modifies material mechanical properties.

BP 7.19 Mon 15:00 P5

MatrixModel: Building a Computational Model of the HSPC niche — •Julia Käsehagen and Sophia Rudorf — Institute for Cell Biology and Biophysics, Leibniz Universität Hannover, Germany

Haematopoietic stem and progenitor cells (HSPCs) rely on finely tuned adhesion to extracellular matrix (ECM) proteins within the bone marrow niche to balance quiescence, self-renewal, and differentiation. As part of the research consortium Matrix Evolution [1], MatrixModel develops a multiscale computational framework to predict how ECM composition, architecture, and mechanics regulate HSPC behavior, including adhesion and motility. We implemented two pipelines to use and adapt models by other goups: (i) a mechanochemical ODE model of integrin-talin-vinculin adhesion dynamics (by Honasoge et al. [2]) and (ii) a hybrid Cellular-Potts-Bead-Spring model of ECM fiber networks (by Tsingos et al. [3]).

For (i), we will parameterize the ODE model for HSPCs to predict adhesion lifetimes and tractions per adhesion. In (ii), the Cellular-Potts-Model (CPM) governs HSPC shape and contract energies, while a nonlinear fiber network captures density, crosslinking, and anisotropy. Cell-fiber links inherit rate laws from results of the ODE model.

[1] https://www.cell.uni-hannover.de/en/research/main-research-areas/matrix-evolution

[2] Honasoge et al., 2023, PLoS Comput Biol.

[3] Tsingos et al., 2023, Biophysical Journal.

BP 7.20 Mon 15:00 P5

Stiffness Characterization of Microtentacles: an optical tweezers study — •Kirill Korneev[1], Thomas John[1], Franziska Lautenschläger[1,2], and Christian Wagner[1,2] — [1]Department of Experimental Physics, Saarland University, Saarbrücken, Germany — [2]Center of Biophysics, Saarland University, Saarbrücken, Germany

Laser tweezers (LT) are devices used for manipulating, trapping, and measuring forces on particles within optical traps, and they are commonly used in biophysics. Microtentacles (McTNs) are membrane protrusions supported by bundles of microtubules produced inside cells. These McTNs appear in circulating tumor cells and are thought to play a key role in facilitating the cells adhesion and extravasation process from the blood vessel. Although the biological mechanisms underlying McTN formation have been partially characterized, their characterization by physical material parameters is still lacking. The objective of this work is to study the deformation of McTNs using optical trap force measurements. We will show how McTNs behave under the action of external forces in the piconewton range and suggest a method to extract their Young's moduli

BP 7.21 Mon 15:00 P5

Determination of the Human Red Blood Cell Mass Density Distribution — •Luca Hastenteufel[1], Thomas John[1], Karin Kretsch[1], and Christian Wagner[1,2] — [1]Dynamics of Fluids, Experimental Physics, Saarland University, 66123 Saarbrücken, Germany — [2]Physics and Materials Science Research Unit, University of Luxembourg, L-1511 Luxembourg, Luxembourg

Red blood cells (RBCs) survive in circulation for approximately 120 days, during which their mass density increases, leading to the formation of a density distribution (DD). This distribution is commonly used as a diagnostic marker and as an indicator of individual cell age. However, few studies have examined the detailed form of the DD, with only few datapoints. In this study, the DD of erythrocytes was quantitatively derived using microscopic imaging approaches in controlled linear density gradients. Linear gradients were created using Percoll and Optiprep, common density media used for the density separation of cells or subcellular compounds. A custom microscopic scanning setup was developed to image RBC distributions along the gradient with a micrometre spatial resolution over several cm. Through image analysis, the vertical positions of individual cells were detected and by single cell counting, the DD was constructed in high resolution. The measured DD revealed significant deviations from Gaussian behaviour.

BP 7.22 Mon 15:00 P5

Integration of environmental stimuli into the contraction dynamics of *Physarum polycephalum* — •Nora Deiringer and Karen Alim — School of Natural Sciences, Technical University of Munich, Garching, Germany

In many organisms, behaviour and decision-making are guided by environmental stimuli. However, the internal dynamics linking stimuli to behaviour are often complex and not fully understood. Additionally, an organism's response to a stimulus can depend on its past stimulus history. In the unicellular, network-shaped organism *Physarum polycephalum*, migration results from the redistribution of cell mass driven by self-organised rhythmic tube contractions. In this study, we mimic environmental stimuli by exposing the cell's contraction dynamics to patterns of harmful blue light. Through live recordings, we observe the imprints of these patterns in the cell's dynamics and investigate how dynamic stimulus memories arise and decay. By varying the time span between two consecutive stimuli, we aim to elucidate how past stimulus history influences responses to future ones. Our findings provide insight into the mechanisms by which simple, non-neural organisms can organise adaptive behaviour.

BP 7.23 Mon 15:00 P5

Coordination of Migration by Adaptive Mechanics — •Diana Lenski, Lucas Troeger, and Karen Alim — School of Natural Sciences, Technical University of Munich, Germany

Unicellular organisms navigate and adapt to their environment using characteristic migration strategies, among them chemotaxis, the ability to detect and respond to chemical gradients. Although numerous models exist for amoeboid migration, the mechanisms governing directional sensing and movement in dynamical systems with complex morphologies across various size scales remain partially characterised. Besides continuous locomotion, migration strategies can involve dynamic regulatory phases that modulate the migratory behaviour. One such example in the slime mould *Physarum polycephalum* are stationary oscillations that repeatedly interrupt persistent migration.

This project involves the analysis and modelling of experimentally observed stationary oscillations in *P. polycephalum* across macroscopic and intermediate scales. These oscillations manifest as the periodic, opposing formation of protrusions that define the direction of migration, making them a key observable across spatial and temporal scales. First, we will statistically evaluate the chemotactic efficiency of large and small plasmodia on the macroscopic scale. Subsequently, we will examine oscillation dynamics by tracking contraction patterns to evaluate their contribution to migration phases and energy efficiency.

Integrating both perspectives will provide a deeper understanding of oscillatory migration phases as a fundamental element of amoeboid migration strategies.

BP 7.24 Mon 15:00 P5

Deep learning architecture combining Vision Transformers and U-Nets for robust traction force microscopy — •Yunfei Huang[1], Elena Van der Vorst[2,3], and Benedikt Sabass[1,2,3] — [1]Faculty of Physics, Technical University Dortmund, Dortmund, 44227, Germany — [2]Faculty of Physics and Center for NanoScience, Ludwig Maximilian University of Munich, Munich, 80752, Germany — [3]Department of Veterinary Science, Ludwig Maximilian University of Munich, Munich, 80752, Germany

Traction force microscopy (TFM) quantifies cellular forces on the extracellular matrix. Although deep learning has advanced TFM analysis, challenges remain in achieving reliable inference across spatial scales, estimating uncertainty, and integrating biological information such as cell type. In this study, we propose a robust deep learning architecture, ViT+UNet, which integrates a U-Net with a Vision Transformer. Our results show that this hybrid model outperforms either U-Net or ViT alone in predicting traction force fields. In addition, ViT+UNet achieves superior generalization across a wide range of scales, which allows one to use the algorithm for TFM with different setups and equipment. We extend the model with an uncertainty estimation module that enables simultaneous prediction of traction forces and confidence levels. Incorporating cell-type information further improves accuracy. Simulated results show that the algorithm effectively reconstructs 3D traction fields in non-linear elastic matrices.

BP 7.25 Mon 15:00 P5

Identifying the proteins controlling the intracellular active mechanics — •Noemie Veyret, Till Muenker, and Timo Betz — Third institute of Physics, University of Göttingen, Germany

Over the past few years, the study of cell mechanical properties has allowed new insights on the understanding of biological processes and life complexity. According to previous work, intracellular mechanical properties can be narrowed down to a fingerprinting of only 6 parameters. Through the use of active and passive microrheology measurements via optical tweezers, frequency dependent viscoelastic properties and intracellular activity were found to vary for different cell types. The aim of this project is to find a correlation between changes in protein expressions and mechanical fingerprint of cells. To do so optical tweezers measurements will be performed during the differentiation process of induced Pluripotent Stem Cells (iPSC) into different cell types such as skeletal muscles or cardiac fibroblasts. This measurement allows the characterization of the mechanics during the iPSC differentiation process. In parallel, the cell proteome will be studied using mass spectroscopy. Combining both, we hope to find the connection between proteins and their mechanical role, the intracellular "mechanome".

BP 7.26 Mon 15:00 P5

Characterization of filamentous cyanobacteria using force-sensing micropipettes — •Paul Dufke and Stefan Karpitschka — Fachbereich Physik, Universtität Konstanz

Filamentous cyanobacteria strongly influence nearly all ecosystems, sometimes with harmful impacts. It is believed that their dominance is based on collective traits such as aggregation, entanglement and dispersal, but the details remain elusive. To understand the collective behaviour that arises in ensembles of many filaments, it is necessary to quantify the mechanical properties of individual filaments. We characterize their bending stiffness using force-sensing micropipettes with nanonewton resolution, quantifying three different species across various growth stages, which affect the filament diameter and thus their bending stiffness. The observed diameter dependence of the bending modulus suggests that most of the structural rigidity emerges from a thin region near the cell wall. The connection between culture age and mechanical properties indicates that modulations of flexural rigidity may also influence the collective behaviour at different stages in the life cycle of a colony.

BP 7.27 Mon 15:00 P5

Passive vs active shells: from spectrin to actin cortex — •Tim Kutz[1], Bart Vos[1], Bart Jan Ravoo[2], Andreas Janshoff[3], and Timo Betz[1] — [1]Third Institute of Physics, Georg August Universität Göttingen, Göttingen, Germany — [2]Institute of Physical Chemistry, Georg August Universität Göttingen, Göttingen, Germany — [3]Organic Chemistry Institute and Center for Soft Nanoscience, University of Münster

The viscoelastic and tensile properties of the cell surface are key regulators of processes such as migration, division, and shape control, yet the respective roles of membrane and cortex remain only partially understood. Here, we use a combined experimental approach integrating atomic force microscopy (AFM) and micropipette (MPA) aspiration to dissect surface mechanics in two paradigmatic systems: red blood cells (RBCs) and Xenopus tadpole cells (XTCs). RBCs provide a membrane-dominated reference state with a passive spectrin network, while XTCs feature an active actomyosin cortex coupled to the plasma membrane. AFM-based tether pulling and creep compliance measurements yield local effective tension and viscoelastic response, whereas MPA reports global surface tension and large-scale deformation behaviour. From the combined data, we identify clear differences in relaxation behavior and tension build-up between RBCs and XTCs, reflecting the presence of active contractile elements in the cortex. Our results demonstrate how multi-modal micromechanical probing can disentangle membrane- versus cortex-dominated contributions to cell surface tension.

BP 7.28 Mon 15:00 P5

Deciphering the role of flagellar membrane glycoproteins in ciliary adhesion of *Chlamydomonas reinhardtii* — •Lea Rupprecht[1], Adrian Nievergelt[2], Rodrigo Catalan[1], Lara Hoepfner[3], and Oliver Bäumchen[1] — [1]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [2]Max Planck Institute of Molecular Plant Physiology, 14476 Potsdam, Germany — [3]Human Technopole, 20157 Milan, Italy

Elucidating the physical mechanisms of microbe-surface interactions is essential for developing novel technologies to control the formation of microbial biofilms. While most studies focus on bacteria as model systems, the adhesion of eukaryotic photosynthetic microorganisms to surfaces remains rather elusive. *Chlamydomonas reinhardtii* has been shown to adhere to surfaces with its two cilia under blue light [1], yet the underlying molecular mechanism remains unclear. For decades, the N-glycosylated proteins FMG1-B were considered the main adhesive components of the ciliary glycocalyx, with FMG1-A also contributing to its organization and function. We performed *in vivo* single-cell micropipette force spectroscopy [2] and adsorption/desorption [3] experiments on CRISPR/Cas9-generated FMG1-B-, FMG1-A-, and double-knockouts of *C. reinhardtii*. Thereby we examine how the absence of specific glycocalyx components affects ciliary adhesion forces in different light conditions.

[1] Kreis *et al.*, *Nature Physics* **14**, 45-49 (2018).
[2] Backholm and Bäumchen, *Nature Protocols* **14**, 594-615 (2019).
[3] Catalan *et al.*, *Soft Matter* **19**, 306-314 (2023).

BP 7.29 Mon 15:00 P5

Probing the micromechanics and fluidity of cellular spheroids — •Tom Sosniok[1], Antoine Girot[1], Gabriel de Barros Righes[2], Rodrigo Catalán[1], Ada Cavalcanti-Adam[2], and Oliver Bäumchen[1] — [1]University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany — [2]University of Bayreuth, Cellular Biomechanics, 95447 Bayreuth, Germany

Characterizing the mechanical properties of multicellular spheroids is crucial to elucidate the dynamics of biophysical processes such as pathological tissue development, tumor metastasis and disease progression. Spherical cellular aggregates

often serve as valuable tissue models, yet, they cannot be readily characterized with conventional techniques that are optimized for single cells. By combining micropipette force spectroscopy [1] with optical shape tracking, we provide an experimental approach to measure the mechanical properties of spheroids. Here, we first applied this technique to the model organism *Volvox globator*, a photosynthetic microbe that naturally forms spherical aggregates. We show that the compression and relaxation dynamics of *Volvox* can be described by a viscoelastic model, with the viscous component exhibiting a shear-thinning behaviour that is accurately described by a power-law fluid. We find that the viscoelasticity of the aggregates as well as their elastic modulus depend on their life stage. Finally, we applied the same methodology and modelling to aggregates of human colorectal adenocarcinoma cells with epithelial morphology and analysed their mechanical properties.

[1] M. Backholm and O. Bäumchen, *Nat. Protoc.* **14**, 594 - 615 (2019).

BP 7.30 Mon 15:00 P5

Intracellular mechanics in migrating cells — •Jannis Fischer[1], Mohammad Amin Eskandari[1], Sarah Louisa Lädke[1], Till Moritz Münker[1], Matthias Krüger[2], and Timo Betz[1] — [1]Third Institute of Physics, Göttingen, Germany — [2]Institute for Theoretical Physics, Göttingen, Germany

To fulfill their incredibly large number of different tasks, biological cells have developed mechanisms to adapt their physical properties and appearance, for example cell shape variation or cell migration. It is still not clear whether the changes in these mechanical properties are due to passive or active processes. Investigating and understanding these processes is the core of this work. For this, I will analyze the behavior of migrating cells, which are induced to move alternately on adhesive patterns. To connect the observed dynamics with the underlying mechanical properties and activities, I will use the new quantity of mean back relaxation (MBR). This can not only overcome the low throughput of optical tweezers, but also determine activity and mechanical properties through purely passive observations. With the MBR, we want to answer the question of how cellular shape influences mechanical properties.

BP 7.31 Mon 15:00 P5

Passive microrheology reveals anisotropic intracellular activity — •Sarah Louisa Lädke[1], Till Moritz Münker[1], Matthias Krüger[2], and Timo Betz[1] — [1]Third Institute of Physics - Biophysics, Georg August Universität Göttingen — [2]Institute for Theoretical Physics, Georg August Universität Göttingen

To investigate intracellular activity and the associated deviations from thermodynamic equilibrium, we study the fluctuations of endogenous vesicles and phagocytosed beads in various cell types and conditions. Experimentally, we combine darkfield microscopy with high-speed imaging and advanced image post-processing techniques, enabling the acquisition of trajectories with spatial and temporal resolution in the order of nanometers and milliseconds, respectively. We apply a novel observable, termed Mean Back Relaxation (MBR) [Münker et al., Nature Materials, 2024], to these trajectories. The MBR quantifies non-equilibrium in confined systems and establishes a link between intracellular particle fluctuations and their effective energies. In doing so, we aim to extend the principles of passive microrheology to non-equilibrium environments. The MBR derived from our trajectories breaks time-reversal symmetry and exhibits pronounced anisotropies, indicating not only heterogeneous cellular structures but also anisotropic activity.

BP 7.32 Mon 15:00 P5

Forces in oocyte deformation analyzed via shear flow deformability cytometry — •Merle Duchêne[1], Bart Vos[1], Jordan Dieter Groh[1], Pratima Sawant[2], and Timo Betz[1] — [1]Third Institute of Physics - Biophysics, Georg August University Göttingen — [2]Institute for X-Ray Physics, Georg-August-Universität Göttingen

Oocytes form the origin of many developing organisms and display distinct mechanical responses compared to smaller somatic cells. Their nuclei are unusually deformable, mimicking whole-cell shape during external compression. Apart from chemical signaling, mechanosensing in the nucleus plays a central role in gene expression. However, the forces involved in oocyte deformation are not quantified and still poorly understood.

Here, we aim to employ microfluidic methods to investigate deformations of cells and nuclei in a well-controlled, high-throughput method via shear flow deformability cytometry, commonly referred to as real-time deformability cytometry (RT-DC). We modified this method for oocytes, by first generating a preliminary channel design using COMSOL simulations. To evaluate device performance after fabrication, polyacrylamide beads are studied and provide a reference for estimating oocyte behavior in the same geometry. Finally, oocyte deformation is recorded to obtain mechanical properties. This helps us to better understand forces involved oocyte development and migration on its journey from the ovaries to an embryo.

BP 7.33 Mon 15:00 P5

Linking Theory and Experiment: RBC Deformation in a Cross-Shaped Microfluidic Channel — •Clara Gremmelspacher[1], Stephan Gekle[1], and Manouk Abkarian[2] — [1]Universität Bayreuth — [2]Centre de Biologie Structurale, Montpellier

Red blood cells (RBCs) must deform significantly to pass through narrow capillaries, a process governed by membrane mechanics such as shear elasticity and membrane viscosity. We use a combined experimental and computational approach to study RBC stretching under extensional flow. The investigated setup consists of two opposing inflow channels and two perpendicular outflow channels arranged in a cross shaped geometry creating a stagnation point at the intersection. By comparing deformation patterns and timescales between microfluidic experiments and Bounday-Integral-Simulations, we extract key mechanical properties of the RBC membrane. This approach links theoretical descriptions to observed dynamics, providing insights into microcirculatory behavior.

BP 7.34 Mon 15:00 P5

Mechanistic Insights into PFAS Interactions with Biological Membranes — •Samuel Türken[1], Doreen Biedenweg[2], Janet Krüger[1], Stefanie Spiegler[2], Bob Fregin[2], Wibke Busch[1], and Oliver Otto[2] — [1]Helmholtz Centre for Environmental Research - UFZ, Leipzig, Germany — [2]Institute of Physics - University of Greifswald, Greifswald, Germany

Per- and polyfluoroalkyl substances (PFAS) are widely used, highly persistent organic chemicals that accumulate in humans and the environment. PFAS exposure is associated with a range of adverse health and environmental effects, yet their mechanisms of action in human cells remain poorly understood. Molecular simulation studies show that PFAS integrate into phospholipid membranes and alter membrane fluidity in a structure-dependent manner.

To investigate how PFAS influence whole-cell mechanics, we used real-time deformability cytometry (RT-DC), which provides single-cell, millisecond-scale measurements of deformation and cell elasticity, i.e., the Young's modulus. This approach captures the mechanical response of HL60 cells after 1 minute PFAS exposures, reducing the contribution of slower cellular adaptive processes. Complementing this, we quantified PFAS-induced changes in membrane order using a Laurdan-based assay. We found that PFAS exposure decreased cell deformability and increased cell stiffness, detectable even at environmentally relevant concentrations in a dose- and structure-dependent manner. Combined membrane-order and RT-DC results show that PFAS alter membrane physical state and thereby modulate whole-cell mechanics.

BP 7.35 Mon 15:00 P5

Bat thermomechanics of red and white blood cells as a blueprint for human hibernation — •Bob Fregin[1,2], Doreen Biedenweg[1], Gerald Kerth[3], and Oliver Otto[1,2] — [1]Institute of Physics, University of Greifswald, Greifswald, Germany — [2]German Center for Cardiovascular Research, Greifswald, Germany — [3]Applied Zoology and Nature Conservation, Zoological Institute and Museum, University of Greifswald, Greifswald, Germany

Hibernation lets mammals conserve energy by sharply slowing metabolism during cold or resource-poor periods. A key challenge is sustaining blood flow at low body temperatures ($\leq 10\,^{\circ}$C). Here, the mechanical properties of red (RBCs) and white blood cells (WBCs) could play a crucial role, which we studied for the hibernating common noctule bat, the non-hibernating Egyptian fruit bat, and humans. Using dynamic real-time deformability cytometry, RBC and WBC elasticity and viscosity were measured at physiologically-relevant time scales (Milliseconds) and temperatures (37 $^{\circ}$C, 23 $^{\circ}$C, and 10 $^{\circ}$C).

Our analysis revealed a temperature-driven increase in RBC elasticity and viscosity, which is mainly influenced by membrane properties and not the cytosol. This effect is significantly enhanced in bats. Finally, our data demonstrate that RBC membranes of both bat species display a transition to a viscous-like state at lower temperatures, which is not explained by seasonal variations of environmental factors but seems to originate from physical properties of the cell membrane. Our results suggest blood cell thermomechanics as a target for future research on human hibernation.

BP 7.36 Mon 15:00 P5

Enhancing optical parameters of platelets in real-time deformability cytometry — •Tristan Franke, Bob Fregin, Doreen Biedenweg, Lucia Wegbünder, and Oliver Otto — Institute of Physics, University of Greifswald, Greifswald, Germany

Real-time deformability cytometry (RT-DC) is a high-speed, label-free cytometric method for imaging and analyzing cell mechanical properties. Cells are flushed through a narrow microfluidic channel and deform by hydrodynamic stresses, while being illuminated by a stroboscopic high-power LED and imaged by a high-speed CMOS camera.

Using RT-DC allows for investigating platelet mechanics, which are key to blood coagulation and may help explain underlying causes of, e.g., coagulopathy and thrombosis. However, with a cell size of only a few micrometers, platelets appear to be difficult to analyze optically, resulting in low image quality, often

characterized by motion blurring, low brightness, and a low level of morphological detail.

We investigated the interplay between various parameters, including LED exposure time (brightness), hydrodynamic flow rate, objective magnification, numerical aperture, and camera settings, to identify optimal imaging parameters. To further enhance image quality, we inserted a 2.18x intermediate lens in our inverted microscope setup to increase image magnification, previously not possible to achieve, while preserving the depth of focus. In combination with an extended exposure time of 9.3 μs, and a 2x digital gain our results demonstrate a balance between image brightness and motion blurring while achieving improved contrast and resolution in RT-DC.

BP 7.37 Mon 15:00 P5

Microparticle traction force microscopy for DNA microparticles based on experimental and computational advances — •Bastian K. Kraus[1,2], Simon Brauburger[1,2], Tobias Walther[3], Tobias Abele[3], Kerstin Göpfrich[3], and Ulrich S. Schwarz[1,2] — [1]Institute for Theoretical Physics (ITP), Heidelberg University — [2]BioQuant, Heidelberg University — [3]Center for Molecular Biology (ZMBH), Heidelberg University

Traction force microscopy quantifies cellular forces by inferring traction fields from the displacements of fiducial markers embedded in soft elastic substrates. Microparticle traction force microscopy extends this concept by employing elastic spherical microparticles as finite-sized force sensors. Traction fields can be recovered by two methods: the volume method, which tracks nanoparticles inside the microparticle, and the surface method, which only considers the deformed microparticle surface. Here, the two approaches are compared systematically, each as a pipeline combining image processing and elasticity theory. Moreover, they are both implemented in the same experimental system, using soft DNA microparticles with different fluorescent labels, which are held and deformed in micropatterned wells. We find that the two methods can lead to similar results, but have different advantages. While the volume method requires fewer assumptions in the elasticity equations, the surface method is less sensitive to imaging artifacts.

BP 7.38 Mon 15:00 P5

A fast & quantitative method to study membrane elasticity of suspended cells — •Eric Sündermann, Bob Fregin, Doreen Biedenweg, Jan Wilder, Stefanie Spiegler, and Oliver Otto — Institute of Physics, University of Greifswald, Greifswald, Germany

Current research acknowledges the importance of bulk and membrane mechanics for understanding cell state and function under pathophysiological conditions. While microfluidic technologies allow for measuring bulk mechanical properties at rates exceeding 1,000 cells per second, traditional approaches for assessing membrane elasticity lack the throughput required to screen entire cell populations.

Here, we utilise membrane tension cytometry (MTC), a microfluidic method combining shear-induced deformation of cells with the capabilities of Flipper-TR, a fluorophore with fluorescence lifetime proportional to the cell membrane elasticity. We established a calibration procedure using thousands of osmotically stressed red blood cells, and confirmed a quantitative relation between surface area and membrane elasticity introduced earlier for different cell models. Next, we focused on HL60 cells, a myeloid precursor cell line. We disturbed cholesterol and filamentous actin, and demonstrated that MTC is sensitive to changes in lipid composition, while being insensitive to cytoskeletal alterations. Finally, we directly measured the mitochondrial membrane elasticity inside living cells using Mito Flipper-TR. Interestingly, mitochondria seem to respond to an external hydrodynamic stress by an increase in membrane elasticity, which might be relevant to understand fission and fusion processes from a mechanical perspective.

BP 7.39 Mon 15:00 P5

The nature of correlations in the fractional Kelvin-Voigt model — •Dorian Marx[1], Raffaele Mendozza[2], Till Moritz Münker[1], Peter Sollich[2], and Timo Betz[1] — [1]Third Institute of Physics - Biophysics, Georg-August-University Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Institute for Theoretical Physics, Georg-August-University Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The inside of cells is a complex, non-equilibrium system. We are interested in the mechanics of this intracellular space, which typically are phenomenologically well described by a complex double-power law (fractional Kelvin-Voigt model). There have been multiple studies on intra- and extracellular systems using different measurement methods that indicated a correlation in the model parameters. We present an analytical and numerical analysis of the complex double-power law model, uncovering the nature of such a correlation and its dependency on measured frequency range. This results in a tool to judge experimental findings and to discern significant, possibly meaningful correlations from those stemming from the nature of the model. As complex double-power law models (or a subclass of them) seem to continue being used in the study of intracellular mechanics, we expect this theoretical investigation to be relevant going forward.

BP 7.40 Mon 15:00 P5

The biophysical response of HL60 cells to a millisecond osmotic stress — •Lucia Wegbünder[1], Eric Sündermann[1], Lea Graichen[1], Doreen Biedenweg[1], Marta Urbanska[2], and Oliver Otto[1] — [1]Institute of Physics, University of Greifswald, Greifswald, Germany — [2]Department of Physiology, Development and Neuroscience, University of Cambridge, Cambridge, United Kingdom

Local differences in the concentration of osmolytes within the human body require cells to consistently regulate their water in- and efflux. While cells are known to change their volume and mechanical properties on the timescale of seconds to minutes, their millisecond response to an osmotic stress has been, so far, unexplored.

Here, we leverage real-time deformability cytometry to apply osmotic challenges to cells and measure their physical properties including size and elastic modulus 0.5 to 10 milliseconds after exposure. We focus on HL60 cells (a myeloid precursor cell line), which are flushed through a microfluidic channel and in which they are in contact with a sheath fluid of varying osmolality. Similar to longer timescale regimes, we observe swelling under hypoosmotic, and shrinkage under hyperosmotic conditions. Independent of stress direction there is a decrease in the Young's modulus of cells. This is in contrast with long timescale findings, where cells are consistently reported to increase their stiffness under hypertonicity. The ability of cells to physically respond to osmotic stress within milliseconds can be of physiological consequences in situations where cells are exposed to steep osmotic gradients, as is the case for immune cells migrating through changing environments.

BP 7.41 Mon 15:00 P5

Mechanical and Viscoelastic Characterisation of *Giardia duodenalis* Trophozoites Using SCFS and nDMA — •Johannes Mischo[1,2], Maike Derenek[1], Markus Bischoff[1], Karin Jacobs[2], Chistian Klotz[3], Anton Aebischer[3], and Philipp Jung[1] — [1]Institute of Medical Microbiology and Hygiene, Saarland University, Homburg, Germany — [2]Experimental Physics, Saarland University, Saarbrücken, Germany — [3]Department of Infectious Diseases, Unit 16, Robert Koch-Institute, Berlin, Germany

Giardia duodenalis trophozoites use a ligand-independent, mechanically dominated suction or clutching mechanism mediated by the ventral disc to resist intestinal shear [1]. Little is known about the mechanical and viscoelastic properties of the cell. We used single-cell force spectroscopy (SCFS) on individual trophozoites to record detachment force-distance profiles. These datasets provide mechanical information of whole-cell deformation during pull-off, including contributions from the cell body, ventral disc and ventrolateral flange. Complementarily, we measured cell-body elasticity by nano-dynamic mechanical analysis (nDMA). Ventral disc and flange are inaccessible to nDMA because stationary cells keep them in surface contact. We observed single-digit kPa storage and loss moduli with a negative correlation between stiffness and approach speed. Together, SCFS and nDMA provide complementary mechanical information and a framework for understanding how *Giardia* balances elasticity and structural rigidity during its adhesion cycle and survival in the small intestine.

[1] Gunaratnam et al. Nanoscale, 2024, 16 (14), 7145-7153.

BP 7.42 Mon 15:00 P5

Dynamics of confined immune cell migration — •Santiago Kuhl and Joachim Rädler — Ludwig-Maximilians-Universität, München, Germany

Immune cells must invade tissue to reach their targets, but the dynamics and mechanics of their invasiveness are not well understood at the single cell level. Photolithographically fabricated 3D hydrogel micro-structures provide a promising platform for probing cellular invasiveness. Here we use nonadhesive 3D dumbbell-microcavities to enforce repeated encounters between single cells and pores of varying dimensions, simulating migration in a dense extracellular matrix. This platform enables us to record trajectories of macrophages and dendritic cells and measure dwell times and transmigration probabilities as a function of confinement.

BP 7.43 Mon 15:00 P5

Structural changes of sarcomeres in iPSC-derived 3D engineered skeletal muscle after laser-induced injury — •Lisa-Marie Scharfenstein[1,2], Daniel Härtter[1], Mahboubeh Farajian[2], Mattias Luber[2], Timo Betz[2], Wolfram Zimmermann[1], and Arne Hofemeier[1] — [1]Department of Pharmacology and Toxicology, University Medical Center Göttingen, Göttingen, Germany — [2]Third Institute of Physics, University of Göttingen, Göttingen, Germany

Skeletal muscle injury models are employed to study mechanisms of muscle repair and regeneration. Commonly used muscle injury models such as cryo-injury, crush-injury and cardiotoxin-treatment do not allow for precisely localized muscle damage. Here, we introduce precise laser-based injury in human iPSC-derived 3D engineered skeletal muscle (ESM) tissue grown in a custom-made culture platform. Using high-resolution live microscopy and a sarcomere reporter model (ACTN2-Citrine), we monitor Z-band morphology on timescales of seconds to several days using the previously by our group introduced AI-based Sarcomere Analysis Multi-tool (SarcAsM). In doing so, we

find an average sarcomere elongation of (0.45 +- 0.061) mum (mean +- sem) within 50 mum distance from the injury, that further decays exponentially from the location of injury towards the periphery, suggesting local impaired tensional homeostasis in myofibers surrounding the injury. Taken together, we report first data obtained in a novel human iPSC-based skeletal muscle injury model, which we intend to use for repair and regeneration inducing drugs.

BP 7.44 Mon 15:00 P5

What we learned from 6000 patient blood samples measured with deformability cytometry: age, biomarkers, and disease mechanotypes — •Markéta Kubánková[1,2], Lena Summa[1,2], Maximilian Schlögel[1,2], Martin Kräter[1,2], Manfred Rauh[3], Markus Metzler[3], and Jochen Guck[1,2] — [1]Max Planck Institute for the Science of Light, Erlangen, Germany — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany — [3]Department of Pediatric and Adolescent Medicine,University Hospital Erlangen, Germany

Deformability cytometry is a label-free microfluidic imaging technique that quantifies mechanical and morphological properties of single cells at ~1000 cells/s directly from brightfield images. Here we analyse >6000 whole-blood measurements from a clinical cohort ranging from newborns to adults. We developed an automated analysis pipeline combining feature extraction with clustering and classification of the main blood cell populations, replacing manual gating. Using this framework, we established age-dependent baselines of size and deformation for the major cell classes. We correlated the features with routine biomarkers such as CRP, IL-6 and PCT. Specific mechanotypes, particularly of neutrophils and monocytes, showed associations with these markers and provided information beyond simple cell counts. We also quantified the impact of pre-analytical confounders, such as the time between blood draw and measurement. Finally, by stratifying samples according to clinical information, we identified disease-related patterns in cell mechanotypes, providing a biophysical basis for future diagnostic applications.

BP 7.45 Mon 15:00 P5

Investigating the role of the membrane-associated cytoskeleton in neuronal action potential propagation — •Julia Butzke[1] and Kristian Franze[1,2,3] — [1]Chair of Neuronal Mechanics, Medical Institute of Biophysics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany — [3]Department of Physiology, Development and Neuroscience, University of Cambridge, Cambridge, UK

During maturation, neuronal axons develop submembraneous F-actin rings as a part of the membrane-associated periodic skeleton (MPS). The MPS has been shown to regulate axon diameter, provide mechanical support and contribute to axonal transport. However, the role of the MPS in successful action potential propagation in single axons is not yet fully understood. In this project, we investigate the impact of submembraneous F-actin rings on the mechanical aspects of action potentials. Using super-resolution microscopy, we study the effect of different F-actin-disrupting drugs on the presence and periodicity of F-actin rings in primary hippocampal mouse neurons. We then use atomic force microscopy to measure the mechanical waves that accompany action potentials in axons with different levels of F-actin ring periodicity. By analysing the possible correlation between F-actin ring periodicity and the propagation properties of the mechanical waves, we will contribute to a better understanding of the mechanical aspects of neuronal signal transmission.

BP 7.46 Mon 15:00 P5

Characterizing the Effective Membrane Tension Response to Substrate Stiffness Using AFM and Optical Tweezers — •Tina Borić[1,2], Maria Villamarin[1,2], Julia Butzke[1,2], Eva Kreysing[4], and Kristian Franze[1,2,3] — [1]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany — [2]Friedrich-Alexander-Universität, Erlangen-Nürnberg, Erlangen, Germany — [3]Department of Physiology, Development and Neuroscience, University of Cambridge, Cambridge, UK — [4]University of Warwick, Coventry, UK

Cellular membranes change their physical properties in response to mechanical stimuli, such as changes in tissue stiffness. Membrane tension transduces these mechanical signals into intracellular responses via mechanosensitive ion channels. However, how and if a change in tissue stiffness affects the surface mechanics of the cell, which in turn would contribute to the activation of mechanosensitive ion channels, is not yet known. To investigate the dependence of the effective membrane tension on substrate stiffness, we culture HEK293T cells and hippocampal neurons on custom made compliant substrates, and measure tether forces using optical tweezers and AFM. Furthermore, we use pharmacological treatments that primarily affect the actin cortex and membrane composition to characterize their contributions to the effective membrane tension. Ultimately, our aim is to understand how stiffness induced changes in membrane tension lead to the activation of the mechanosensitive ion channel Piezo1. Our work will contribute to the understanding of how mechanosensitive ion channels are gated, which may have important implications for drug design in the future.

BP 7.47 Mon 15:00 P5

Topologically invariant coordinates for dynamic epithelia undergoing morphogenesis — •Paweł Korzeb[1], Marko Popović[1,4], and Frank Jülicher[1,2,3] — [1]Max Planck Institute for Physics of Complex Systems, Dresden, Germany — [2]Center for Systems Biology, Dresden, Germany — [3]Cluster of Excellence Physics of life, Technische Universität Dresden, Dresden, Germany — [4]Rudjer Bošković Institute, Zagreb, Croatia

Epithelia are two-dimensional tissues, sheets of tightly connected cells that form many structures in organs. Such tissues acquire their shape and function through morphogenesis, a process that involves changes in both their geometry and cellular network topology. A key question in morphogenesis is to understand how cellular processes, such as cell division or T1 transitions, contribute to tissue morphology by changing its geometry and topology. For a curved epithelium, this problem can be formulated in a continuous covariant description on the tissue surface. In this work, we propose two sets of topologically invariant coordinates, describing cellular networks, obtained by embedding a graph representation of the network into $\mathbb{R}^2$ using only its connectivity, without the need to take into account the underlying tissue geometry. We construct these embeddings using the spectrum of the graph Laplacian and a spring-meshwork representation. Local changes of these topologically invariant coordinates allow us to identify the cellular processes occurring during tissue development. This formalism provides a framework to investigate the coupled evolution of epithelial geometry and topology.

BP 7.48 Mon 15:00 P5

BeadBuddy: Multiscale shape analysis of in-vivo stress sensors for force inference — •Alejandro Jurado Jiménez[1], Jonas Isensee[3], Arne Hofemeier[2], Lea Johanna Krüger[4], Raphael Wittkowski[5], Ramin Golestanian[3], Philip Bittihn[3], and Timo Betz[1] — [1]Third Institute of Physics-Biophysics, University of Göttingen — [2]Institute of Pharmacology and Toxicology, University Medical Center Göttingen — [3]Max-Planck-Institute for Dynamics and Self-Organization, Göttingen — [4]Institute of Theoretical Physics, University of Münster — [5]Department of Physics, RWTH Aachen University, DWI - Leibniz Institute for Interactive Materials

The measurement of stresses and forces at the tissue level has proven to be an indispensable tool for the understanding of complex biological phenomena such as cancer invasion, embryo development, or wound healing. One of the most versatile tools for force inference at the cell and tissue level are elastic force sensors, whose biocompatibility and tunable material properties make them suitable for many different experimental scenarios. The evaluation of those forces, however, is still a bottleneck due to the numerical methods seen in the literature until now, which are usually slow and render low experimental yield. Here, we present BeadBuddy, a ready-to-use platform for the evaluation of deformation and stresses from fluorescently labeled sensors within seconds. The strengths of BeadBuddy lie in the precomputed analytical solutions of the elastic problem, the abstraction of data into spherical harmonics, and a simple user interface that creates a smooth workflow for force inference.

BP 7.49 Mon 15:00 P5

Mechanics of reconstituted cardiac microtissues — •Polina Malova, Mattias Luber, Noemie Veyret, Anna Mukhina, Till Münker, and Timo Betz — Georg-August Universität Göttingen

Cardiovascular diseases remain the leading cause of mortality in Western countries [1]. Heart failure, which characterized by reduced cardiac output, myocardial thickening, and diminished contractile strength is among them and is highly prevalent. Human induced pluripotent stem cells (hiPSCs) are widely used for cardiac disease modelling and drug screening due to a preservation of patient-specific genetic backgrounds [2]. hiPSC-derived engineered human myocardium (EHM) microtissues provide an opportunity for *in vitro* research of the cardiac environment in a three-dimensional (3-D) system. Despite extensive characterization of the heart as a complex 3-D system, the mechanics of cellular interactions within the cardiac tissue still require detailed clarification. This work examines how cells within EHM microtissues mechanically interact with neighbouring cells and the extracellular environment to generate observed load curves. We compare contraction profiles of tissues composed of cardiomyocytes with cardiac fibroblasts to those containing cardiomyocytes with human foreskin fibroblasts. In addition, we investigate the contribution of extracellular matrix homeostatic tension to the mechanics of the 3-D system. These findings support the further development of 3-D tissue models for patient-specific drug screening.

[1] World Health Organization, 2022
[2] Takahashi K, Yamanaka S., 2006

BP 7.50 Mon 15:00 P5

Connecting tissue stiffness and glycosylation patterns in the developing brain — •Sarah Fritsche[1,2], Sebastián Vásquez-Sepúlveda[1,2], Leonhard Möckl[3,4], and Kristian Franze[1,2,5] — [1]Medical Institute of Biophysics, FAU Erlangen-Nuremberg, Germany — [2]MPZPM, Erlangen, Germany — [3]Department of Medicine 1/CITABLE, University Hospital Erlangen, FAU

Erlangen-Nuremberg, Germany — [4]MPL, Erlangen, Germany — [5]Department of Physiology, Development and Neuroscience, University of Cambridge, United Kingdom

Mild malformation of cortical development with oligodendroglial hyperplasia and epilepsy (MOGHE) is a pathological entity leading to drug resistant epilepsy that is characterised by increased density of oligodendroglial cells, hypomyelination, and heterotopic neurons in the white matter. This malformation has been linked to mutations of the galactose transporter SLC35A2. At the same time, processes like brain folding involve motion and must therefore be driven by large scale forces. This is why, in order to comprehend this disease to a greater extent, we are investigating the connection between the physical properties of brain tissue and its glycosylation patterns to emulate brain malformations in the Xenopus laevis embryo. The physical properties are measured via atomic force microscopy and the glycosylation patterns via super-resolution microscopy of metabolically labelled galactose, as well as antibody- and lectin stainings. With this approach we aim to understand the relation between the mechanical properties of brain tissue and developmental pathologies.

BP 7.51 Mon 15:00 P5

Cellular shape anisotropy couples to morphogen transport to drive pattern formation — •Stefan Nienhaus[1] and Diana Khoromskaia[1,2] — [1]Institut für Theoretische Physik, Universität Münster, 48149 Münster, Germany — [2]Center for Soft Nanoscience, Universität Münster, 48149 Münster, Germany

To attain their intended structures, many tissues have been shown to rely on morphogens that induce concentration-dependent changes in cell fate and in cellular mechanical properties. These changes can alter the transport properties of the morphogen within the affected tissue. Hence, a feedback loop may arise in which tissue patterning influences morphogen distribution, which in turn influences tissue patterning (bioRxiv:658228). This concept also applies to tissues with nematic order, which has been shown to be crucial to certain morphogenetic processes that predominantly occur at topological defects.

In this work, we explore the complex couplings between morphogens and nematics and aim to investigate the role of topological defects in localising cellular signalling for morphogenesis. Previous work has shown that cellular shape anisotropy may lead to anisotropic diffusion (bioRxiv:683494). Here, through numerical simulations of a reaction-diffusion system coupled to a nematic order parameter, we study how locally anisotropic diffusion affects the observed patterns. Introducing a concentration-dependent nematic alignment as a next step, we will investigate mechanisms of self-organisation that arise from this inherent coupling of morphogens and nematic order in tissues.

BP 7.52 Mon 15:00 P5

Quantifying vascular morphology on a chip — •Leonie Karr — TUM, Munich, Germany

Our human vasculature is dynamic, growing and reorganising not only in development but also continuously adapting its morphology. Yet, what determines vessel formation and branching in healthy and disease states seems complex, given the multitude of contributing factors. Our focus lies in growing a human vasculature within the controlled environment of a chip, with the goal of quantifying the flow properties of self-organised in vitro networks. Employing image analysis techniques in conjunction with flow simulation methods, our objective is to accurately quantify how flow and related properties, such as shear stress and absorption determine network architecture. The results obtained from our analyses will significantly contribute to the development of next-generation therapeutics aimed at targeting vessel development.

BP 7.53 Mon 15:00 P5

Mechanics of spinal cord regeneration in Xenopus laevis — •Maria Tarczewska[1,2] and Kristian Franze[1,2,3] — [1]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany — [2]Medical Institute of Biophysics, Friedrich-Alexander- Universität Erlangen-Nürnberg, Erlangen, Germany. — [3]Department of Physiology, Development and Neuroscience, University of Cambridge, Cambridge, UK

In mammals, spinal cord injury (SCI) often leads to paralysis due to the limited regeneration of damaged neurons in the central nervous system (CNS). The African clawed frog (Xenopus laevis) can regenerate CNS neurons during its early life stages - pre-metamorphosis. However, this ability is lost post-metamorphosis, in frogs adult form. Biochemical differences between pre- and post-metamorphosis frog spinal cord tissue identified so far cannot fully explain the differences in their regenerative capacity, suggesting that other signals may contribute to the regeneration. Following SCI, the composition of the extracellular matrix changes, and scar tissue forms. In mammals, this scar tissue, which is softer than healthy tissue, inhibits axon regeneration. In zebrafish, whose CNS neurons regenerate after SCI, tissue stiffens after injury. Mechanical properties of frog spinal cord tissue have not been measured yet. Because mechanosensing of tissue stiffness is critical for axon growth, we test the hypothesis that tissue stiffness is a critical factor in axon regeneration after SCI. We investigate the mechanical differences in the SCI lesion environment in Xenopus. By examining both tissue stiffness and molecular changes, we will illuminate the relationship between these factors and the regenerative capabilities.

BP 7.54 Mon 15:00 P5

Dimensionality and confinement reshape competition in cellular renewing active matter — •Patrick Zimmer[1,2], Philip Bittihn[1,2], and Yoav G. Pollack[1,2] — [1]MPI for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, Göttingen University, Germany

Cellular renewing active matter—assemblies of proliferating and apoptotic cells—underlies tissue homeostasis, morphogenesis, and clonal competition. Previous work in one-dimensional periodic systems identified a fitness advantage associated with rapid dead-cell clearance, an "opportunistic" competition mechanism. Extending this framework, we study two-dimensional cellular aggregates and show that dimensionality modifies the interplay between competition mechanisms for clones with different clearance rates: in 2D, opportunistic and homeostatic-pressure-based competition jointly shape clonal selection. We introduce an explicit circular confinement to probe how boundaries modulate this interplay. While opportunistic competition persists, distinct timescale-dependent behaviors emerge through weakened homeostatic-pressure-based competition near boundaries. Structural analysis reveals that confinement promotes tangential alignment and spatially heterogeneous homeostatic pressure, thereby reshaping competitive outcomes at tissue edges. Our study connects newly discovered competition mechanisms with more realistic biological contexts, highlighting how dimensionality and spatial constraints influence tissue structures and modulate competition in heterogeneous cell populations, with implications for tumor growth dynamics and tissue development.

BP 7.55 Mon 15:00 P5

Remotely Actuated Elastic Meta-Lattices using Bjerknes Forces — •Laurin Sartori[1], Peer Fischer[1,2], and Athanasios G. Athanassiadis[1,2] — [1]Heidelberg University, Heidelberg, Germany — [2]Max-Planck Institute for Medical Research, Heidelberg, Germany

Acoustically-responsive elastic structures have recently gained interest as tools for gentle, wireless manipulation of biological materials. By combining acoustic effects with elastic structures, they can be actuated dynamically to even manipulate single cells in fluidic chambers. However, there is currently a large gap between existing manipulators designed for single cells and larger-scale acoustically-actuatable materials that could be integrated with larger biological tissues or organoids.

Here, we introduce a dynamic acoustic metamaterial that can be change both its geometric configuration and elastic properties in response to sound. The metamaterial consists of an elastic lattice with embedded gas bubbles, and is actuated leveraging the secondary radiation forces between embedded bubbles. By tuning the driving or the microscopic structures the specific response of the material can be tailored. We introduce a numerical model to predict the response of arbitrary lattices, and validate the model experimentally using carefully designed structures that achieve the desired motion.

The engineered lattices shown in this work can be used as building blocks for metamaterials with a remotely tunable stiffness, auxetic properties and memory behavior, providing new interaction paradigms for applications in bio-interfaced soft robotics.

BP 7.56 Mon 15:00 P5

Direct Measurement and Enhancement of Piezoelectric Fields around Microparticles in an Ultrasound Field — •Mareike Stoll[1,2], Honorata Kazimierczak[1,2], Peer Fischer[1,2], and Athanasios Athanassiadis[1,2] — [1]Institute for Molecular Systems Engineering and Advanced Materials, Heidelberg University, Heidelberg, Germany — [2]Max Planck Institute for Medical Research, Heidelberg, Germany

There is growing interest in designing ultrasound-responsive materials that broaden the possibilities for non-invasive, remotely controlled therapies. In this context, piezoelectric micro- and nanoparticles are emerging as promising mediators, generating electric fields and reactive chemical species that can interact with biological tissues. Despite growing evidence suggesting macroscopic effects, a direct measurement of the piezoelectric response of individual particles under an applied ultrasound field has not yet been demonstrated. This knowledge gap presents a hurdle to further design and targeting of piezoelectric particle-mediated therapies. In this work, we introduce a new methodology and provide the first direct measurements of electric potential generated by piezoelectric microparticles during ultrasonication. By mapping the time-varying potential around microparticles we are able to quantify the ultrasound-induced fields and identify enhancement strategies. These results provide a first step to disentangling the contributions of different physical processes involved in sonopiezoelectric therapies, and provide insights into the feasibility and design strategies for therapies based on ultrasound-activated piezoelectric materials.

BP 8: Systems and Networks Biophysics

Time: Monday 16:45–18:30 Location: BAR/0106

BP 8.1 Mon 16:45 BAR/0106

Origins of the Fittest: Clonal interference in the World Aviation Network — •Adrian Zachariae, Pascal Klamser, and Dirk Brockmann — Technische Universität Dresden, Dresden, Deutschland

Clonal interference, the competition between strains carrying different beneficial mutations, plays a crucial role in shaping evolutionary outcomes in asexual populations. Since the spread of new mutations is critical for CI, it is strongly influenced by the structure of the population. For example, long-range connections can rapidly distribute new mutations, reducing CI. We investigate how this phenomenon unfolds in the the World Aviation Network, which shapes the population structure of microorganisms that use humans as hosts, including pathogens. We developed a novel analytical framework that models the succession of adaptive mutations as a Markov Renewal Process. The process is built by leveraging epidemic modeling methods to model mutation spread in the network. Or approach reveals how the interplay between mutation rate and network topology gives rise to distinct evolutionary regimes: At low mutation rates, strains originating from globally central nodes have higher fixation probabilities, while at higher mutation rates, meso-scale and local properties become more important. Applied to the WAN, affluent, western regions are most likely origins of high-fitness lineages in the low-rate regime, shifting to more populous nations in Asia at high rates. The framework provides valuable insights how spatial structure shapes evolutionary outcome, with particular relevance for pandemic preparedness.

BP 8.2 Mon 17:00 BAR/0106

Polymerization of prebiotic building blocks in a wet-dry cycling system — •Almuth Schmid — LMU, Geschwister-Scholl-Platz 1, München

When it comes to the question on how life could have emerged on an early Earth, not only the setting plays an important role but also the chemistry that helped forming the first building blocks of life. Prebiotic chemistry is limited in multiple ways since many of the common catalysts life uses nowadays are too complex to have been present in such an early stage. In addition, the existing compounds were diluted and only available in low concentration. To overcome these problems, systems like wet-dry cycles can help accumulating molecules while at the same time lowering the reaction activation barrier.[1] In addition, amino acids promote RNA copolymerization more than 100-fold via acid-base catalysis, starting from prebiotically plausible ribonucleoside-2',3'-cyclic phosphates.[2] MD simulations and X-ray crystallography confirmed that water is still present in the dry state, limiting the condensation reaction and hydrolyzing the material. Preliminary experiments showed that by using ammonium salts instead of sodium salts, including nucleotides and hydroxide to adjust the pH, overall longer polymers and yields 5-fold higher than before were obtained. Expanding this adapted wet/dry cycling system with an NH3/CO2 enriched atmosphere [3] would re-create a day and night rhythm on the early Earth, providing a prebiotic way to synthesize RNA.

Invited Talk BP 8.3 Mon 17:15 BAR/0106

Constructing synthetic life-like vesicle systems by integration of artificial metabolic reaction networks — •Laura Heinen — DWI - Leibniz Institut für interaktive Materialien, Aachen, Germany

Life emerges as a systemic property of the interplay of complex chemical reaction networks out of equilibrium. Living cells, for example, need energy to grow, divide, process information and synthesize their own constituent building blocks. In my group we develop minimal metabolic reaction networks to fuel out of equilibrium behavior in synthetic lipid vesicles, to finally, build active cell-like compartments bottom-up, called synthetic cells. In my talk I will demonstrate the construction of autonomous, active behavior in vesicles by the example of cross-feeding in between synthetic vesicles. Key to such sustained out-of-equilibrium behavior is the selective transport of energy molecules across the lipid membrane. One population of vesicles produces and exports adenosine triphosphate (ATP) while a second population of vesicles takes up the ATP and uses this chemical energy to fuel ATP-consuming reactions. The hydrolyzed ATP feeds back into the first vesicle population where it will be recycled, and the interdependent metabolic cycle can be sustained. The vesicles are a platform to enable active behavior in synthetic systems in a continuous, autonomous and adaptive fashion. Fundamentally, they allow us to study non-equilibrium processes in an energy-controlled environment and will promote our understanding of constructing life-like materials and systems.

BP 8.4 Mon 17:45 BAR/0106

Living Network Dynamics: From pH-Stimulated Growth to Resistance Optimization — •Mathieu Le Verge-Serandour, Alexandra Bienau, Karen Alim, and Friedrich Simmel — School of Natural Sciences, Technical University of Munich

In this work, we explore how vascular-like functionality can be integrated into bioelectronic interfaces using the unicellular slime mold Physarum polycephalum. This organism forms a dynamic, self-organized tubular network that exhibits emergent behaviors such as optimization, adaptation, and self-healing, making it an ideal model for studying decentralized, stimulus-responsive growth. By leveraging electrochemically induced pH gradients, we experimentally translate designed network layouts into biological structures and characterize the key dynamics underlying their responses to pH stimuli.

We further analyze Physarum morphological evolution, where the network reorganizes over several hours to evacuate a defined area by sequentially pruning competing parallel veins, ultimately forming a tree-like architecture. Drawing an analogy with power-grid networks, we investigate how sequential pruning depends on the ratio of tube to network resistance. Analytical and numerical results show that regular graphs undergo pruning until the average node degree falls below four, a finding that remains robust in simulations of random networks. Incorporating mass redistribution into this process leads to resistance homogenization, revealing fundamental physical constraints that shape adaptive transport networks.

BP 8.5 Mon 18:00 BAR/0106

Simulation of autoimmune and autoinflammatory diseases: the novel mechanism of psoriasis progression. — •Nadezhda Esenkova[1,2], Lukas Pöschl[1,2], Gerard C. L. Wong[3], and Vasily Zaburdaev[1,2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany — [2]Max-Planck-Zentrum für Physik und Medizin, Germany — [3]University of California, Los Angeles, USA

Autoimmune and autoinflammatory diseases (AIIDs) still remain an unsolved problem. One of the most studied diseases which carries features of both types is psoriasis. In this study, we are focusing on the novel mechanism of disease enhancement, driven by antimicrobial peptides (AMPs) and AMP-like fragments organizing innate immune ligands for enhanced binding to Toll-Like Receptors in immune cells. These fragments have a diverse origin: there is strong recent evidence that serine proteases can digest viral and host proteins into AMP-like fragments. In order to explore the effect of this emerging pathway, we developed a new unified interaction network model for psoriasis, based on the current extant measurements. The model was reduced to a system of nonlinear differential equations, which were studied by using dynamical system theory and numerical methods. Importantly, we find that the proposed model can reproduce the full spectrum of disease progression from healthy response to uncontrolled inflammation and allows comparison of different therapeutic interventions. Finally, by expanding the model to include diffusion, we can successfully predict the geometry of psoriatic plaques, the precise measurements of which may inform modulation of treatment.

BP 8.6 Mon 18:15 BAR/0106

Network-induced control of sustained oscillations in SIRS epidemics — •Samuel Ropert[1,2], Tomas Perez-Acle[2], and Dirk Brockmann[1] — [1]Technische Universität Dresden, Dresden, Germany — [2]Universidad San Sebastián, Santiago, Chile

Sustained oscillations in SIRS epidemic models are well understood in well-mixed populations when infectious and immune periods deviate from exponential waiting times. In contrast, the role of contact network structure in generating or suppressing such oscillations has received little attention. Existing work on small-world networks reports oscillations but does not relate them to effective transition-time distributions. This work investigates how network topology shapes oscillatory SIRS dynamics by simulating a stochastic SIRS process on self-similar modular hierarchical (SSMH) networks. These networks interpolate between random-like graphs and strongly modular, hierarchical structures while preserving system size and mean degree. A single structural parameter controls edge placement across hierarchical levels, reshaping effective distances between communities. Preliminary results show that random-like networks support robust, coherent oscillations in global prevalence, whereas increasing hierarchical modularity desynchronizes outbreaks across communities and gradually destroys the global limit cycle, leading to damped or irregular fluctuations. These findings support an interpretation of epidemic oscillations as a synchronization phenomenon of individual SIRS cycles, where network topology promotes or inhibits global coherence by reshaping the time-to-infection distribution through changes in effective distances.

BP 9: Single Molecule Biophysics

Time: Monday 16:45–18:30 Location: BAR/0205

Invited Talk BP 9.1 Mon 16:45 BAR/0205

Breaking the photobleaching limit in single-molecule FRET with nanophotonic DyeCycling. — Benjamin Vermeer[1], Dong Hoon Shin[2,3], Alexander Vogel[4], Fabian Zundel[1], Sabina Caneva[2], and •Sonja Schmid[1,4] — [1]University of Basel, Basel, Switzerland — [2]Delft University of Technology, Delft, The Netherlands. — [3]Korea University, Sejong, Republic of Korea — [4]Swiss Nanoscience Institute, Basel, Switzerland

Paradoxically, single-molecule FRET studies rely on ensemble averaging during data analysis, because early photo-bleaching prohibits sufficient sampling of single molecules. As a result, the FRET-based study of inter- and intra-molecular heterogeneity in biomolecular function - a specific hallmark of single-molecule techniques - is hardly possible, preventing insights into dynamic disorder, the effects of post-translational and other modifications, of rare but decisive states, etc. Here, we demonstrate hour-long single-molecule FRET observations using DyeCycling in zero-mode waveguides, which circumvents photobleaching through reversible fluorophore binding. We detect the conformational dynamics of single molecules over four orders of magnitude in time (milliseconds-hour), enabling us to directly observe slow kinetic regime changes within individual molecules that were intractable previously. Moreover, we demonstrate the versatility of DyeCycling with DNA and protein molecules. Together, these advances establish DyeCycling/FRET as a powerful new approach that vastly expands the information gain of single-molecule FRET, enabling the study of important biological questions that were previously inaccessible.

BP 9.2 Mon 17:15 BAR/0205

Monitoring the ribosome dynamics at the single molecule level — •Baptiste Bouhet[1], Sandra Blanchet[2], Charles Truong[3], Olivier Namy[2], and Karen Perronet[1] — [1]Light, Matter and Interactions lab, Gif/Yvette, France — [2]Institute for Integrative Biology of the Cell, Gif/Yvette, France — [3]Centre Borelli, Gif/Yvette, France

Protein synthesis is a complex multi-step process involving factors that need to interact in a coordinated manner to properly translate mRNA. As translating ribosomes cannot be synchronized over many elongation cycles, single molecule studies, mainly using total-internal-reflexion fluorescence microscopy, have been introduced to better understand translation dynamics. We decided to monitor the passage of individual, unmodified eukaryotic ribosomes from wheat germ extracts at specific fluorescent primers hybridized along mRNA. Because of the ribosome helicase activity, the double strand formed by the oligonucleotide and the mRNA is opened while the ribosome translates this region of the mRNA. Thus, the consecutive loss of fluorescence signal of two oligonucleotides allows us to measure the translation speed distribution of single ribosomes. We use this system to measure simultaneously the initiation and the elongation kinetics for linear mRNA and during -1 frameshifting, which is induced by a secondary structure on mRNA. We are also currently developing a magnetic tweezers assay to get complementary information on the opening dynamics of these structures. Thanks to its versatility, this method is a valuable tool to investigate translation machinery modifications in human diseases.

BP 9.3 Mon 17:30 BAR/0205

Single-molecule force and torque spectroscopy reveals conformational transitions in DNA and proteins — •Jan Lipfert — Universität Augsburg

Magnetic tweezers are a powerful tool to probe single molecules under precisely controlled forces, down to well below 1 pN, and, in addition can control twist and torque. Here, I highlight recent developments and applications of magnetic tweezers. In particular, I will present how we use magnetic tweezers to probe regulatory conformational changes in protein complexes, including pathogen-cell adhesion and the initiation of primary hemostasis by von Willebrand factor. In addition, I will show how we use the capabilities of magnetic tweezers to precisely measure DNA helicity under changes in environmental conditions and upon small-molecule binding.

BP 9.4 Mon 17:45 BAR/0205

Direct measurement of ultra-weak plant kinesin steps using silicon nanospheres as optical tweezers probes — •Aleksandr Kostarev[1], Shu Yao Leong[1], Anita Jannasch[1], Minoru Fujii[2], Hiroshi Sugimoto[2], and Erik Schäffer[1] — [1]Eberhard Karls Universität Tübingen, Tübingen, Germany — [2]Kobe University, Kobe, Japan

Kinesin motor proteins are essential for transport along cytoskeletal microtubules and cell division. In plants, cytokinesis relies on phragmoplast orienting kinesins (POKs). The kinesin-12 paralog POK2 can generate only about 300 fN of force. This low force is consistent with the idea that POK2 does not transport cargo, similar to weak kinesin-8 motors, the function of which is unknown in plants. To understand the function and mechanochemistry of these ultra-weak motors, it is necessary to detect their individual steps during ATP hydrolysis. However, the spatiotemporal resolution achieved with conventional probes in optical tweezers is insufficient for detecting fast steps at such low forces. To overcome this limitation, we used high refractive-index silicon nanospheres for optical trapping. With these nanospheres, we achieved an unprecedented force resolution of 60 aN at room temperature in liquids with a force sensitivity of 2.7 fN Hz^(-1/2). We bound single POK2 or plant kinesin-8 motors to the nanospheres and were able to detect individual 8-nm steps with 4-nm substeps within a force range of 100-400 fN. These in vitro measurements establish a path toward identifying plant kinesin function and demonstrate the potential of silicon nanospheres for studying ultra-weak molecular machines.

BP 9.5 Mon 18:00 BAR/0205

Ultrafast sensing of single nanoparticles with an optofluidic microcavity — •Shalom Palkhivala[1], Larissa Kohler[1], Christian Ritschel[1], Christoph Pauer[2], Tim Liedl[2], Claus Feldmann[1], and David Hunger[1] — [1]Karlsruhe Institute of Technology, Karlsruhe — [2]Ludwig Maximilian University, Munich

The characterisation of single, unlabelled particles in water is of much interest in biophysics and chemistry, where most processes occur in an aqueous environment. We report measurements of single nanoparticles in aqueous suspension using a fibre-based Fabry-Perot microcavity. For quantitative analysis of the nanoparticles' diffusion dynamics, we developed an analytical autocorrelation function to model diffusion in a standing wave field. This enabled the accurate sizing of nanoparticles having diameters down to 3 nm. [1]

Additionally, the rotational dynamics of anisotropic particles were investigated. Via the polarization modes of the cavity, the orientation of a nanorod was tracked with high temporal resolution (~ 20 ns), orders of magnitude faster than most other current techniques. As an application of our sensor to biosensing, we demonstrate measurements of individual DNA "origami" structures and of few protein molecules, which already enabled their hydrodynamic sizes to be determined.

We further expect our nanosensor to give an insight into the structural properties and conformation of single bioparticles, and to become a powerful tool for diagnosis in biomedicine and for biochemical and environmental assays.

[1] Palkhivala *et al.* (2025), *ACS Nano*, 19, 45, 39320-39326

BP 9.6 Mon 18:15 BAR/0205

Indications for Ultrafast Energy Transfer and Subsequent Disulfide Bond Cleavage in Lysozyme upon Ultrafast Excitation of Aromatic Residues — •Philip Wehling[1], Jessica Harich[1], Antonia Freibert[1], Ru-Pan Wang[2], Tae Gyun Woo[3], Junho Lee[3], Seonghyeon Jeong[3], Sungin Yu[3], Haneol Oh[3], Migel Ochmann[1], Victoria Kabanova[4], Emma Beale[4], Philip Johnson[4], Claudio Cirelli[4], Camila Bacellar[4], Briony Yorke[5], Tae Kyu Kim[3], and Nils Huse[1] — [1]University of Hamburg, Hamburg, Germany — [2]DESY, Hamburg, Germany — [3]KAIST, Daejeon, Republik of Korea — [4]Paul Scherrer Institute, Villigen, Switzerland — [5]University of Leeds, Leeds, U.K.

Disulfide bonds play a crucial role in stabilizing the tertiary structure of proteins. Ultraviolet (UV) radiation leads to S-S bond cleavage, possibly compromising the functionality of proteins. Femtosecond X-ray absorption spectroscopy at the sulfur K-edge revealed ultrafast geminate disulfide bond reformation in aliphatic disulfides [1]. These findings raise the question how disulfide bridges behave in proteins upon UV irradiation. Disulfide photochemsitry in Lysozyme by UV excitation across the dominant absorption of the aromatic residues leads to efficient sulfur radical formation which must stem from energy transfer. We discuss yields and possible mechanisms of energy transfer in competition with direct photocleavage of disulfide bridges, and implications for energy dissipation and structural integrity of proteins.

[1] M. Ochmann et al, Nat. Commun. 15, 8838 (2024).

BP 10: Active Matter III (joint session BP/CPP/DY)

Time: Tuesday 9:30–12:45 Location: BAR/SCHÖ

BP 10.1 Tue 9:30 BAR/SCHÖ

inertia-driven re-entrant coil-Globule transition of active ring polymers — •Sunil P Singh[1], Roland G Winkler[2], Rakesh Palariya[1], and Arindam Panda[1] — [1]Indian Institute of Science Education and Research Bhopal, India — [2]Theoretical Physics of Living Matter, Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Germany

The role of inertia in the collective dynamics of active systems has been a subject of increasing interest in recent studies. The present study investigates the inertial effects on active agents. We present the conformational and dynamical characteristics of an active Brownian ring polymer using Langevin dynamics simulations. We show that a long active ring polymer shrinks into globular-like structures even in the absence of attractive interactions. This transition becomes sharper and the structures more compressed as the reduced moment of inertia of the monomers increases, particularly in the intermediate range of activity. We demonstrate that the ring polymer undergoes a coil-globule-coil transition, which is modulated by both activity and rotational inertia. The coil-to-globule transition is mapped in the inertial parameter space (J-M) using the radius of gyration. Additional physical quantities, including bond-bond correlations, scaling behavior in the compressed state, monomer contact probability, geometric distances, coordination number, and effective temperature, further elucidate the physical mechanism driving the collapse. Finally, we show that the effective diffusivity of the ring polymer increases with the reduced moment of inertia as $D_p \sim \sqrt{J}$.

BP 10.2 Tue 9:45 BAR/SCHÖ

Shape selectivity by complex buckling dynamics in poroelastic active gels — •Kinjal Dasbiswas[1], Subhaya Bose[1], Arnab Roy[1], Michael Vennettilli[1], and Anne Bernheim[2] — [1]University of California, Merced, USA — [2]Ben Gurion University, Israel

Shape change in animal cells is prototypically driven by active forces, generated by myosin molecular motors bound to the actin cytoskeleton. Inspired by experiments on disc-shaped extracts of crosslinked actomyosin gels, we aim to show how a family of 3D shapes can arise from buckling caused by non-uniform active stresses. Although synthesized with identical composition of actin, myosin and the crossliker fascin, these gels contract and buckle into different shapes depending on the initial aspect ratio of the disc: thinner gels tend to wrinkle, while thicker gels tend to form domes. By incorporating active stresses, actin alignment, and stress-dependent myosin binding kinetics into a 2D poroelastic gel model, we qualitatively capture trends in gel contraction dynamics observed from quantitative particle image velocimetry (PIV). Next, we carry out numeric simulations of a geometric elastic model for thin sheets to obtain 3D buckled shapes from the strain rates predicted by the poroelastic model. Our results show that the coupling of elasticity to solvent flow, motor binding and fiber alignment play an important role in shape changes in living matter. Our studies have implications for shape changes during tissue morphogenesis and cell migration.

BP 10.3 Tue 10:00 BAR/SCHÖ

The energy cost to build a spindle — •Dongliang Zhang[1], Xingbo Yang[4], Jan Brugués[2,1,3,4], and Frank Jülicher[1,3,4] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [3]Center for Systems Biology Dresden, Dresden, Germany — [4]Physics of Life, Cluster of Excellence, TU Dresden, Dresden, Germany

Spindle is a structure actively build from microtubules (MTs), and plays an important role for chromosome segregation during cell cycle. It's observed in experiments that the spindle size and shape depends on the cell level metabolic rate. In this work, we developed a minimal model that captures the active, energy-consuming processes such as MT turnover and active stress generation, which shows the energy cost for spindle mass maintenance and spindle-shape formation. We show that a spindle can be self-organized through these active processes. We aim to predict how the size and shape of the spindle depends on the energy input, and explain relative experimental phenomena, e.g. spindle shrinkage when the metabolism level is reduced.

BP 10.4 Tue 10:15 BAR/SCHÖ

Cytoskeletal oscillations drive large-scale flows and nuclear organization in early embryonic systems. — •Lara Koehler, Elissavet Sandaltzopoulou, and Jan Brugués — Physics Of Life, TU Dresden

Synchronization drives early embryonic development, enabling simultaneous cell divisions and the spatial organization of nuclei within the embryo. In organisms such as Xenopus, Drosophila, and zebrafish, mitotic waves coordinate cell cycles across distances that exceed diffusion limits, guided by a chemical oscillator. At the same time, global cytoplasmic flows in these syncytial tissues contribute to the large-scale self-organization of nuclei, yet the coupling between biochemical signaling and cytoskeletal mechanics that underlies these directed flows remains poorly understood. Here, we relax the geometric constraints of the embryo and investigate nuclear dynamics in Xenopus egg extracts and complementary simulations. We show that the periodic polymerization and depolymerization of microtubule asters are sufficient to generate robust large-scale directed flows, even though the asters are intrinsically isotropic. Furthermore, we demonstrate that cell division stabilizes short-range order in a global synchronized system. Together, these findings reveal a minimal physical mechanism by which cytoskeletal dynamics and biochemical oscillations jointly organize flows and patterns, with implications for understanding the emergent principles that shape early development across species.

BP 10.5 Tue 10:30 BAR/SCHÖ

Geometric control of cell migration in disordered porous media — •Laeschkir Würthner[1] and Frederik Graw[2] — [1]European Molecular Biology Laboratory, Heidelberg, Germany — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg and Universitätsklinikum Erlangen, Erlangen, Germany

Cell migration is a dynamic process that plays a central role in development, wound healing, and immune responses. Active cell movement is controlled by several biochemical and mechanical cues, including chemokine gradients and the mechanical properties of the extracellular matrix (ECM). Although the biochemical pathways underlying directed cell motion are increasingly well understood, the influence of the porous structure of the ECM on active cell motion remains largely unexplored. Using a combination of computational modeling and theory, we investigate how active cells move through 3D disordered porous environments. We show that cell migration in disordered porous media can be understood as a generalized random walk among "traps", with the effective diffusivity determined by the geometry of the microenvironment. A key implication of our work is that spatial heterogeneities in porosity effectively direct cell motion, revealing a guidance mechanism that we refer to as porotaxis. Overall, our work connects geometry with cell motility and underscores the microenvironment as a key regulator of cell migration.

BP 10.6 Tue 10:45 BAR/SCHÖ

Motility-induced mixing transition in exponentially growing multicellular spheroids — •Torben Sunkel[1,2], Lukas Hupe[1,2], and Philip Bittihn[1,2] — [1]MPI for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, University of Göttingen, Germany

Growth drives cellular dynamics in various dense aggregates, but its effects on other relevant activities have only received limited attention. Here, we investigate the interplay of unconstrained growth, steric repulsion and motility in a minimal agent-based model of exponentially growing, three-dimensional spheroids. Our results reveal a diverging mixing time scale at a critical motility threshold, below which mixing of cells is completely suppressed. Above the threshold, large-scale mixing is enabled. Using an effective phenomenological model parameterized from full simulations, we identify two fundamental mechanisms governing this transition: On the cell scale, weak motility-induced active motion is locally suppressed by growth-induced steric repulsion, consistent with an Active Brownian Particle type description of single-cell dynamics. Beyond this, the expanding nature of the system inhibits global mixing purely geometrically by limiting the exploration range of diffusive cell motion. Both mechanisms naturally scale with the growth rate, highlighting the nature of the transition as an interplay between proliferation and motility. The results provide a baseline for identifying additional biological mechanisms in experiments and could be relevant for competition, heterogeneous tumor evolution and other manifestations of motile proliferating active matter.

15 min. break

BP 10.7 Tue 11:15 BAR/SCHÖ

Fluctuation-Response Theory of Non-Equilibrium Complex Fluids — •Ryota Takaki[1] and Frank Jülicher[1,2,3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Center for Systems Biology Dresden, Dresden, Germany — [3]Cluster of Excellence Physics of Life, TU Dresden, Dresden, Germany

Active soft materials such as cytoplasm and tissues are constantly driven by chemical reactions and often retain long-lived mechanical memory. In this work, we develop a generalized hydrodynamic framework applicable to non-equilibrium fluids with memory at finite wavevectors and frequencies. Our approach is based on exact correlation-function identities, leading to a fluctuation-response relation for steady states, including non-equilibrium. Applying the theory to chemically driven active fluids, we uncover Active Viscoelastic Memory, in which reaction cycles dynamically renormalize the viscous response and can generate negative storage moduli at finite frequency, absent in conventional viscoelastic materials. Our results provide a first-principles basis for modeling memory-dependent dynamics in a broad class of biological and synthetic active

systems, and suggest concrete rheological signatures of chemical driving that can be tested experimentally.

BP 10.8 Tue 11:30 BAR/SCHÖ

Chemically Active Liquid Bridges Generate Repulsive Forces — •Noah Zierthen — DAMTP, University of Cambridge, UK

Intracellular droplets help organize cells by compartmentalizing biomolecules and mediating mechanical interactions. When such droplets bridge two structures, they generate capillary forces that depend on the surface properties and the separation between the structures. While the forces exerted by passive liquid bridges are well understood, the impact of active chemical reactions, ubiquitous in biological condensates, remains unclear.

Here, we investigate a single liquid bridge with continuous chemical turnover, in which the production and degradation of droplet material maintain a non-equilibrium steady state. In this active bridge, the reactions dynamically set the bridge radius, thereby controlling the force-distance relation. In striking contrast to passive systems, we find that activity can generate purely repulsive forces over a broad range of separations. These results show that chemical activity can qualitatively alter capillary forces generated by liquid bridges, suggesting a potential route for cells to actively regulate mechanical coupling via droplets.

BP 10.9 Tue 11:45 BAR/SCHÖ

Shared Laws of Pattern Formation in Reaction-Diffusion and Phase Separation — •Daniel Zhou[1] and Erwin Frey[1,2] — [1]Arnold Sommerfeld Center for Theoretical Physics — [2]Max Planck School Matter to Life

Many nonlinear field theories generate a strikingly similar repertoire of patterns: arrested coarsening, traveling waves, and spatiotemporal chaos appear both in phase-separating systems and in classical reaction-diffusion models. These descriptions have different physical origins, yet recent studies on Turing mixtures and foams in protein systems [1] and on chemotaxis-driven phase separation in cell populations [2] have already highlighted unexpected connections between these ostensibly different mechanisms, linking foam-like, phase-separating, and reaction-diffusion-type patterns. The present work revisits the relation between kinetic and phase-separating descriptions from a more general viewpoint. A unifying perspective is developed that places different modeling frameworks on comparable footing, identifies the conditions under which they yield effectively equivalent patterns, and suggests how stability criteria and design principles can be translated between them. This points toward a more systematic classification of pattern-forming dynamics that cuts across traditional divides between reaction-diffusion, chemotactic, and phase-separating systems.

[1] H. Weyer et. al, Deciphering the Interface Laws of Turing Mixtures and Foams, arXiv:2409.20070 (2024).

[2] H. Weyer et. al, Chemotaxis-Induced Phase Separation, Physical Review Letters 135, 208402 (2025).

BP 10.10 Tue 12:00 BAR/SCHÖ

Spatial self-organization of enzymes in complex reaction networks — •Vincent Ouazan-Reboul[1,2], Ramin Golestanian[2,3], and Jaime Agudo-Canalejo[2,4] — [1]LPTMS, CNRS, Université Paris-Sud, 91400, Orsay, France — [2]Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, D-37077, Göttingen, Germany — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, OX1 3PU, Oxford, UK — [4]Department of Physics and Astronomy, University College London, WC1E 6BT, London, UK

Living systems contain intricate biochemical networks whose structure is closely related to their function and allows them to exhibit robust behavior in the presence of external stimuli. Such networks typically involve catalytic enzymes, which can have non-trivial transport properties, in particular chemotaxis-like directed motion along gradients of substrates and products. Here, we find that taking into account enzyme chemotaxis in models of catalyzed reaction networks can lead to their spatial self-organization in a process similar to biomolecular condensate formation. We develop a general theory for arbitrary reaction networks, and systematically study all closed unimolecular reaction networks involving up to six chemicals. Importantly, we find that network-wide propagation of concentration perturbations can be key to enabling self-organization, in a manner which is highly sensitive on the global network structure.

BP 10.11 Tue 12:15 BAR/SCHÖ

Spatial organisation of the cell's metabolic power plant via phase separation — •Kathrin S. Laxhuber[1,2] and Frank Jülicher[1,2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck School Matter to Life

Cell metabolism is the power plant that fuels the active processes essential to life. Recent experimental results show that glycolytic enzymes, central to sugar metabolism, phase-separate to form foci under energetic stress and can localise to sites of demand. To understand this phenomenon, we build and study a minimal theoretical model. We show that droplet formation can act as a metabolic switch that enables the system to maintain energetic homeostasis at higher output power. Notably, the metabolic droplets that emerge from this switch can self-organise to colocalise with demand. We discuss the non-equilibrium features and spatial energetic profiles in this system.

BP 10.12 Tue 12:30 BAR/SCHÖ

Emergent interactions lead to collective frustration in robotic matter — •Onurcan Bektas[1,3], Adolfo Alsina[2,3], and Steffen Rulands[1,3] — [1]Arnold-Sommerfeld-Center for Theoretical Physics and Center for NanoSciences, Ludwig-Maximilians-Universität München, Theresienstr. 37, 80333 München, Germany — [2]GISC, Universidad Rey Juan Carlos, Tulipán, 28933, Móstoles, Spain — [3]Max-Planck-Institute for the Physics of Complex Systems, Noethnitzer Str. 38, 01187 Dresden, Germany

Current artificial intelligence systems show near-human-level capabilities when deployed in isolation. Systems with intelligent agents are deployed to perform tasks collectively. This raises the question of whether robotic matter, where many learning and intelligent agents interact, shows emergence of collective behaviour. And if so, what kind of phenomena would such systems exhibit? Here, we study a paradigmatic model for robotic matter: a system composed of a large collection of stochastic interacting particles where each particle is endowed with a deep neural network that optimizes its transitions based on the particles' environments. For a 1D model, robotic matter exhibits complex phenomena arising from emergent interactions, including transitions between long-lived learning regimes, the emergence of particle species, and frustration. We also find an abrupt, density-dependent change in the behaviour of particles. Using active matter theory, we show that this phenomenon is a reflection of a phase transition with signatures of criticality. Our model captures key phenomena observed in more complex forms of robotic systems.

BP 11: Franco-German Session: Bacterial Biophysics I

Time: Tuesday 9:30–12:45 Location: BAR/0106

BP 11.1 Tue 9:30 BAR/0106

Monitoring of biofilms formation using a QCM-D — •Philipp Sievers[1], Andreas Böttcher[1], Günther Räcker[2], Felix Bosch[2], and Diethelm Johannsmann[1] — [1]Institute of Physical Chemistry, Clausthal University of Technology, Arnold-Sommerfeld-Str. 4, 38678 Clausthal-Zellerfeld, Germany — [2]Feindrahtwerk Adolf Edelhoff GmbH & Co. KG, Am großen Teich 33, 58640 Iserlohn, Germany

Biofilms formed by bacteria are a severe problem in many industries. Biofilm formation leads to biofouling, which limits the heat transfer (e.g. in heat exchangers) or contaminates process water. Regular biofilm removal often is necessary. In order to reduce cost, an online detection of biofilm formation is highly desirable.

An instrument is described, which monitors biofilm formation based on a quartz crystal microbalance with dissipation monitoring (QCM-D). In contrast to a conventional gravimetric QCM, which would rely on the shift in the resonance frequency, the most useful parameter to quantify biofouling was found to be the increase in the resonance bandwidth. This is due to the fact that biofilms consist of soft material loosely attached to the resonator, mostly leading to the dissipation of energy. This behavior is recognized based on a specific overtone dependence of the bandwidth, namely increased bandwidth (**) being the same on the different overtones. This feature is best explained with a mechanical equivalent circuit containing a single dashpot coupled to the resonator surface.

BP 11.2 Tue 9:45 BAR/0106

Following bacterial biofilm formation with X-rays: From scanning gradients towards real-life studies. — •Matthias Schwartzkopf[1], Joanne Neumann[1], Edina Klein[1,2], and Holger Sondermann[1,2] — [1]Deutsches Elektronen-Synchrotron (DESY), Notkestr. 85, D-22607 Hamburg, Germany — [2]Centre for Structural Systems Biology (CSSB), Notkestr. 85, D-22607 Hamburg, Germany

Bacterial biofilm formation is a complex multi-step process yielding microbial communities encapsulated in an extracellular matrix of polymeric substances. Biofilms are a significant problem in treating bacterial infections and are one of the main reasons for the persistence of infections. Their increased resistance to classical antibiotics poses a severe threat to global health issues. Therefore, following and understanding the process of biofilm formation are essential for early detection and suppressing biofilm-associated infections. In this context, surface-sensitive X-ray scattering (GI-SAXS) is successfully applied to observe initial thin film growth morphologies and kinetics at various metal/organic in-

terfaces [Schwartzkopf and Roth, Nanomaterials, 6, 239 (2016)]. In this contribution, we present the capabilities and first results of our combinatorial X-ray study on *Pseudomonas aeruginosa* biofilms aiming to provide nanoscale insight into the structure and dynamics of growing biofilms.

BP 11.3 Tue 10:00 BAR/0106

Nonlinear rheology of biofilm streamers: An eDNA-driven stress-hardening mechanism — Giovanni Savorana[1,2] and •Eleonora Secchi[1] — [1]ETH Zurich, Switzerland — [2]Princeton University, US

Biofilms are aggregates of microorganisms embedded in a self-secreted polymeric matrix that protects the community from physicochemical insults, enhancing their resilience across environmental, industrial, and medical settings. Because most biofilms develop in moist, flowing environments, they are constantly exposed to hydrodynamic forces. Yet how biofilms withstand strong or fluctuating flow conditions remains poorly understood.

Our work investigates how biofilms assemble under flow and how their morphology and rheology adapt across different flow regimes. Using a microfluidic platform enabling reproducible formation and in situ rheological testing, we show that biofilm streamers-filamentous assemblies that develop within the bulk of the flow-display stress-hardening: under flow-induced axial stress, both the differential elastic modulus and the effective viscosity increase linearly. This non-linear rheological response is conserved across several bacterial species. We develop a physical model showing that extracellular DNA (eDNA) is the key component enabling this stress-hardening behavior, allowing streamers to withstand both rapid and sustained variations in hydrodynamic load. Our work advances the physical understanding of biofilm development, reveals the molecular drivers of their mechanical resilience, and informs strategies for preventing biofilm-induced clogging.

BP 11.4 Tue 10:15 BAR/0106

Matrix-Microbe-Metabolite: Re-thinking transport phenomena in microbially-active soft matrices — •Juan Pablo Carmona Almazán[1] and Anupam Sengupta[1,2] — [1]Physics of Living Matter, Department of Physics and Materials Science, University of Luxembourg, Luxembourg — [2]Institute for Advanced Studies, University of Luxembourg, Luxembourg

The diffusion of biological metabolites through soft matrices is central to microbial biophysics, mediating healthy microbe-host interactions as well as diverse infections and biodegradation. An interplay of mechano-chemical cues, together with the microbe-induced remodeling of the local environments, impacts the metabolite transport in these settings. Yet, currently, we lack a mechanistic model of the Matrix-Microbe-Metabolite interactions. Here, we use a combination of high resolution imaging and quantitative image analysis techniques to study metabolite transport in diverse synthetic matrices with varying mechanical stiffness, composition, and biochemical complexity. Using suitable fluorescent probes as proxies, we quantify the transport kinetics in agarose as well as Matrigel, a model mammalian extracellular matrix. By interfacing atomic force microscopy, we map the results to the matrix structure, focusing on two key metabolites, formate and citrate. Finally, we embed bacterial cells to capture microbe-mediated impact on the diffusion kinetics, which together with the mechano-chemical datasets, provide a biophysical framework for active metabolite distribution in soft environments.

BP 11.5 Tue 10:30 BAR/0106

Differential pili interactions trigger colony eversion and dissemination of bacteria — Stephan Wimmi[1], •Isabelle Wielert[1], Kai Zhou[2], Marc Hennes[1], Benedikt Sabass[2], and Berenike Maier[1] — [1]Institute for Biological Physics, and Center for Molecular Medicine Cologne, University of Cologne, Germany — [2]Institute for Infectious Diseases and Zoonoses, Ludwig-Maximilians-Universitaet Munich, Germany

Attractive forces between cells determine the shape and sorting behaviour of bacterial colonies. During colony development, chemical gradients form within the colony but it is unclear how they affect cohesion. Here, we discover global eversion of colonies formed by Neisseria gonorrhoeae. Like a jet, the inner core flows towards the periphery where it is partially dispersed and partially spreads around the core of the colony. Living dispersed cells leading to fast dissemination. The eversion depends on local oxygen depletion that reduces cellular attraction: prior to eversion the colony consists of a weakly cohesive spherical core surrounded by a strongly cohesive shell. A computational model reveals when the thickness of the strongly interacting shell falls below a critical value a non-linear instability initiates colony-wide eversion. Simulations predict that an increase of cohesion forces among the bacteria suppresses colony eversion. This was confirmed experimentally by a genetic modification that increases attractive forces among bacteria. Overall, we conclude that a gradient of oxygen pushes the colony out of its equilibrium state and that non-linear instabilities trigger cellular fluxes during relaxation to a new stationary state.

BP 11.6 Tue 10:45 BAR/0106

How substrate stiffness and roughness tune early biofilm development: designing platforms for in situ observation of bacterial behavior — •Mathieu Letrou[1], Sofia Gomes[1], Kennedy Chagua Encarnacion[2], Rebecca Matthias[1], Yeraldinne Carrasco Salas[1], Elena Murillo Vilella[1], Lionel Bureau[1], Karin John[1], Delphine Débarre[1], and Sigolène Lecuyer[2] — [1]Université Grenoble Alpes, CNRS, LIPhy, Grenoble, France — [2]Laboratoire de Physique, ENS de Lyon, CNRS, Lyon, France

Biofilm formation begins with bacterial colonization of substrates, a process that occurs across diverse living tissues and abiotic surfaces. Early bacterial exploration of solid-liquid interfaces, governed by adhesion and individual motility, is a known determinant of the subsequent development and persistence of bacterial colonies. Yet, how bacteria integrate environmental cues at these interfaces and adapt their behavior accordingly remains poorly understood. In this talk, I will present recent experimental approaches to generate microenvironments with precisely controlled properties, that also enable the in situ imaging of bacterial behavior within microfluidic channels. Using the pathogen Pseudomonas aeruginosa, I will show how substrate stiffness, rigidity gradients, and the presence of dispersed obstacles can alter surface exploration, thus modifying the onset of colony formation [1]. These results highlight how physical properties of solid-liquid interfaces can regulate early biofilm development and suggest new avenues for controlling surface colonization.

[1] Letrou et al., Eur Phys J E Soft Matter, 48(10-12):70 (2025)

15 min. break

Invited Talk BP 11.7 Tue 11:15 BAR/0106

Physics of bacterial adhesion: heterogeneity, patchiness, and surface interactions — •Karin Jacobs — Saarland University, Experimental Physics & Center for Biophysics, Saarbrücken, Germany

Bacterial cells interact with solid interfaces through a heterogeneous cell envelope, giving rise to rich physical behavior at solid-liquid boundaries. From a physics perspective, bacteria can be regarded as soft objects whose adhesion is governed by collective interactions of many fluctuating macromolecules. In this talk, I summarize recent experimental and theoretical work on bacterial adhesion using concepts from soft matter and surface physics.

Using atomic force microscopy-based single-cell force spectroscopy, we determine interaction forces between individual microbial cells and well-defined substrata. These experiments reveal heterogeneity of adhesion across the surface of single bacteria [1,2]. In particular, Gram-positive bacteria such as S. aureus exhibit a patchy adhesion landscape, reminiscent of patchy colloids, where a small number of adhesive regions dominate surface interactions.

We further show how surface properties such as wettability and protein coatings control bacterial adhesion by modulating the accessibility of tethering macromolecules [3]. Overall, these results place bacterial adhesion in the framework of condensed matter physics and illustrate how physical principles can guide the design of bio-interactive materials, ranging from simple functional interfaces to artificial cells. [1] C. Spengler et al., Soft Matter 20 (2024) 484; [2] E. Maikranz et al., Nanoscale 12 (2020) 19267; [3] F. Nolle et al., ACS Omega 10 (2025).

BP 11.8 Tue 11:45 BAR/0106

Bacterial motility and chemotaxis in porous media: lophotrichously flagellated *Pseudomonas putida* exhibits run motility with mechanical trapping and active turning events that enable chemotaxis based on a turn-angle bias — •Sönke Beier[1], Agniva Datta[1], Veronika Pfeifer[1], Robert Grossmann[1], and Carsten Beta[1,2] — [1]University of Potsdam, Institute of Physics, Germany — [2]Kanazawa University, Nano Life Science Institute, Japan

Chemotaxis has been extensively studied in bulk liquid, particularly for the peritrichously flagellated *Escherichia coli* with its run-and-tumble motility, where navigation toward chemoattractants relies on a run-time bias, which extends runs when cells swim up nutrient gradients. Less is known about chemotaxis in environments, where confinement limits free swimming and reduces the effectiveness of a run-time bias. Previous studies suggest that *E. coli* also bias its turning angle, adjusting reorientations to favor subsequent runs toward the chemoattractant. By analyzing the soil bacterium *P. putida* in porous media, we identify run phases and active turning events -known from bulk liquid- and additional mechanical trappings caused by the environment[1]. We provide evidence that the bacterium performs chemotaxis by employing a turn-angle bias and show that the resulting directional preference of runs arises from the active, motor-induced turning events, while passive mechanical trapping in the porous matrix weakens the preference[2]. Agent-based simulations indicate that the turn-angle bias is the predominant chemotactic strategy[2]. [1] Datta et al.:Sci Rep 15, 20320 (2025), [2] Beier et al.:arXiv:2503.05286 (2025)

BP 11.9 Tue 12:00 BAR/0106

Patchy Adhesion of Staphylococcus aureus on Structured Surfaces Uncovered via Single Cell Force Spectroscopy — •Samer Alokaidi[1], Hannah Heintz[1], Michael A. Klatt[1], Markus Bischoff[2], and Karin Jacobs[1] — [1]Saarland University, Saarbrücken, Germany — [2]Institute for Microbiologie, Homburg/Saar, Germany

Investigating bacterial adhesion at the single-cell level provides critical insights into bio-film formation and the influence of surface properties on microbial attachment. This study examines the adhesion behavior of Stapylococcus aureus on wrinkled polydimethylsiloxane (PDMS) surfaces using single cell force spectroscopy (SCFS) [1]. While conventional SCFS typically evaluates a single contact point, our approach-utilizing structured surfaces-enables mapping of adhesion across the lower portion of the bacterial cell envelope. This method reveals considerable variation in adhesion strength at different points on the cell surface, supporting the "patchy colloid" model originally proposed for Escherichia coli. Simulations, incorporating angle-dependent molecule-substrate interactions, suggest that localized adhesive "hotspots" on S. aureus may arise from surface roughness, chemical composition, and the clustering of specific adhesive proteins. These findings emphasize the significance of surface structuring in bacterial attachment and provide insights that inform the design of antimicrobial materials.

[1] C. Spengler, E. Maikranz, et. al: "The adhesion capability of Staphylococcus aureus cells is heterogeneously distributed over the cell envelope", Soft Matter, 20 (2024) 484

BP 11.10 Tue 12:15 BAR/0106

Drug interactions between translation and transcription-targeting antibiotics result from differences in ribosome regulation — •Natawan Gadjisade and Tobias Bollenbach — Institute for Biological Physics, Cologne, Germany

Combining antibiotics has the potential to improve treatment efficacy and slow the evolution of resistance. When two antibiotics are combined, their effect on bacterial growth may be stronger or weaker than expected. Recent work has shown that such interactions between ribosome-targeting antibiotics can often be predicted using a biophysical model based on bacterial growth laws. Here, we aim to understand the interplay between translation and transcription inhibitors. We identified different types of drug interactions by measuring E. coli growth in two-dimensional concentration gradients of the transcription inhibitor rifampicin and several translation inhibitors. We systematically quantify proteome allocation and individual protein regulation using mass spectrometry-based proteomics measurements. Notably, some translation inhibitors, such as kasugamycin, exhibit signs of disrupted coordination between the two ribosomal subunits. The ribosome concentration does not increase in response, thus violating the usual growth law. The way ribosomes respond to each translation inhibitor influences drug interactions with rifampicin, which itself causes a decrease in ribosome concentration. Based on the quantification of these different responses, we aim to build a biophysical model of antibiotic action that can explain the interaction patterns. Our work has the potential to facilitate quantitative predictions of drug interactions.

BP 11.11 Tue 12:30 BAR/0106

How transformation affects evolution in changing environments — •Ariana Leu, Mona Förster, Melih Yüksel, and Berenike Maier — Institute for Biological Physics, Cologne

Horizontal gene transfer (HGT) is known to play a critical role in bacterial evolution. However, it is still poorly understood under which exact conditions it can confer a fitness advantage and how it affects the dynamics of an evolving bacterial population. We study the effect of transformation on the adaptation of a bacterial population to a new environment depending on cell history.

First, the laboratory strain is adapted to two different environments, exponential growth in liquid and to growth in a structured environment. The pre-adaptation is driven purely by mutation. By selecting one of the two environments for further evolution we compare the adaptation pathways of a well adapted and a poorly adapted strain. We evaluate the fitness of the evolved populations relative to their ancestor, taking into account the effect of HGT. For well-adapted strains growing exponentially in a liquid environment, we see that the distribution of fitness effects broadens for hybrid populations. In a structured environment the adaptation of a poorly adapted strain is accelerated by transformation. We also find that transformation opens up a new genotypic pathway for adaptation that is not available through mutation. In addition, each cell is labeled with a unique genetic barcode at the beginning of evolution. By analyzing the ratio of barcodes at different time points, we gain insight into the evolutionary dynamics within the population.

BP 12: Cytoskeleton I

Time: Tuesday 9:30–12:45 Location: BAR/0205

Invited Talk BP 12.1 Tue 9:30 BAR/0205

Tuning the Tracks: Functional Diversity Encoded in Microtubule Lattice States — •Lukas Kapitein — Utrecht University

Microtubules are active polymers that power intracellular transport and signaling. In cells, functionally distinct microtubule subsets are known to coexist, but the underlying mechanisms that specify these subsets have remained unclear. I will show that microtubule lattice conformation, specifically expanded and compacted states, acts as a tunable structural parameter that regulates both motor-driven transport and cytoskeletal signaling. Whereas expanded lattice states define tracks for Kinesin-1 driven transport, compacted states sequester specific signaling factors, both independently of tubulin chemical modification. These findings identify microtubule lattice plasticity as a fundamental mechanism by which active cytoskeletal matter encodes functional diversity.

BP 12.2 Tue 10:00 BAR/0205

Mechanical tension extends the microtubule lattice and modulates kinesin-1 binding in an isoform-dependent manner — Yannic Lurz[1], Benedikt Fischer[1], Laura Muras[2], Antoine Rittaud[3], Hevré Morhbach[4], Igor Kulic[3], E. Michael Ostap[5], Erik Schaffer[1], and •Serapion Pyrpassopoulos[1] — [1]University of Tübingen — [2]University of Uppsala — [3]ICS, Strassburg — [4]ICPM, Metz — [5]University of Pennsylvania

Recent work has shown that the microtubule lattice possesses remarkable structural plasticity, with its conformation modulated by MAPs and motor binding. However, how this plasticity responds to mechanical forces remains poorly understood. We developed assays to measure the effect of tensile forces on single microtubules using optical tweezers and fluorescence microscopy. Decorating microtubules with quantum dots enabled us to measure, with nm-precision, mechanical distortions of ~0.4% under changes in average tensile force <ΔF> = 10.4 pN, within the rage of Fmin = 1.29 pN to Fmax = 20.4 pN, forces comparable to those generated by one to three kinesin-1 motors. Under forces in this range, the average binding rate of KIF5B decreased by ~20%, while its dissociation rate increased by ~10%, reducing its average run length. In extreme cases, run length dropped by up to 46% under tension. By contrast, no statistically significant effects were observed for KIF5C at the same forces. Together, these experiments provide new insights into how microtubules can act as sensors and transducers of mechanical and biochemical cues across the cell.

BP 12.3 Tue 10:15 BAR/0205

Beyond the tip: lattice dynamics, seams, and the mechanism of microtubule fracture — •Amir Zablotsky[1], Subham Biswas[2], Laura Schaedel[2,3], and Karin John[1] — [1]Université Grenoble-Alpes, CNRS, Laboratoire Interdisciplinaire de Physique 38000 Grenoble, France — [2]Experimental Physics and Center for Biophysics, Saarland University, 66123 Saarbrücken, Germany — [3]PharmaScienceHub (PSH), 66123 Saarbrücken, Germany

The structural integrity of microtubules is paramount for cellular function. While tip behavior has been extensively studied, the dynamics of the microtubule lattice remain less explored. We present a theoretical analysis of lattice fracture mechanisms, focusing on the influence of multi-seam structures arising from monomer defects and aiming to provide a more accurate estimation of GDP lattice parameters.

Our findings reveal that seams function as pre-existing pathways that accelerate damage propagation. Consequently, monomer vacancies destabilize the lattice due to the inherent structural loss of tubulin-tubulin contacts and the additive acceleration of fracture through multiple seams. Furthermore, comparison of our simulations with experiments on lattice fracture suggests that the intrinsic ratio of longitudinal to lateral binding energies is bounded at approximately 1.5, challenging previous predictions of lattice anisotropy from tip-growth models.

These results emphasize the urgent need to revise current microtubule growth models to incorporate parameters obtained from lattice dynamics and reassess their implications for overall microtubule stability and tip dynamics.

BP 12.4 Tue 10:30 BAR/0205

Microtubule mechanics in actin network — •Komal Bhattacharyya, Sarah Köster, and Stefan Klumpp — University of Göttingen, Göttingen, Germany

The cytoskeleton provides structural support while enabling dynamic cellular processes such as growth and migration. Actin filaments and microtubules are key cytoskeletal components: actin is semiflexible, whereas microtubules are comparatively stiff and rod-like. The interplay between these two filament systems underlies many biological behaviors. For example, microtubules exhibit increased resistance to compressive forces when embedded within an actin network. In our work, we use the simulation package Cytosim to investigate composite actin-microtubule networks. In particular, we examine the buckling behavior of microtubules subjected to compressive loads and thermal fluctuations,

and how these responses are altered by mechanical coupling to actin. Our results show that the mechanical response of a probe filament such as a microtubule is governed primarily by its immediate local interactions rather than by the bulk properties of the surrounding network. Indicating the actin network can not influence the microtubule dynamics as an uniform elastic medium but only through direct interactions through crosslinkers or molecular motors.

BP 12.5 Tue 10:45 BAR/0205

Polydispersity-Induced Traveling Waves in Microtubule-Motor Mixtures — •Katrina Wharam[1], Ivan Maryshev[1], Filippo De Luca[2], and Erwin Frey[1] — [1]Ludwig-Maximilians Universität München, Germany — [2]University of Cambridge, United Kingdom

Microtubule-motor mixtures are exemplary active systems that self-organize into a variety of non-equilibrium phases, including asters, bilayers, and active foams. While previous theoretical work has largely assumed monodisperse filament lengths, we investigate a mixture with two microtubule populations of distinct lengths and derive a continuum field theory using a Boltzmann-Ginzburg-Landau approach. Analytical and numerical analysis shows that, despite reciprocal microscopic interactions, the system develops emergent asymmetric behaviour at the macroscopic scale. We identify the filament length ratio as a key control parameter: small length ratios yield stationary nematic bands, whereas increasing the disparity leads to traveling waves - a pattern absent in monodisperse models. Our results reveal a generic, collective route to traveling states in non-self-propelling active matter and connect ad-hoc asymmetric-alignment theories with biologically realistic microtubule systems.

15 min. break

BP 12.6 Tue 11:15 BAR/0205

Hold on tight no matter what! How cholesterol and cytoskeletal fibers affect microtentacles formation. — •Enrique Colina Araujo[1,2], Lucina Kainka[1,2], and Franziska Lautenschläger[1,2,3] — [1]Department of Experimental Physics, Saarland University, Saarbrücken, 66123, Germany — [2]Center for Biophysics, Saarland University, Saarbrücken, 66123, Germany — [3]Max Planck School, Matter to Life, Heidelberg, 69120, Germany

Following the formation of a primary tumor, cancer cells in the outer areas may detach and undergo an epithelial-to-mesenchymal (EMT) transition, enabling them to migrate and colonize new tissues, ultimately leading to metastasis. Circulating tumor cells (CTCs) play a key role during this invasion. Invasion can only occur after CTCs have attached to the blood vessel wall and extravasated from the bloodstream. Recent work suggests that such adhesion is mediated by microtubule (MT)-based membrane protrusions, known as microtentacles (McTNs). However, it remains unclear how McTNs protrude from the CTC and how they facilitate cell adhesion. In this work, we analyzed McTN formation in MDA-MB-231 cells. Using the actin depolymerizing drug latrunculin A and the cholesterol-depleting drug methyl-β-cyclodextrin (MβCD), we show that McTNs growth results from a reorganization of the actin cortex into areas of high actin concentration as well as from variations in cholesterol distribution in the plasma membrane of CTCs. Furthermore, McTNs' adhesion is integrin-based. Integrin-β-2 is evenly distributed across the surface of McTN, enabling adhesion at every potential contact with the blood vessel walls.

BP 12.7 Tue 11:30 BAR/0205

Coexistence and selection of branched actin networks — •Valentin Wössner[1,2], Falko Ziebert[1,2], and Ulrich S. Schwarz[1,2] — [1]Institute for Theoretical Physics, Heidelberg University, Philosophenweg 19, 69120 Heidelberg, Germany — [2]BioQuant, Heidelberg University, Im Neuenheimer Feld 267, 69120 Heidelberg, Germany

The actin cytoskeleton is crucial for essential cellular processes such as division, migration, and shape regulation. Most cellular actin structures are continuously turned over while keeping similar sizes. However, they are coupled through a shared and finite pool of actin monomers, which begs the question of how they can control their sizes. For branched actin networks, we suggest that local depletion of actin monomers at the leading edge constitutes a generic negative feedback mechanism between the current state of a structure (filament density) and its growth rate (creation of new branches). We derive a single equation capturing this local feedback and the global competition between different networks. Our theory leads to well-defined steady states even in the case of multiple networks sharing the same pool of monomers, without any need for specific molecular processes, in agreement with recent experiments on reconstituted systems. We also present the phase diagram for the transition from coexistence to selection under increased competition.

BP 12.8 Tue 11:45 BAR/0205

Phase Separation Strength Controls Actin Filament Treadmilling — •Beatrice Nettuno[1], Davide Toffenetti[1], Timon Nast-Kolb[2], Moritz Striebel[1], Erwin Frey[1], and Andreas Bausch[2] — [1]Arnold Sommerfeld Center for Theoretical Physics (ASC), Department of Physics, Ludwig-Maximilians-Universität München, Theresienstrasse 37, München, D-80333, Germany — [2]Heinz Nixdorf Chair in Biophysical Engineering of Living Matter, Technical University of Munich, Ernst-Otto-Fischer Str.8, Garching bei München, D-85748, Germany

Actin treadmilling underlies diverse forms of cellular motility, yet the physical principles enabling stable, persistent turnover remain unclear. In our work, we reconstitute a minimal system in which phase-separated condensates of zyxin and VASP balance cofilin-driven severing to produce robust treadmilling and higher-order actin organization. To uncover the mechanistic basis of this emergent behavior, we develop agent-based simulations that quantitatively recapitulate the experimental dynamics. Our modeling reveals that persistent treadmilling requires an optimal condensate cohesion: phase separation must be strong enough to locally concentrate and crosslink filaments, yet sufficiently fluid to permit barbed-end growth and internal rearrangements. Too weak a cohesion fails to stabilize bundles, whereas overly cohesive condensates suppress filament dynamics and prevent sustained turnover. Together, experiments and theory identify a physical mechanism by which the material properties of multivalent protein condensates regulate cytoskeletal turnover.

BP 12.9 Tue 12:00 BAR/0205

Anisotropic stretch biases the self-organization of actin fibers in multicellular Hydra aggregates — •Anais Bailles, Giulia Serafini, Heino Andreas, Christoph Zechner, Carl Modes, and Pavel Tomancak — Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany

Hydra displays a striking planar pattern of actin fibers at the organism scale, and mechanics influence the morphogenesis of biological structures during its prepatterned regeneration. However, how mechanics participate in the formation of an ordered pattern from a totally disordered state remains unknown. To study this, we used cellular aggregates formed from dissociated Hydra cells, which initially lose all actin polarity yet regenerate a long-range actin pattern. We showed quantitatively that the actin meshwork evolves from a disordered symmetric state to an ordered state in which rotational symmetry is broken, and translation symmetry is partially broken, with the nematic and smectic order parameters increasing over days. During the first hours, the actin meshwork displayed spatial heterogeneity in the nematic order parameter, and ordered domains separated by line defects progressively grew and fused. This suggests that local cell-cell interactions drive the transition from disorder to order. To understand the mechanism of ordering, we perturbed the tissue's physical constraints. We showed that while topology and geometry do not have a direct effect, anisotropic stretch biases the emerging orientation of the actin meshwork within hours. This demonstrates the role of tissue mechanics in the alignment of the actin fibers during the disorder-to-order transition.

BP 12.10 Tue 12:15 BAR/0205

Bridging Scales in the Cytoskeleton: Towards a nonperturbative renormalization group framework — •Patrick Jentsch, Thomas Quail, Niccolò Banterle, and Anna Erzberger — European Molecular Biology Laboratory, Heidelberg, Germany

Microtubules (MTs) and their interactions are microscopically well characterized, yet the connection between these interactions and the emergent, functionally relevant collective behavior of the cytoskeleton remains incomplete. To develop an analytic framework that links these scales, we aim to explore the use of nonperturbative renormalization group (NPRG) methods to derive large-scale effective theories of MT networks from a microscopic model of interacting MTs. Using *Xenopus laevis* egg extract as a model system, we have begun inferring a phenomenological theory of interacting MTs at the micrometer scale based on TIRF microscopy data. In the next stage, this model will be coarse-grained using NPRG methods to obtain an effective description at the millimeter scale, enabling us to track the scale dependence of interaction couplings and the emergence of new dynamical processes. Ultimately, the resulting effective theory will be evaluated by comparing predicted correlation functions with experimental measurements of spontaneously formed MT asters which we are currently imaging using millimeter-scale widefield and confocal techniques.

BP 12.11 Tue 12:30 BAR/0205

Bayesian inference of bond parameters from interactions between single filaments — •Kristian Angeli Pajanonot[1,2], Sascha Lambert[1,2], Pallavi Kumari[1], Stefan Klumpp[2], and Sarah Köster[1] — [1]Institute for X-Ray Physics, University of Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, University of Göttingen, Germany

Interactions among cytoskeletal filaments-actin, microtubules, and intermediate filaments-regulate cell structure, movement, and transport. Single-filament direct interactions can be measured using a quadruple optical tweezers setup. In this approach, filaments are attached to two separate bead pairs held in optical traps and positioned in a cross configuration. As the vertical filament is pulled across the other one, the bond that forms between these filaments experiences increasing mechanical load until it breaks. Previous analysis using Kolmogorov-Smirnov (KS) tests allows for the estimation of bond parameters but lacks a probabilistic interpretation. Here, we present a Bayesian inference framework to estimate bond parameters from the interaction data. Using published data on

the interaction between two vimentin filaments, we show that Bayesian inference provides consistent results with the KS test and with narrower parameter estimates. We then investigate how the pulling velocity influences the bond parameters and find that probing different pulling velocities improves inference compared to using a single velocity. Finally, we apply the method to other cytoskeletal filament interactions demonstrating broader applicability and offering guidance for future experimental optimization

BP 13: Active Matter IV (joint session DY/BP/CPP)

Time: Tuesday 14:00–15:30 Location: ZEU/0160

See DY 29 for details of this session.

BP 14: Poster Session II

Active matter; bacterial biophysics; bioimaging; computational biophysics; membranes, vesicles and life-like systems; protein structure and dynamics; single molecule biophysics; statistical physics of biological systems; systems and networks biophysics; FS integrated structural modelling; FS sequence spaces, populations and evolution

Time: Tuesday 18:00–21:00 Location: P2

BP 14.1 Tue 18:00 P2

Controlling Cell Motility and Morphology by Microscale Stripe Patterns — •Henrik Groh and Matthias Weiss — University of Bayreuth, Experimental Physics I, 95447 Bayreuth, Germany

Cells are highly responsive to the architecture of the substrate on which they adhere. In particular, cell morphology and motility can be influenced by providing microstructured adhesion patterns, e.g. fibronectin-coated lanes of varying width, as this determines how cellular adhesion sites form and organize. To study this in more detail, we generated fibronectin-coated lanes through the Primo technique with widths ranging from 2.5 μm to 40 μm on which highly migratory breast cancer cells (MDA-MB-231) adhered. As the lane width was changed, cells exhibited significant changes in their morphology, including alterations in aspect ratio and orientation angle relative to the lanes. In addition, the cells' motility, specifically velocity and migration mode composition, underwent pronounced changes as the lane width decreased. Our findings provide important insights into how cell migration might be guided with simple physico-chemical cues and highlight the potential of micro-patterned substrates as a tool for cancer cell migration analyses, possibly providing a core mechanism that underlies cell migration in development and disease.

BP 14.2 Tue 18:00 P2

Computational Modelling of Active-Polymer Dynamics in Gliding Filamentous Cyanobacteria — •Krishna Iyer Vadakkeputhanmadom Subramanian[1], Stefan Karpitschka[2], and Stefan Klumpp[1] — [1]Georg-August University, Göttingen, Germany — [2]University of Konstanz, Konstanz, Germany

Filamentous cyanobacteria such as *Oscillatoria lutea*, *Kamptonema animale* and *Nostoc commune* constitute a natural realization of active polymers: long, flexible filaments that self-propel by gliding motility and whose activity can be tuned with light. Dense colonies display a rich repertoire of collective phenomena—nematic lanes, topologicaldefects, spirals, clusters etc.—yet the physical mechanisms that connect single-filament properties (bending rigidity, propulsion force, reversal rates) to these emergent states remain largely unexplored. We develop a Browinan-dynamics framework, each filament represented as a chain of active particles with tangential self-propulsion and stochastic direction-reversal events, and explore the collective-state phase diagram in the space of activity, rigidity and length of filaments. Through comparisons with experiments, we seek to understand the mechanisms behind reversal events, both at collective and filament levels.

BP 14.3 Tue 18:00 P2

Filamentous cyanobacteria in model complex environments — •Jakob Gönnenwein, Elias Illing, and Stefan Karpitschka — Fachbereich Physik, Universität Konstanz

Cyanobacteria are pervasive throughout most ecosystems, ranging from open water bodies to porous media like soil or sandstone. Their accelerated growth in a warming climate constitutes rising ecologic and economic threats. Besides harmful blooms in natural water bodies, their degrading effect on buildings and sculptures has been identified as a threat to cultural heritage sites.

In our work we investigate the motility, individual behaviour and collective mechanics of filamentous cyanobacteria. We use well-controlled quasi-two-dimensional model porous media that mimic properties of natural habitats like soil or sandstone, while allowing direct observation of their dispersal characteristics. Using this system, we derive characteristic persistence scales of orientational order and density fluctuations in relation to the porosity parameters of the model medium.

Characterizing their collective behaviour in porous media allows us to understand and potentially mitigate their adverse effects on porous structural materials.

BP 14.4 Tue 18:00 P2

Motility Modes and Deformation Dynamics in *Trypanosoma brucei* — •Hannes Wunderlich[1], Marinus Thein[2], Lucas Brehm[2], Geena Eglmeier[2], Klaus Ersfeld[2], and Matthias Weiss[1] — [1]Experimental Physics I, University of Bayreuth, Germany — [2]Laboratory of Molecular Parasitology, University of Bayreuth, Germany

Trypanosoma brucei is a unicellular parasitic microswimmer whose flagellum-driven motion and cell-body elasticity are essential for navigating host environments and maintaining immune evasion.

Although run-and-tumble dynamics have been described for both the procyclic and bloodstream forms of T. brucei, details of motility changes and cell deformation during locomotion remain poorly understood. To address this gap, we performed a comparative analysis of the motility of bloodstream- and procyclic-form trypanosomes in controlled microfluidic environments. Using high-resolution recordings in bulk and in confining single-emulsion droplets (allowing tracking over extended periods), we extracted and analyzed positional trajectories and cell-shape time series. As a result, we reveal marked differences in swimming efficiency and overall motion patterns between the two trypanosome forms. Our findings indicate that cell-body elasticity and deformation play a crucial role in motility and may be directly relevant for biological processes such as surface-protein exchange.

BP 14.5 Tue 18:00 P2

A microfluidic device for probing microbial adhesion phenotypes in light and flow gradients — •Florian Böhme and Oliver Bäumchen — University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany

The unicellular photosynthetic microbe *Chlamydomonas reinhardtii* has naturally evolved the ability to unspecifically adhere to surfaces under sufficient illumination with blue light [1]. Their natural habitats are porous, liquid-infused soil and temporary pools. Thus, the cells regularly experience spatiotemporal light variations as well as external flows. *Chlamydomonas* employs its two cilia to firmly attach to surfaces, a mechanism which is hypothesized to sustain a stable photosynthetic yield while providing protection from external flows at low energetic costs.

We mimic such complex natural habitats by creating artificial microscale flow systems with tailored light and fluid flow conditions. Our microfluidic devices entail sections featuring continuous light-intensity gradients of certain wavelengths. At the same time the cells may experience external flows through precise pressure control in the channels. This allows for quantifying population statistics of microbial adhesion phenotypes in terms of threshold intensities of individual light switches and adhesion strengths during exposure to external flows. Our microfluidic devices can be employed for the high-throughput screening of adhesion phenotypes of wild-type and genetically modified photosynthetic microorganisms.

[1] R. Catalan et al., *Soft Matter* **19**, 306 - 314 (2023).

BP 14.6 Tue 18:00 P2

Active stresses induce bending instabilities and oscillatory dynamics in semiflexible filaments — •Sreehari Choorikkat, Jonas Bosche, Ludger Santen, and Reza Shaebani — Theoretical Physics and Center for Biophysics, Saarland University, 66123 Saarbrücken, Germany

Despite their high structural rigidity, cytoskeletal filaments can undergo large deformations driven by active stresses generated by motor proteins. We investigate

this phenomenon by developing a two-dimensional model in which a discretized filament interacts with an underlying array of molecular motors. Using Monte Carlo simulations, we show that stochastic motor binding and unbinding events can produce a wide range of deformation patterns, including bending, buckling, knot formation, and oscillatory motion. We characterize these dynamical regimes by analyzing the time-resolved mean curvature and by determining how the frequency and amplitude of oscillations depend on key physical parameters such as filament length, bending stiffness, and motor density. Our results delineate the parameter space that supports robust, sustained oscillations and clarify how the coupling between motor activity and filament mechanics generates dynamical instabilities.

BP 14.7 Tue 18:00 P2

Modeling host-pathogen interactions via stochastic simulations and neural network-driven Bayesian inference — •Soham Mukhopadhyay[1], Jonathan Pollock[2], David Voehringer[2], and Vasily Zaburdaev[1] — [1]MPZPM, Erlangen, Germany — [2]Department of Infection Biology, University Hospital Erlangen, Friedrich-Alexander University Erlangen, Germany

Helminth infections affect a large proportion of the world's population and cause significant morbidity. There are no vaccines against helminths, and the mechanisms of anti-helminth immune responses are often not well-understood. Taking the murine hookworm *N. brasiliensis* as our experimental system, we develop a mechanistic model that describes the parasite load in different host organs — which the parasite migrates through over the course of its lifecycle — as a function of time. We abstract infection progression as a state-transition process and simulate it via kinetic Monte Carlo, thereby linking the infective dose of larvae to the number of eggs shed to the environment by adult worms from the host intestines, which can then be compared to experimental data. To infer model parameters — the various transition rates — from experimental data, we employ emerging techniques from the domain of neural network-driven Bayesian inference to infer the posterior probability distribution of parameters conditioned on data. Using this model and inference framework, we plan to compare the population dynamics for different immune perturbations.

BP 14.8 Tue 18:00 P2

Structural Analysis of Cyanobacterial Monolayers — •Rodewald Lars and Karpitschka Stefan — Department of Physics, University of Konstanz, Germany

Cyanobacteria are interesting organisms from several perspectives e.g., due to their ecological importance and biotechnical potential but also as model active matter systems as they constitute active polymers that exhibit a wide variety of collective behavior.

Here we investigate dense quasi-2-dimensional layers of filaments and analyze the patterns that emerge from their motility and mutual interactions. In contrast to molecular systems here the complete microstate of the system can be accessed by optical microscopy, which allows for a more complete understanding and description of the global dynamics and structures including nematic and polar order parameters and defect formation.

In this contribution we discuss the design of a confining structure to generate monolayers while providing a healthy environment allowing for long term experiments. Using this structure we investigate the impact of light intensity on the behavior of the individual cyanobacteria and therefore the structures present the associated emerging order in the monolayer.

BP 14.9 Tue 18:00 P2

Mathematical modeling of larvae motility in complex environments — •Sreya Chatterjee[1], Jhanvi H. Patel[2], David Voehringer[2], and Vasily Zaburdaev[1] — [1]MPZPM, Erlangen,Germany — [2]Department of Infection Biology,University Hospital Erlangen,Friedrich-Alexander University,Erlangen.Germany

N. brasiliensis is one of the most widely-studied helminth parasites due to the relatively simple life cycle for parasite production and its ability to be used in animal models, especially rodents. The larvae mature into adult worms in the lumen of the small intestine, which is composed of mucus produced by goblet cells. Studying their interactions with the surrounding host tissue will help us understand how helminths trigger and modulate immune responses. The mucus layer of the extracellular matrix is viscoelastic which influence their motility. We model these adult worms as active agents exhibiting persistent motion within this viscoelastic environment. To capture their dynamics, we formulate the problem using the well-established framework of Active Brownian Particles (ABPs). As a first step, we study the behavior of a simple system of two ABPs connected by a spring through analytical approaches as well as numerical simulations. Next we will extend this model to simulate N-particles connected by springs to capture a more realistic model of the movement of the worm in viscoelastic environment.

BP 14.10 Tue 18:00 P2

Modeling the aging dynamics of confluent endothelial cells — •Anselm Hohlstamm, Andreas Deussen, Stephan Speier, and Peter Dieterich — Institut für Physiologie, TU Dresden

Coordinated movements of endothelial cells are essential for maintaining the barrier function of blood vessels while adapting to disturbances. Understanding the underlying dynamics of these movements can provide valuable insights into the complex biological processes and help to detect changes under pathophysiological conditions. Therefore, we cultured human umbilical vein endothelial cells and stained their nuclei to enable cell tracking. We obtained several tens of thousands of cell paths with durations of up to 48 hours (dt=10 min). Bayesian inference was applied to estimate model parameters and probabilities. Our analysis revealed an age-dependent reduction of mean cell velocities, with cells never coming to a complete standstill. Furthermore, the velocity autocorrelation function indicated correlated movement patterns that persist for approximately 1-2 hours and may be linked to the movements of neighboring cells. The active motion is further influenced by strong repulsive cell-cell interactions, which become particularly relevant shortly after cell division. By combining elements of generalized stochastic processes and cell-cell-interactions, we constructed models that integrate these characteristics and generate collective dynamics in simulations similar to those observed in experiments. In summary, our study provides a comprehensive characterization of endothelial cell movement dynamics and develops a stochastic model that can be used for future simulations and predictions.

BP 14.11 Tue 18:00 P2

Mechanosensing by active singularities — •Fabian Knüpfer[1], Jonas Neipel[1,2], and Frank Jülicher[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute for Molecular Cell Biology and Genetics, Dresden, Germany

During the development of an animal, the self-organized formation of chemical patterns establishes the body plan, defining body axes as well as the midline. However, the overall symmetry of an embryo is typically broken before, in particular due to environmental cues. Here we investigate how mechanical cues can control pattern formation. Motivated by the egg-shell that confines various embryos, we consider a rigid heterogenous substrate coupling to an active fluid surface. We focus on localized centers of mechanical activity, i.e. multipoles and topological defects of the active stress field. We ask how variations in friction and substrate curvature impact on the movement of such active singularities. We show that monopoles of isotropic active tension are advected towards maxima in friction. We then discuss how on a curved surface gradients in Gaussian curvature map to friction gradients to explain the localization of stress multipoles in anisotropic geometries. Finally, we explore how in an active nematic, topological defects move along gradients in friction and substrate curvature.

BP 14.12 Tue 18:00 P2

Swimming With and Against Confined Microscale Flows — •Vishu Saini and Marisol Ripoll — Theoretical Physics of Living Matter (IAS-2), Institute for Advanced Simulation, Forschungszentrum Jülich , Germany

Bacteria in real-world settings are typically navigating heterogeneous porous media, such as soil [1]. Such environments involve a complex interplay between geometric confinement and fluid flow [2], which can be understood as networks of channels with varying cross sections [3]. By means of Brownian Dynamics simulations, we investigate the properties of microswimmers in the presence of both confinement and flow to identify universal mechanisms that microorganisms employ to traverse complex environments. Since self-propelled particles tend to accumulate at the walls, the strength of the flow will determine the upstream or downstream nature of swimming. This will be importantly modified by the intrinsic rotational noise of the self-propelled and the channel width, which is known to vary together with the geometric characteristics of the media. The interaction between self-propelled particles will also importantly affect the dynamics with the formation of percolating clusters. We systematically characterize these dynamics for varying flow strengths and channel sizes, as often encountered in soil-like porous environments.

[1] Bhattacharjee et al (2019). Nature communications, 10(1), 2075. [2] Conrad, J. C et al. Annual review of chemical and biomolecular engineering, 9(1), 175-200. [3] Monteiro et al. Commun Biol 8, 662 (2025).

BP 14.13 Tue 18:00 P2

Synthesis and characterization of platinum (pt)-decorated se-tio2@fcnts nanocomposite and their photocatalytic antibacterial mechanism — •Asif kamal[1], Akhtar munir[2], Jinguang yang[3], and Yingwen wang[4] — [1]Department of Plant Sciences Quaid-i-Azam University Islamabad, 45320 Islamabad, Pakistan. — [2]Department of Chemistry, Quaid-i-Azam University Islamabad, 45320 Islamabad, Pakistan. — [3]Key Laboratory of Tobacco Pest Monitoring, Controlling and Integrated Management, Tobacco Research Institute of Chinese Academy of Agricultural Sciences, Qingdao 266101, China: — [4]Key Laboratory of Tobacco Pest Monitoring, Controlling and Integrated Management, Tobacco Research Institute of Chinese Academy of Agricultural Sciences, Qingdao 266101, China:

The development of efficient and sustainable antibacterial agents is crucial to address the growing threat of multidrug-resistant pathogens. In this study, we report the synthesis and characterization of a novel nanocomposite Pt-decorated

selenium-doped titanium dioxide supported on functionalized carbon nanotubes (Pt/Se-TiO2@FCNTs) with enhanced photocatalytic antibacterial performance under visible light. This new material was synthesized through sol gel method by in situ pt NPs decoration to achieved uniform dispersion and strong interfacial coupling between the components. Comprehensive characterization using XRD, TEM, SEM-EDS, FTIR, Raman, XPS and UV confirmed successful Se doping, Pt decoration, and improved optical absorption in the visible range. The photocatalytic antibacterial activity was evaluated against E. coli and Ralstonia solanacearum.

BP 14.14 Tue 18:00 P2

Laser-cell interactions in a microorganism model: Influence of irradiation with 1064 nm on *E. coli* — •Katja Schmitz and Beatrix Konermann — Trier University of Applied Sciences, Trier, Germany

Lasers are being used more and more in sensor technology, including in biotechnological applications such as fermentation monitoring. However, the biological impact of laser radiation on microorganisms is not clarify understood. Depending on the wavelength, the radiation can induce DNA damage, protein denaturation, or thermal effects, which can inhibit growth or kill cells. Additional parameters, such as irradiation duration and intensity, also influence these interactions.

This study investigates the effects of a 1064 nm laser on the growth and metabolism of *E. coli* under different irradiation conditions. An *E. coli* culture was exposed to a 100 mW laser radiation with variable irradiation times. After treatment, the samples were either cultivated immediately or returned to the culture medium. Growth behavior was evaluated by determining total and viable cell counts, which were then compared to those of untreated reference samples.

Initial results showed no detectable influence of 1064 nm irradiation on cell growth or metabolic processes. A literature review was conducted to contextualize these findings and summarize the reported positive, negative, and neutral effects of laser exposure on microorganisms. These results contribute to a more detailed understanding of laser-cell interactions and highlight the need for further research, particularly regarding wavelength- and organism-specific effects.

BP 14.15 Tue 18:00 P2

Agent-based modeling of short range cell-cell communication — •Ricardo Santander[1,3], Noam Golan[2], Lior Kreindler[2], Avigdor Eldar[2], and Vasily Zaburdaev[1,3] — [1]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany — [2]School of Molecular Cell Biology & Biotechnology Tel Aviv University, Israel — [3]Friedrich-Alexander-Universität, Erlangen, Germany

We use agent-based simulations to model synthetic gene regulatory networks that mediate short-range cell-cell communication in bacterial monolayers. These circuits couple intracellular dynamics of transcription factors and inhibitors with extracellular concentration fields driven by diffusion, secretion, and uptake of signaling peptides. Individual bacteria are represented as elongating, dividing capsules that act as point-like sources and sinks shaping the extracellular concentration field. The model is nondimensionalized to expose key parameter groups that govern the balance between secretion, import, diffusion, and dilution. Simulations reproduce the influence of nearby inhibitor-producing cells on their neighbors observed in microfluidic experiments and provide detailed insight into how spatial organization and transporter-driven accumulation control signaling range, spatial patterns, and circuit behavior in dense bacterial populations

BP 14.16 Tue 18:00 P2

Effects of extracellular DNA on material properties of bacterial biofilms — •Mandus Aldag, Isabelle Wielert, Stephan Wimmi, and Berenike Maier — Institute for Biological Physics, University of Cologne

Many bacterial species form spatially structured biofilms that protect the bacteria from external stresses. In *Neisseria gonorrhoeae*, a human pathogen, early biofilms are characterized by the formation of spherical colonies with liquid-like local order via active attractions between single cells. An important component of biofilms is extracellular DNA (eDNA), that is predominantly released from lysed cells and is proposed to have biofilm-stabilizing properties. Here, we use a combination of confocal microscopy, laser tweezers and tolerance assays to explore the spatial distribution of eDNA and how it affects structure, dynamics and attractive forces in gonococcal colonies. We find that after 16h of growth, *N. gonorrhoeae* colonies show filamentous, network-like eDNA structures, that can span over large parts of the colony and often interconnect lysed cells. Treatment with DNase prevents the formation of the eDNA network while the spherical colony shape is maintained. Furthermore, we find that the presence of eDNA is associated with a lower bacterial within-colony motility, compared to DNase-treated colonies. The results suggest that even though gonococcal colonies can still form in DNase presence, eDNA affects the cohesive properties of cells within biofilms which potentially influences the biofilm's susceptibility to antibiotics.

BP 14.17 Tue 18:00 P2

Probing Bacterial Adhesion on Functionalized Silicon Surfaces Using AFM-Based Single-Cell Force Spectroscopy — •Hannah Heintz, Hendrik Hähl, and Karin Jacobs — Experimental Physics & Center for Biophysics, Campus E2 9, 66123 Saarbrücken, Germany

Understanding bacterial adhesion to solid surfaces is crucial for biomedical as well as technical applications ranging from implants to antifouling strategies. In this study, we investigate how chemical functionalization and nanoscale roughness influence microbial attachment. We employed silicon surfaces that were modified by (i) coating with octadecyltrichlorosilane (OTS) to render them hydrophobic, (ii) pre-conditioning with a protein film of the hydrophobin HFBI from *Trichoderma reesei*, and (iii) controlled etching with hydrofluoric acid to introduce varying roughness levels. Adhesion forces of *Staphylococcus aureus* and *Shewanella oneidensis* were quantified using Atomic Force Microscopy (AFM)-based Single-Cell Force Spectroscopy (SCFS), employing both polydopamine-mediated and FluidFM vacuum-based cell immobilization. Complementary AFM and confocal microscopy enabled simultaneous characterization of topography, elasticity, and cell wall architecture. Our results reveal distinct adhesion profiles depending on surface chemistry and bacterial species, highlighting the interplay between hydrophobicity and roughness. These findings provide mechanistic insights into biointerface design and pave the way for tailored surface engineering to control microbial colonization.

BP 14.18 Tue 18:00 P2

Exploring Chemotaxis in Magnetotactic Bacteria: A Biophysical Approach — •Diego Roesch — nstitut de Biosciences et Biotechnologies d'Aix-Marseille, Aix en Provence, France

Magnetotactic bacteria (MTB) navigate complex microenvironments by integrating magnetic, chemical, and physical cues. Although magnetotaxis and aerotaxis have been extensively studied, the mechanisms governing chemotaxis in MTB remain largely unexplored, particularly at the level of the bacterial flagellar motor. This work aims to establish a quantitative steady-state model of motor dynamics in Magnetospirillum gryphiswaldense (MSR-1) as a foundation for studying how the motor adapts to and integrates chemical stimuli.

Using tethered-cell assays, high-speed recording, and a custom Python analysis pipeline, individual MSR-1 motors were characterized, revealing three well-defined rotational states: counterclockwise (CCW), clockwise (CW), and pausing. MSR-1 motors exhibited frequent directional reversals and extensive time spent in transient failed-switch pauses, whereas genuine long pauses formed rare but highly persistent states following lognormal distributions, likely reflecting regulatory or mechanistic resets of the motor.

Switching intervals, long pauses, and most run durations follow non-Poissonian, lognormal-like statistics, suggesting structured rather than memoryless regulation. Since MSR-1 possesses two polar flagella, this framework also opens the way to investigate the synchronicity and coordinated behavior of both motors under chemical stimulation.

BP 14.19 Tue 18:00 P2

Controlling transport for RNA enrichment in alkaline hydrothermal vents at the emergence of life — •Mona B. Michelsen[1], Almuth Schmid[2], Dieter Braun[2], and Karen Alim[1] — [1]Theory of Biological Networks, School of Natural Sciences, Technical University of Munich, Garching, Germany — [2]Systems Biophysics, Ludwig Maximilians University, Munich, Germany

Reactive mineral surfaces within alkaline hydrothermal vents (AHVs) at the prebiotic ocean floor are compelling candidates for mediating the accumulation and stabilization of early biomolecules such as RNA. The intricate hierarchical architecture of AHVs, featuring central conduits branching into finely ramified networks, creates dynamic microenvironments that may promote selective adsorption of RNA onto mineral surfaces and enhance local concentrations through flow-driven accumulation. These mineral-RNA interactions could have influenced both the persistence and the catalytic potential of primitive RNA species, potentially facilitating steps toward replication and evolution.

In this project, we apply microfluidics to construct quasi-2D analogues of hydrothermal vents in the laboratory, enabling direct observation of mineral precipitation, flow patterns, and RNA transport under controlled chemical and physical conditions. This approach allows us to investigate how mineral surfaces and flow dynamics influence RNA accumulation and the potential for mineral-assisted RNA catalysis and replication in prebiotic environments.

BP 14.20 Tue 18:00 P2

Molecular Dynamics Simulations as a tool to investigate the impact of novel imidazole-based cholesterol analogs in lipid bilayers — •Clara Rickhoff and Andreas Heuer — Institut für Physikalische Chemie, Universität Münster, Münster, Germany

In biological membrane systems of eukaryotic cells, the cholesterol plays an important role, impacting for example the fluidity and structure of the membrane. To gain a deeper understanding of the behaviour of cholesterol a range of analogs were developed to add functionalities required for lab experiments such as fluorescence to the sterol. In order to investigate cholesterol via these tools, it is es-

sential that the anaolgs show a similar behaviour to that of the wildtype molecule. In a previous study a similar behaviour was observed between a non-charged imidazole-based cholesterol analog (CHIM-N) and cholesterol itself [1].

The present study focuses on a novel group of imidazole-based cholesterol analogs with a more flexible linker between imidazolium and cholesterol and a fully retained cholesterol backbone. Via Molecular Dynamics (MD) Simulations it can be assessed how accurate these new analogs mimic cholesterol in terms of order parameter, tilt angle and position within the membrane. Furthermore, a comparison of the different new analogs as well as with the molecules already applied in cells can be made.

[1] M. Pierau et al, Langmuir 2025, 41 (17), 10991-11002

BP 14.21 Tue 18:00 P2

Modelling genome condensation and membrane bending in SARS-CoV-2 — •Nils O. Winkler, Sarah M. Seibert, Falko Ziebert, and Ulrich S. Schwarz — Institut Theoretische Physik & BioQuant, Uni Heidelberg

While many enveloped RNA-viruses use a rigid protein capsid to package and protect their genome, SARS-CoV-2 uses a high density of the transmembrane protein M to structurally reinforce its membrane, which then bends around the viral genome condensed by the cytosolic protein N. Interestingly, the RNA-genome seems to be further subdivided into smaller subunits, leading to a nested egg structure. We theoretically study the energetics of this situation by miminizing appropriate energy functions for genome condensation, membrane bending, droplet wetting and wrapping. In particular, we investigate which of these energy contributions can explain the nested egg structure as observed experimentally.

BP 14.22 Tue 18:00 P2

Modelling Wave Propagation on Monolayers — •Philipp Zolthoff and Jan Kierfeld — TU Dortmund University, Dortmund, Germany

Recent experimental advances have enabled precise studies of pressure wave propagation through monolayers at the air-water interface, triggered by light-induced conformation changes of embedded azobenzenes. We model wave generation and propagation using a fractional Lucassen-type wave equation and compare experimental results on pulse shape and pulse propagation in detail with numerical simulations in order to describe experiments quantitatively and unravel the influence of possible non-linearities and different rheological monolayer models. Particular attention is paid to the question how the influence of non-linearities and rheology changes for different states of the monolayer, i.e., in different regions along its Langmuir isotherm.

BP 14.23 Tue 18:00 P2

A synthetic flow system for modelling the vascular margination effect using microbeads — •Teresa M. Maunz, Alexandra Bienau, Friedrich Simmel, and Karen Alim — School of Natural Sciences, Technical University of Munich, Germany

The margination effect in the blood vasculature causes particles to migrate toward the blood vessel walls due to interactions with red blood cells (RBCs). Margination plays an important role in particle-based drug delivery targeted at the vascular endothelium, which requires contact with the endothelium for delivery. While margination has been studied with simulations and (some) experiments, how to control margination for synthetic particles is underexplored and requires thorough experimental testing of multiple variable parameters. Here, we present a synthetic microfluidic system dedicated to investigating the margination effect. The base system consists of a microfluidic channel carrying a binary suspension of beads, mimicking RBCs and marginating particles. Physiological conditions are emulated by tuning parameters that have been predicted to be crucial for the emergence and prominence of the margination effect, such as vessel diameter, RBC volume fraction, RBC deformability, the size ratio between RBCs and particles, and flow characteristics. We anticipate that our system will contribute to identifying key parameters that enable the margination effect, thereby improving our understanding of blood flow and facilitating the development of future drug delivery testing models.

BP 14.24 Tue 18:00 P2

Effects of perfluorocarbons on lipid monolayers and protein adsorption — •Jaqueline Savelkouls[1], Michael Paulus[1], Christian Thiering[1], Michelle Dargasz[2], Lena Friedrich[1], Mike George[1], Prashant Hitaishi[3], Svenja Hövelmann[3,4], Oleg Konovalov[5], Eric Schneider[1], Gordon Scholz[1], Chen Shen[4], and Metin Tolan[1] — [1]Technische Universität Dortmund, Germany — [2]Universität Siegen, Germany — [3]Christian-Albrechts-Universität zu Kiel, Germany — [4]DESY, Hamburg, Germany — [5]ESRF, Grenoble, France

Lipid monolayers serve as biomimetic models to study structural and functional aspects of protein-membrane interactions, which are essential for understanding physiological functions. Investigating how perfluorocarbon (PFC) effects on these interactions may aid new therapeutic strategies. This study examines the influence of various PFCs on structural changes of lung-surfactant-like DPPA and DPPC monolayers at different initial surface pressures, as well as on the adsorption behavior of surface-active proteins. Experiments were conducted at beamlines ID10 (ESRF, Grenoble) and P08 (PETRA III, Hamburg) under ambient conditions using a combined grazing incidence X-ray diffraction and X-ray reflectivity study. The results demonstrate that the effect of the PFCs on the lipid structure and protein adsorption depends on the chemical characteristics of the PFCs, the lipid type, and the lipid phase. This work will discuss how the adsorption of PFCs at the membrane promotes protein association.

BP 14.25 Tue 18:00 P2

Local dynamical properties of lipid bilayers using Scanning Ion Conductance Microscopy (SICM) — •Eric Lieberwirth[1], Franziska Dorn[1], Regina Lange[1], Una Janke[2], Mihaela Delcea[2], Ingo Barke[1], and Sylvia Speller[1] — [1]Physics of Surfaces and Interfaces, Institute of Physics & LLM, University of Rostock, Germany — [2]Biophysical Chemistry, Institute of Biochemistry, University of Greifswald, Germany

To determine dynamical properties of lipid bilayers, various experimental methods have been established, e. g. contour analysis and fluctuation spectroscopy. Based on Helfrichs theory from 1973 [1], bending rigidity and membrane tension of lipid bilayers can be derived. We demonstrate a local measurement approach by Scanning Ion Conductance Microscopy (SICM) on Giant Unilamellar Vesicles (GUVs) for evaluation of dynamic lipid bilayer properties. Using a nanopipette controlled via a feedback loop to maintain constant membrane-tip distance, we record time traces of local membrane height fluctuations with nanometer precision. In a contour analysis like approach [2], we obtain a bending rigidity of a few $k_B T$ and membrane tension of a few $\mu\mathrm{Nm}^{-1}$. Computation of the power spectral density (PSD) based on [3] combined with a global-local fit provides a second evaluation route with same data set, yielding in similar results. Differences and limitations of both methods are discussed.

[1] W. Helfrich, Zeits. für Naturfor. 28c (1973), p. 693-703
[2] J. F. Faucon et al., J. Phys. France 50 (1989), p. 2389-2414
[3] T. Betz & C. Sykes, Soft Matter 8 (2012), p. 5317-5326

BP 14.26 Tue 18:00 P2

Influence of PLIN5 and Lipid Composition on Lipid Droplet Contact Sites with other Organelles — •Mahsa Mohammadian, Shima Asfia, and Ralf Seemann — Department of Experimental Physics and Center for Biophysics, Saarland University, Saarbrücken, Germany

Lipid droplets (LDs) maintain cellular lipid homeostasis through dynamic interactions with other organelles. Understanding how these contact sites form is crucial for uncovering the mechanisms of lipid exchange and signaling. In this study, we used an in vitro model to investigate how lipid composition and the LD-associated protein perilipin 5 (PLIN5) influence contact formation between an LD monolayer and a bilayer membrane. Artificial LDs consisting of triolein and coated with either a DOPE or DOPC monolayer containing PLIN5 or not were incubated with large unilamellar vesicles (LUVs) that mimic the bilayer membrane of the organelle. Using double fluorescence labeling of the LUV bilayer and the core, we can distinguish between fusion of the LUV bilayer with the LDs and stable attachment of LUVs to the LD's surface. Our results show that the probability of fusion between LDs and LUVs is greatly increased for DOPE-coated LDs, while PLIN5 promotes the stable attachment of LUVs to the LD's surface and prevents fusion. These observations illustrate how certain lipid and protein components can modulate contact formation between LDs and membranes in a controlled in vitro system, and provide a basis for future studies on the molecular mechanisms of organelle communication.

BP 14.27 Tue 18:00 P2

Elucidating the dynamics of DNA-based Transmembrane Receptors through Molecular Dynamics Simulations — •Cyrille Ngueldjou Tahabo[1], Doruk Baykal[2], Lorena Baranda Pellejero[2], Andreas Walther[2], and Lukas Stelzl[3,4] — [1]Institute of Physics,University of Johannes Gutenberg,Mainz,Germany — [2]Department of Chemistry,University of Johannes Gutenberg,Mainz,Germany — [3]Institute of Molecular Physiology, University of Johannes Gutenberg, Mainz, Germany — [4]Institut of Molecular Biology, Mainz (IMB), Germany

Building an artificial cell is an essential step to creating artificial life-like systems and a critical step in this endeavour is to design molecular systems which enable the communication of an artificial cell with its environment. Such artificial life-like systems hold great promise for biomedical engineering. By mimicking biological mechanisms to enable the transmission of information from the exterior of artificial cells across membranes to their interior, we will contribute to creating new artificial life-like systems and gain insights to essential biological information processing mechanisms and advance simulation method development, using an atomistic molecular dynamics and Coarse Grained simulations approaches, who can be synthesized to function as receptors in artificial life-like systems. we study DNA attached to an anchor insert in lipid membranes. In the simulations we investigate how Anchor interacts with the membranes and how DNA-Anchor changes local membrane structure.

BP 14.28 Tue 18:00 P2

Ray-based simulation and experimental analysis of red blood cell imaging in brightfield microscopy

— •Aaron Kreis, Sarah Tabea Hermes, Thomas John, and Christian Wagner — Experimental Physics, Saarland University

The interpretation of brightfield microscopy images of red blood cells (RBCs) requires a quantitative understanding of how light propagates through their biconcave geometry. We present a numerical ray-tracing framework that models refraction and reflection at the cell–medium interface according to Snell's and Fresnel's laws, explicitly reproducing the optical configuration of a brightfield microscope. The simulated intensity distributions show excellent quantitative agreement with experimentally measured axial intensity profiles acquired using a conventional inverted microscope. This confirms that geometrical optics adequately describe light propagation through RBCs, as diffraction effects remain negligible for micrometer-scale objects. The approach enables label-free prediction of contrast and focus-dependent image formation, paving the way for future quantitative assays of single-cell oxygenation and advanced label-free imaging.

BP 14.29 Tue 18:00 P2

Photothermal imaging of autofluorescent retinal pigment epithelium (RPE) granules — •Sicheng Tian[1,2], Maryam Ali[1,2], Hanan Alderzy[1,3], Christoph Krafft[1,2], Martin Hammer[1,3], and Daniela Täuber[1,2] — [1]Friedrich Schiller University Jena — [2]Leibniz Institute of Photonic Technology, Jena — [3]Jena University Hospital, Jena, Germany

The retinal pigment epithelium (RPE) plays an important role in the photocycle. RPE cells contain varied amounts of micrometer-sized autofluorescent granules, including melanosomes (M), lipofuscin (L) and melanolipofuscin (ML), whose distribution varies throughout the RPE layer and with increasing age. Non-invasive fundus autofluorescence is used for clinically monitoring the distribution of L and ML. Specific alterations in the distribution of L, ML and M are linked to age-related macular degeneration (AMD)[Bermond et al., IOVS, 2020, 61, 35]. In spite of their importance, their chemical composition is not fully understood. Mid-IR Photo-induced Force Microscopy (PiF-IR) can provide a chemical evaluation of cell and organelle surfaces with less than 5 nm spatial resolution [Ali et al., Anal. Chem., 2025, 97, 23914] by combining powerful infrared illumination with mechanical detection using atomic force microscopy (AFM-IR). We utilized PiF-IR for the investigation of isolated M in a dried droplet. We complemented our study by sub-micron photothermal images using Optical Photothermal Infrared spectroscopy (O-PTIR) under illumination at visible wavelengths. We compare the results to PiF-IR spectra and conventional Fourier-transform IR spectra obtained on membrane phospholipids.

BP 14.30 Tue 18:00 P2

Multimodal imaging with light microscopes and scanning small angle X-ray scattering — •Boram Yu[1], Mangalika Sinha[1], Rita Mendes da Silva[1,2], Ulrike Rölleke[1], Manfred Burghammer[2], and Sarah Köster[1] — [1]Institute for X-Ray Physics, University of Göttingen, Germany — [2]The European Synchrotron, Grenoble, France

Imaging biological cells using X-rays is a complementary approach to electron and fluorescence microscopy due to their high penetration depth and the possibility for label-free imaging. One such technique is scanning small angle X-ray scattering (SAXS), which enables the acquisition of a real-space overview image with moderate resolution and reciprocal-space information with high resolution of cells in aqueous environment. However, intracellular structures in aqueous environment are very sensitive to radiation; therefore, the investigation of such damage requires additional imaging techniques beyond scanning SAXS. We present a scanning SAXS configuration, which integrates a mobile fluorescence microscope and an on-axis bright field microscope with a microfluidic sample chamber. The microfluidic sample chamber is compatible with X-ray measurement, as well as two microscopes, owing to its very thin design. While the fluorescence microscope enables obtaining correlative images before and after X-ray scanning within a short time span, the bright field microscope produces bright field images simultaneously during the scan. Our approach provides complementary information on specimens to X-ray measurements, thereby demonstrating its applicability in various fields.

BP 14.31 Tue 18:00 P2

Receptor-Mediated Binding Kinetics of Ligand-Functionalized Lipid Nanoparticles for Targeted mRNA Delivery — •Tianyi Cao — Faculty of Physics and Center for NanoScience, Ludwig Maximilians University, Munich 80539, Germany

For targeted mRNA delivery, lipid nanoparticles (LNPs) are functionalized with PEG-lipid tethers that display affinity ligands–such as full antibodies, Fab fragments, or peptides–to enable receptor-specific cell binding.

We establish a quantitative single-cell binding assay to characterize these receptor-mediated interactions using functionalized LNPs. Using time-lapse live-cell imaging on single-cell arrays (LISCA), we track individual particles via fluorophore-labeled lipid components incorporated directly into the LNP membrane. We systematically vary the molar fraction of functionalized PEG-lipids to quantify how ligand density influences binding probability and saturation behavior.

From these trajectories we extract apparent on-rates, binding capacities, and cell-to-cell variability arising from heterogeneous receptor expression. Under controlled shear flow, we distinguish diffusion-limited from reaction-limited binding and quantify how hydrodynamic forces modulate bond formation and stability.

We further extend the framework to multivalent LNPs carrying mixtures of different ligands that target distinct receptors on the same cell. This assay provides a mechanistic, single-cell-resolved readout of receptor-mediated LNP binding, enabling rational optimization of selective mRNA delivery formulations.

BP 14.32 Tue 18:00 P2

Optical properties of red blood cells and refractive index of hemoglobin — •Sarah Tabea Hermes, Agatha Belén Pinto Pino, Thomas John, and Christian Wagner — Experimental Physics, Saarland University

As the determination of the oxygen saturation of whole blood is common practice in medicine, the research of the oxygenation state of individual red blood cells (RBCs) remains challenging. When observing RBCs under a light microscope, the image is a composition of absorption as well as refraction (since the refractive index inside the RBC is higher than in the medium) and further depends on the focal plane, see Poster Aaron Kreis. This is important both for determining the composition of the cell via absorption as well as for edge detection because the refraction leads to "ghost edges". It is thus relevant to research the optical properties of RBCs and in particular the refractive index of the hemoglobin inside the RBCs. This allows for better comparison with numerical simulations and enables to precisely match the refractive index of the medium and the RBCs. We will present a detailed measurements about the refractive index of hemoglobin solutions in comparison with literature values.

BP 14.33 Tue 18:00 P2

Time resolved fluorescence anisotropy of single phalloidin-dye complexed F-Actin fibrils: MD simulation and experiments. — Phillip Seeber[1], •Shangjun Cheng[1,2], Lukas Spantzel[1,3], Rainer Heintzmann[1,2], and Daniela Täuber[1,2] — [1]Friedrich Schiller University Jena — [2]Leibniz Institute of Photonic Technology, Jena — [3]Jena University Hospital, Jena

Phalloidin conjugates are widely used to visualize actin filaments (F-Actin) due to their high binding affinity [1]. Fluorescence polarization imaging adds information on cellular structures known from other approaches [2, 3]. Moreover, super-resolution techniques such as STED and SIM often employ polarization optics. For aligned samples, such as actin filaments, insights in fluorophore orientation and wobbling dynamics will improve the interpretation of experimental results. Here, we apply quantum chemical methods including DFT, TD-DFT and ADC(2) to study the trajectory of the dye*s transition dipole moments during thermal fluctuations. We correlate the MD simulations with fluorescence anisotropy measurements acquired using time-resolved fluorescence lifetime imaging (FLIM) and 2D polarization fluorescence imaging (2D-POLIM) [3]. [1] Melak M., Plessner M., et al. Journal of cell science, 2017, 130, 525. [2] Rimoli, C. V., Valades-Cruz C.A., et al. Nat Commun 2022, 13, 301. [3] Camacho R., Täuber D., et al. Communications Biology, 2018, 1, 157.

BP 14.34 Tue 18:00 P2

Nanomechanical ultrastructure of native skin — •Mario Zerson[1], Martin Dehnert[1], Paul Zech[1], Melanie Knaak[2], Korinna Jöhrens[2], Martin Kaatz[3], and Robert Magerle[1] — [1]Fakultät für Naturwissenschaften, TU Chemnitz — [2]Institut für Pathologie, Klinikum Chemnitz gGmbH — [3]Hautklinik, DRK Krankenhaus Chemnitz-Rabenstein

Native skin has a complex, layered structure across the epidermis and dermis. In this study, we explore the use of atomic force microscopy (AFM) to examine the nanomechanical morphology of skin under controlled relative humidity conditions that maintain water content close to physiological levels. We examined cryosections of native, unfixed rabbit skin with tapping mode AFM and AFM-based nanoindentation measurements. This enables imaging the nanomechanical ultrastructure of the stratum basale in the epidermis and of collagen fibrils in the dermis with 20 nm spatial resolution. The results are compared with optical micrographs of adjacent stained sections of the same specimen and with scanning electron micrographs reported in the literature.

BP 14.35 Tue 18:00 P2

Red Blood Cell shape classification using curvature flow and spherical harmonics — •Nikolas Lerch, Felix Maurer, Diana Örüm, and Thomas John — Universität des Saarlandes

The morphological characterization of erythrocytes deformed due to pathology or disease has traditionally relied on manual assessment, which introduces subjective sources of error and hampers the differentiation of closely related morphologies such as echinocytes and acanthocytes. We present an automated method for the objective classification of deformed erythrocytes. The approach employs a bijective mapping of surface curvature onto a reference sphere via curvature flow and decomposes the resulting features into spherical harmonics. The

resulting spectral signatures enable the assignment of cells to morphologically distinct clusters. The method is quantitative and reproducible, explicitly identifies transient shapes and transition regions between morphologies, recognizing them as such and distinguishing them from clearly defined class expressions, and thereby opens new perspectives for computer-assisted hematology.

BP 14.36 Tue 18:00 P2

Diffusion and deoxygenation/oxygenation of hemoglobin solutions in microfluidics — •Agatha Belén Pinto-Pino, Sarah Tabea Hermes, Thomas John, and Christian Wagner — Experimental Physics, Saarland University

The observation of red blood cells (RBCs) under bright field microscopy allows the study of how absorption and refraction combine to form image contrast. In this work, we use the absorption of light to investigate the diffusion of hemoglobin in water in microfluidic channels. By analyzing how intensity profiles evolve over time, we characterize the diffusion behavior of hemoglobin in water. The setup will also be used to study the transition from deoxygenated to oxygenated hemoglobin, because the absorptions differ strongly for those states, in particular for different wave length of the light. This study helps for a better understanding of the mechanisms that govern oxygen transport in blood.

BP 14.37 Tue 18:00 P2

Implementation of NIR excitation and detection in 2D-POLIM setup — Shangjun Cheng[1,2], •Zilong Huang[1], Rainer Heintzmann[1,2], and Daniela Täuber[1,2] — [1]Friedrich Schiller University Jena — [2]Leibniz Institute of Photonic Technology, Jena

Two-dimensional polarization fluorescence imaging (2D-POLIM) has been used to probe the orientation/rotation of molecules and the Förster resonance energy transfer between closely located chromophores [Camacho et al., Adv. Mat. 2019, 31, 1805671; Camacho et al., Commun. Biol. 2018, 1, 157]. 2D-POLIM can provide full in-plane information on the polarization state of the sample through synchronized control of the excitation and detection polarizations. Near-infrared (NIR) excitation reduces the background from intrinsic autofluorescence in cells and tissue samples. Here, we show a stable, precisely controllable excitation polarization of a 785 nm laser. We also demonstrate the potential of 2D-POLIM in imaging and analysis of molecular orientation in the NIR range.

BP 14.38 Tue 18:00 P2

Metasurfaces for Oblique Plane Microscopy — •Maike Kreutz[1,2], Martijn Moorlag[1], Ibnun Nur Akash[3], Stephan Daetwyler[4], Sara Lelek-Greskovic[5], Ibnun Nur Akash[3], Yijun Wang[3], Chih-Yao Hsu[6], Yu-Chuan Chang[6], Yao-Wei Huang[6], Reto Fiolka[4], Florian Engert[1], Maryna L. Meretska[3], and Fabian F. Voigt[1] — [1]MCB, Harvard University — [2]RWTH Aachen University — [3]INT, Karlsruhe Institute of Technology (KIT) — [4]UT Southwestern Medical Center — [5]SCRB, Harvard University — [6]Department of Photonics, National Yang Ming Chiao Tung University

A promising emerging bioimaging technique is oblique plane light-sheet microscopy (OPM), which allows volumetric imaging using a single scan mirror but suffers from significant losses due to its complex optical path. To enhance the light-collection efficiency of OPMs, we propose to integrate optical metasurfaces into the optical path of an OPM. Metasurfaces utilize sub-wavelength nanostructures for manipulation of electromagnetic fields and can be produced with CMOS-compatible technology. By implementing tailored metagrating designs, we aim to reduce losses in single-objective light-sheet setups.

BP 14.39 Tue 18:00 P2

Lens-free lab-on-chip fluorescence microscopy using angle-stable polariton filters — •Anja Lindenau[1], Andreas Mischok[1], and Malte Gather[1,2] — [1]Humboldt Centre for Nano- and Biophotonics, Department of Chemistry, University of Cologne, Germany — [2]School of Physics and Astronomy, University of St Andrews, Scotland

Fluorescence microscopy is an essential tool in biomedical research but typically relies on complex optical setups with high-numerical-aperture objectives and specialised colour filters, which results in a large footprint and high acquisition costs. Here, we present a modified commercial CMOS image sensor for lens-free fluorescence microscopy. Lens-free imaging enables compact, low-cost systems with a large field-of-view (> 20 mm) and pixel-limited resolution (1.4 micrometer). To overcome the limitations of conventional colour filters, in particular their strong angular dispersion, we integrate a polariton-based filter directly on the sensor. This novel filter design exploits ultra-strong light-matter coupling between photons and material excitons, maintaining a stable long-pass cut-off below 540 nm over a broad range of incidence angles and thereby drastically improving the signal-to-noise ratio. Initial results highlight the potential for high-resolution on-chip lens-free fluorescence microscopy with significantly enhanced image quality.

BP 14.40 Tue 18:00 P2

Construction of Mueller Matrix Polarimeter with a Polarization Camera — •Kathrin Rott — Georg August Universität, Göttingen, Deutschland

A Mueller matrix polarimeter based on a division-of-focal-plane polarization camera has been developed for microscopy. The setup enables spatially resolved measurements of Mueller matrix elements in a single image acquisition, allowing the extraction of polarization parameters such as retardance, diattenuation and depolarization. The setup includes a polarization state generator (PSG) consisting of a linear polarizer and a rotating compensator, and a polarization state analyzer (PSA) implemented through the micro-polarizer array of the camera. This design allows fast measurement of Mueller matrix images with micrometer-scale resolution. Initial work focused on characterizing the camera, including calibration of nonlinear response, sensor homogeneity, polarization angle accuracy and pixelwise extinction ratio. The aim is to enable label-free imaging of biological cell cultures and to investigate whether polarization-based contrast can provide information about microstructures such as the cytoskeleton or nucleus. Unlike tissue samples, which typically exhibit polarization effects, the focus here lies on exploring polarization contrast in single cells. The project combines optical component development with a potential biophysical application and forms the basis for further studies on polarization contrast in cell culture imaging.

BP 14.41 Tue 18:00 P2

Quantification of in vivo flow of blood cells - adhesion cascade — •Khadija Larhrissi[1], Felix Maurer[1], Selina Wrublewsky[2], Alexis Darras[3], and Christian Wagner[1] — [1]Department of Experimental Physics, University Campus, Saarland University, 66123 Saarbrucken, Germany. — [2]Institute for Clinical and Experimental Surgery, Saarland University, 66421 Homburg, Germany — [3]School of Physics, University of Bristol, Bristol, United Kingdom)

Red blood cells (RBCs) constitute the majority of cells in the blood and play a key role in transporting oxygen to tissues and organs. On the other hand, leukocytes, also known as white blood cells (WBCs), make up approximately 1% of the total blood volume in most mammals. The flow of these cells ensures the body's defense against various viral and bacterial infections. The WBCs exhibit two modes of motion: a fast flow mode where they move with the surrounding fluid, and a slower rolling mode where they partly adhere to the wall, whereas RBCs simply flow with the surrounding fluid. In this study, our objective is to examine the influence of geometry and distribution on the flow of WBCs. To achieve this, we used Golden Syrian Hamsters as a model system to quantify the flow of cells by fluorescence microscopy and compare their behavior in different networks of vessels. Additionally, since some WBCs are larger in size than the capillaries they pass through, we will examine the impact of this size difference on their flow.

BP 14.42 Tue 18:00 P2

Visualizing Immune Cell Behaviour in 3D: An Ex Vivo Lattice Lighsheet Microscopy and Analysis Framework — •Anna Schepers[1], Joannah Fergusson[1], Edward Wheeler[1], Jacky Ko[1], Robert Kochl[2], and Marco Fritzsche[1] — [1]Kennedy Institute of Rheumatology, University of Oxford, UK — [2]King's College London, UK

The inherently multiscale immune response is regulated by diverse cell interactions, relying on cues from tissues down to single cells and subcellular structures. The intricate dynamics of the immune system present challenges for the observation of the immune response. A technological advance has been achieved with the introduction of lattice light sheet microscopy (LLSM), allowing fast and gentle imaging of live samples while achieving subcellular resolution. By complementing LLSM-based volumetric imaging with advanced sample handling of ex vivo tissue samples and perfusion imaging chambers, we provide a system that preserves critical physiological complexity. We present a complex data processing and analysis framework for robust 3D segmentation and tracking cells in the complex tissue environment allowing cell profiling from live cell behaviour. We show that in our setup, we can follow single cells and their interactions in volumes several cell layers deep in living samples within their environment, providing nuanced insights into the immune response.

BP 14.43 Tue 18:00 P2

Large-area AFM SmartMapping for contact lens characterization and mechanobiological tissue analysis — •Jörg Barner, Andre Körnig, Joan-Carles Escolano, and Thomas Henze — BioAFM, Bruker Nano Surfaces, Am Studio 2D, 12489 Berlin, Germany

Atomic force microscopy (AFM) provides quantitative nanoscale characterization of soft materials and biological systems, enabling analysis of surface topography, elasticity, and viscoelasticity under physiologically relevant conditions. We applied AFM to two distinct systems: ophthalmic contact lenses and highly corrugated tissues. For lenses, SmartMapping was used to acquire large-area curvature maps (up to several millimeters) combined with localized high-resolution measurements of nanomechanical properties. Silicone hydrogel lenses were analyzed, revealing heterogeneities in elasticity critical for balancing oxygen permeability and comfort. For biological samples, SmartMapping enabled automated imaging of rough, heterogeneous specimens such as 3D tumor spheroids (>100 um) and brain tissue sections (>300 um), capturing stiffness gradients relevant to mechanotransduction and transport. The synchronized XYZ-piezo and AFM head movement ensured reproducible mapping across extended areas without manual intervention, overcoming limitations of conventional AFM in lateral range and throughput. These results demonstrate that SmartMapping in-

tegrates large-scale imaging with nanoscale precision, establishing AFM as a robust platform for material optimization in ophthalmology and spatially resolved mechanobiological studies.

BP 14.44 Tue 18:00 P2

X-ray holo-tomography reveals 3D structure of protein networks and lipid globules in heat-treated egg yolk — •Felix Wittwer[1,2], Nimmi Das Anthuparambil[2], Frederik Unger[2], Randeer Pratap Gautam[2], Silja Flenner[3], Imke Greving[3], Christian Gutt[2], and Peter Modregger[1,2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Universität Siegen, Siegen, Germany — [3]Helmholtz-Zentrum Hereon, Geesthacht, Germany

Egg yolk is a versatile ingredient for cooking and food processing. As a natural emulsifier, it allows to bind fats and water. Under heating, the texture and consistency of egg yolk changes due to denaturation, aggregation, coagulation and gelation. By using X-ray holo-tomography, we could study the heat-induced changes in egg yolk on the micron to sub-micron length scale. In contrast to other techniques such as electron microscopy, X-ray holography can be used without sample staining, fixation, or drying, which potentially alter or damage the sample. Our results reveal a developing separation between proteins and lipids with fatty components rapidly aggregating into large globules around 40 micrometer in size.

BP 14.45 Tue 18:00 P2

Realignment and realization of polarization-resolved confocal FLIM — •Lizhong Mou[1], Shangjun Cheng[1,2], Subham Adak[1,2], Maryam Ali[1,2], Daniela Täuber[1,2], and Rainer Heintzmann[1,2] — [1]Friedrich Schiller University Jena — [2]Leibniz Institute of Photonic Technology, Jena

Fluorescence lifetime imaging microscopy (FLIM) is an attractive technique in the life sciences that enables quantitative mapping of excited-state lifetimes in the regime of nanoseconds within microscopic images [Le Marois et al., J. Biophot. 2017, 10,1124]. Conventional fluorescence polarization is widely used to assess the orientation and rotation of molecules but typically relies on millisecond acquisition times [Camacho et al., Adv. Mat. 2019, 31, 1805671]. Here, we present an alignment protocol for polarization-resolved confocal FLIM that delivers nanosecond temporal resolution and high-quality imaging. We further investigate time-resolved polarization states of dye molecules from cell and tissue samples.

BP 14.46 Tue 18:00 P2

Physics Informed Neural Networks for Microbial Interaction Network Inference — •Luca Battiston[1,2] and Frank Cichos[1] — [1]Universität Leipzig, Linnestr. 5, 04103, Leipzig, Germany — [2]Helmholtz Centre for Environmental Research GmbH (UFZ), Permoserst. 15, 04318, Leipzig, Germany

Recent advances in machine learning have enabled data-driven modeling of complex dynamical systems, with growing interest in methods that extract meaningful information about the underlying physical laws. Among these, Physics-Informed Neural Networks (PINNs) have emerged as a powerful tool for system identification, particularly in settings where data are scarce or noisy. On the other hand, generalized Lotka-Volterra (gLV) equations are widely used to model microbial community dynamics, provided that the underlying interaction matrix is known. In this work, we aim to reconstruct these interactions by combining PINNs with Least Squares Regression for inference of the interaction network. We evaluate our method using extensive gLV simulations covering a range of interaction matrix complexities and noise levels. Our results demonstrate high accuracy in network recovery and show that the approach retains robustness under measurement noise. This provides a step toward developing a robust and flexible framework for identification of complex interaction patterns in microbial communities.

BP 14.47 Tue 18:00 P2

Experimental Setup for the Irradiation of Organoids with High-Energy Electron Beams — •Laura Andrea Pastor Luque[1], Natascha Thomas[2], Victor Empe[2], Carla Sprengel[1], Antonio Tarzikhan[2], Constantin Aniculaesei[2], Thomas Heinemann[2], Mirela Cerchez[2], and Thomas Heinzel[1] — [1]Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany — [2]Institut für Laser- und Plasmaphysik, Heinrich Heine University, Düsseldorf, Germany

Organoids are three-dimensional cell systems that mimic key physiological and structural characteristics of human tissues, making them highly relevant models for studying biological responses to ionizing radiation. However, experimental platforms for irradiating organoids with high-energy electron beams remain limited, particularly regarding precise dose control and sample handling. In this work, we present the design and development of an experimental irradiation setup specifically adapted for organoid cultures. The system integrates a high-energy electron beam source with a setup to irradiate organoids samples at different energy ranges (MeV).

BP 14.48 Tue 18:00 P2

Evolution-inspired exploration of pattern formation in reaction diffusion systems — •Ming Hong Lui[1,2] and Erwin Frey[1,2] — [1]Faculty of Physics, Ludwig Maximilian University of Munich, Germany — [2]Max Planck Schools Matter to Life, Max Planck Institute for Medical Research, Heidelberg, Germany

Protein reaction networks often contain complex network topology. Modelling them involves numerous variables such as concentrations, diffusion rates and kinetic coefficients. Each variable adds an additional dimension to the phase space that made sweeping parameters challenging and impedes comprehensive understanding of the full dynamics by demanding assumptions or simplifications of biological systems.

Here, we present an alternative pipeline to full parameter sweeps, to characterize pattern-forming regimes, by applying an evolutionary algorithm. We iteratively bootstrapped parameter combinations that demonstrated instability using linear stability analysis. Together with applying mutations, represented by random displacements on the high-dimensional phase space, we could focus our attention in the vicinity of instabilities to reconstruct a heuristic phase diagram more effective than evenly-spaced parameter sweeps.

We shall demonstrate how this algorithm can be applied to various reaction-diffusion models, where it provided more informed choices of diverse systems to run full numerical simulations on, bridging the gap bewteen analytical and numerical solutions.

BP 14.49 Tue 18:00 P2

Pancreatic Network Morphogenesis — •Yasmin Abdelghaffar[1], Coline Schewin[2], Szabolcs Horvát[3], Monalisa Mishra[2], Lydie Flasse[2], Carl Modes[2,4], Anne Grapin-Botton[2], and Benjamin M. Friedrich[1,4] — [1]Cluster of Excellence Physics of Life, Technical University Dresden, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [3]Reykjavik University, Reykjavik, Iceland — [4]Center for Systems Biology Dresden, Dresden, Germany

During the course of development, the mammalian pancreatic ductal network remodels from a fully connected plexus to a tree-like branched network optimized for fluid transport. Previous in silico modeling suggested that this remodeling could be guided by flow through the network [1]. However, the physical mechanism of flow sensing in the developing pancreas remains open.

We quantitatively analyze duct network morphology at subsequent developmental time-points, to reverse-engineer putative physical mechanisms of network remodeling. This includes a spatial zonation of statistical network properties and an empirical Murray's law relating duct diameter to hierarchy level (Strahler number). We put forward theoretical descriptions, e.g., of cilia-based flow sensing, which reproduce distinct variants of Murray's law, which could be distinguished by future experiments.

[1] Dahl-Jesen et al., PLoS Biology, 2018.

BP 14.50 Tue 18:00 P2

A Mathematical Model of Microlesion-Driven Calcium Signalling in Fibroblast Networks — •Kara Nachtnebel[1,2,3,5], Eric Greto[1,2,3], Anna Möller[1,2,3,6], Christian Maueröder[1,2,3], David B. Blumenthal[6], Vasily Zaburdaev[4,5], and Stefan Uderhardt[1,2,3] — [1]Department of Medicine 3 - Rheumatology and Immunology, FAU und Universitätsklinikum Erlangen — [2]Deutsches Zentrum für Immuntherapie, FAU — [3]Exploratory Research Unit, Optical Imaging Centre Erlangen, FAU — [4]Department of Biology, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) — [5]Max-Planck-Zentrum für Physik und Medizin, Erlangen — [6]Department of Artificial Intelligence in Biomedical Engineering, FAU, Erlangen, Germany

Resident tissue macrophages (RTMs) maintain tissue homeostasis by continuously sensing and integrating local environmental signals. The interstitial fibroblast network, an omnipresent, self-interconnected system capable of generating intracellular calcium signals and transmitting them to neighbouring cells, provides signals that RTMs can detect and respond to. For example, in response to calcium elevations associated with tissue lesions, macrophages initiate rapid cloaking behaviour. Disruption of fibroblast networks can amplify unwanted immune activation and may contribute to the development of autoimmune diseases. We present a mathematical model of microlesion-induced calcium signalling in gap-junction-coupled fibroblast networks. It shows how microlesions drive signal propagation via intra- and extracellular pathways and quantifies the factors that shape this process.

BP 14.51 Tue 18:00 P2

Equal Partitioning of the Min Proteins at Cell Division — •Natan Dominko Kobilica[1], Nora Deiringer[2], Vitalii Grigorev[3], Antonia Winter[1], Robin Köhler[4], Sean Murray[5], Viktor Sourjik[3], Henrik Weyer[6], and Erwin Frey[1] — [1]ASC, LMU München, Munich, Germany — [2]Technical University of Munich, Garching, Germany — [3]Max Planck Institute for Terrestrial Microbiology, Marburg, Germany — [4]Geomagic, Leipzig, Germany — [5]IMESO-IT, Giessen, Germany — [6]Kavli Institute for Theoretical Physics, University of California, Santa Barbara, Santa Barbara, USA

The pole-to-pole oscillation of the Min proteins in Escherichia coli plays a crucial role in the process of cell division. The oscillation facilitates the formation of the

FtsZ ring, which determines the division site. It is essential that the Min proteins are distributed equally between daughter cells to ensure precise determination of the division site in subsequent divisions. Previously, experiments and stochastic particle-based simulations have linked protein equipartition to the splitting of the pole-to-pole oscillation. Importantly, the splitting is already triggered before the division is fully completed. The goal of this study is to explain the mechanism underlying the splitting of oscillations using the well-known reaction-diffusion equations for the Min System. We model the constriction during cell division as a reduced diffusion rate between the two parts of the mother cell. This already captures the oscillation splitting and agrees well with realistic simulations of the constricting cell. Additionally, we conduct high-throughput microfluidic experiments which align well with the predicted protein dynamics.

BP 14.52 Tue 18:00 P2

Information Processing and Scaling of Spatially Coupled Complex Networks — •Ambar Neel[1,2,3] and Carl Modes[1,2,3] — [1]Max Planck Institute for Molecular Cell Biology and Genetics (MPI-CBG), Dresden 01307, Germany — [2]Center for Systems Biology Dresden (CSBD), Dresden 01307, Germany — [3]Cluster of Excellence, Physics of Life, TU Dresden, Dresden 01307, Germany

Biological adaptive spatial networks are constantly grappling with increasing the efficiency of the network while minimising the metabolic costs. Simulations demonstrate that incorporating fluctuations in a system's sinks/sources leads to the onset of topological complexity in the network. Additionally, it has recently been shown that coupling two spatial networks also results in topological complexity categorised by the existence of loops. This framework is very well suited to investigating information processing in such spatially coupled networks and is thus the focus of this presentation. Along with organ systems such as the pancreas, kidney and bone marrow, the liver is a prime candidate for this analysis as it consists of bile and blood capillary systems that are interwoven. Another challenge is to understand the packing limit of these complex spatial networks by scaling them until a critical point is reached. This provides a meaningful length-scale for the system, allowing for further investigation into fundamental questions regarding geometrical aspects of these spatially embedded complex networks as well as setting up the template to compare these results to experimentally acquired datasets of sinusoids in the liver lobules of mice.

BP 14.53 Tue 18:00 P2

Chimeric RNA-DNA Oligomers Overcome Template-Product Inhibition in Prebiotic Ligation — •Lena Mühlschlegel, Ludwig Burger, and Ulrich Gerland — Physics of Complex Biosystems, School of Natural Sciences, Department of Bioscience, Technical University of Munich, Garching, Germany

The RNA world hypothesis proposes that DNA-based life evolved from a precursor living system that used RNA alone to store genetic information. However, it is unclear how the transition from a system purely based on RNA to one incorporating DNA could have occurred. At the transition, a lack of specificity in the synthesis of genetic polymers in prebiotic systems likely led to the simultaneous emergence of RNA and DNA, involving molecules comprising RNA-DNA nucleotides, which we refer to as chimeric RDNA strands. Because homogeneous RNA-RNA and DNA-DNA duplexes are highly stable, template-product inhibition can impede template-directed ligation. Experimental data show that RDNA-DNA or RDNA-RNA duplexes tend to be less stable than RNA-RNA and DNA-DNA duplexes, suggesting that RDNA strands might overcome template-product inhibition. We developed a nearest neighbor model parametrized by experimental data to predict RDNA hybridization energies as a function of sequence and used it to simulate template-directed ligation of RNA and DNA in the presence and absence of RDNA strands. We found a hybridization free energy regime in which RDNA strands enable the efficient replication of RNA and DNA, providing a potential pathway for the early evolutionary transition from RNA to DNA.

BP 14.54 Tue 18:00 P2

FRET-guided selection of RNA 3D structures — •Mirko Weber[1], Felix Erichson[1], Maciej Antczak[2,3], Vanessa Schumann[1], Josephine Meitzner[1], Tomasz Zok[3], Fabio D. Steffen[4], Marta Szachniuk[2,3], and Richard Börner[1] — [1]Laserinstitut Hochschule Mittweida, University of Applied Sciences Mittweida, Mittweida, Germany — [2]Institute of Bioorganic Chemistry, Polish Academy of Sciences, Poznan, Poland — [3]Institute of Computing Science, Poznan University of Technology, Poznan, Poland — [4]Department of Oncology, University of Zurich, Zurich, Switzerland

Integrative RNA modeling requires structurally validated ensembles and experimental data that reflect binding and folding behavior. However, predicting such structure collections remains challenging due to rugged energy landscapes and extensive conformational heterogeneity. We address these limitations with a FRET-guided selection strategy that identifies RNA conformational states consistent with single-molecule FRET (smFRET) data. We predicted 3D structures of a ribosomal RNA tertiary contact containing a GAAA tetraloop and a kissing loop using RNAComposer, FARFAR2, and AlphaFold3, and validated them based on Watson-Crick base pairing and an eRMSD threshold. For all retained models, we computed accessible contact volumes of the sCy3/sCy5 dye pair using FRETraj and derived FRET distributions, which were weighted against experimental smFRET data. Our results demonstrate that in silico predicted structures can reproduce the experimental transfer efficiencies, and that our selection reliably identifies RNA conformations consistent with the smFRET data.

BP 14.55 Tue 18:00 P2

Intrinsically disordered regulators of endocytosis - an integrated NMR/single molecule fluorescence approach — •Sigrid Milles — Leibniz-Forschungsinstitut für Molekulare Pharmakologie (FMP), Berlin, Germany

Intrinsically disordered proteins (IDPs) lack clearly defined structure and are therefore highly flexible and easily adaptable to different binding partners. This makes them important players in many biological processes, often with vital regulatory functions. Their dynamic features and broad range of interaction modes, however, render them difficult to study and analyzing their complexes often requires integrated approaches. Integrating complementary parameters from of nuclear magnetic resonance (NMR) and single molecule fluorescence approaches allowed us to describe the conformational landscape of IDPs at molecular resolution and promises to shed new light onto various biological processes. Among those counts clathrin mediated endocytosis. The early phases of clathrin mediated endocytosis are organized through a highly complex interaction network mediated by clathrin associated sorting proteins (CLASPs) that comprise long intrinsically disordered regions (IDRs). We characterize the IDRs of those CLASPs in their entirety and at molecular resolution, uncovering a plethora of interactions of various strengths and dynamic features with their endocytic interaction partners, proposing a rationale for how first interactions and dynamic rearrangement of partners take place during the uptake of a coated vesicle.

BP 14.56 Tue 18:00 P2

Adaptive NK cell analysis by t-SNE — •Andrea Schneider[1], Wiebke Moskorz[2], Jörg Timm[2], and Thomas Heinzel[1] — [1]Heinrich-Heine University Duesseldorf — [2]University Hospital od Duesseldorf

High-dimensional flow cytometry data from Natural Killer (NK) cells, collected using a comprehensive panel of typical and adaptive NK cell markers, poses a challenge for the characterization of complex cell subsets. To visualize the complete receptor expression profile in a two-dimensional cellular plot, we applied t-distributed Stochastic Neighbor Embedding (t-SNE) to the multi-parameter dataset. The resulting t-SNE projection successfully resolved distinct immune subpopulations regarding NK cell development and adaptive NK cells. Crucially, the map enabled the simultaneous visualization and comparison of different definitions of adaptive NK cells (including NKG2C+ and FceRIg- subsets within mature NK cells), visually confirming their close relatedness. Furthermore, while CD95 is known to be increased in adaptive NK cells, the t-SNE visualization clearly confirmed that this high expression level is consistently shared across all defined adaptive cell clusters, which were tightly localized within the embedding. This methodology demonstrates the power of non-linear embedding techniques for validating complex immunological phenotypes. Moreover, it establishes a visual framework for comparative studies of NK cells across different patient groups, including Hepatitis C Virus (HCV) seronegative, chronically HCV infected, and HCV resolved donors, with each cohort further stratified by Cytomegalovirus serostatus.

BP 14.57 Tue 18:00 P2

Exploring coarse graining RNA force fields via Machine Learning — •Anton Emil Dorn[1], Emile de Bruyn[1], Fabrice von der Lehr[3], Stefan Kesselheim[1,4], Philipp Knechtges[3], and Alexander Schug[2] — [1]Forschungszentrum Jülich — [2]KIT — [3]DLR Köln — [4]Universität zu Köln

In Protein structure prediction there have been massive improvements recently with the help of machine learning. In RNA structure prediction however the situation is less ideal due too much sparser experimental data. Here we attempt to solve a modified version of the problem by determining a coarse-grained RNA force field for Molecular Dynamics simulations. The data sparsity can here be alleviated by atomistic RNA simulations using proven and established force fields. In a first step we show the viability of this approach with a limited scenario of only small RNA molecules. We also explore different bead numbers for the coarse graining to determine the best approximation.

BP 14.58 Tue 18:00 P2

Segmentation and classification of retinal pigment organelles in fluorescence lifetime imaging microscopy (FLIM) data — •Maryam Ali[1,2], Hala Alhaj Ahmed[3,4], Martin Hammer[4], Rainer Heintzmann[1,2,5], and Ondrej Stranik[1,2] — [1]Leibniz Institute of Photonic Technology, Jena, Germany — [2]Friedrich Schiller University, Jena, Germany — [3]Ernst-Abbe University of Applied Sciences, Jena, Germany — [4]Jena University Hospital, Jena, Germany — [5]Abbe Centre of Photonics, Jena, Germany

Retinal Pigment Epithelium (RPE) granules can be categorized based on their autofluorescence and morphology like Lipofuscin (L), Melanolipofuscin (ML), and Melanin(M)[1]. Fluorescence lifetime measurements reveal another discriminative feature; however, identifying individual granules remain challenging by human eye. Here, we present a computational analysis pipeline for seg-

menting and classifying RPE granules from fluorescence lifetime imaging microscopy (FLIM) data. The analysis was implemented in a custom Python script employing seeded watershed segmentation to isolate individual granules and discriminate hyperfluorescent lipofuscins, characterized by longer lifetimes. Granules with shorter lifetimes were further analyzed by examining their lifetime distribution across their surfaces, allowing MLs to be distinguished from other melanin-rich granules. The proposed approach achieved high performance, with mean sensitivity 87% and mean specificity 98% compared to manually classified ground truth data. [1] K. Bermond et al., IOVS 2020, 61, 35

BP 14.59 Tue 18:00 P2

Modeling the Clustering of Pma1 in the Yeast Plasma Membrane under Starvation — •Annemarie Quas[1], Roland Wedlich-Söldner[2], and Andreas Heuer[1] — [1]Institut für Physikalische Chemie, Universität Münster — [2]Institut für Zelldynamik und Bildgebung, Universität Münster

Starvation of yeast cells leads to the internalization of most plasma membrane (PM) proteins via endocytosis, strongly reducing the overall protein content of the PM. However, the level of the H^+-ATPase Pma1 is hardly affected by starvation. Instead, clustering of Pma1 is observed under these conditions. FF-EM images reveal 2D crystals composed of hexagonal units corresponding to Pma1 hexamers. Interestingly, deletion of Mrh1 blocks the clustering of Pma1. An interplay between the positively charged C-terminus of Mrh1 and the negatively charged phosphatidylserine (PS) is proposed, as Mrh1 is not required for clustering in the absence of PS. Because experimental insight into the mechanism of cluster formation is limited, we employ a coarse-grained Monte-Carlo model to investigate how interactions between Pma1 hexamers can drive large-scale organization. In our 2D model, Pma1 is represented as hexamers with attractive corner-to-corner interactions. By systematically varying particle density and interaction strength, we explore the system's phase behavior and identify conditions under which extended cluster formation emerges. We analyze cluster sizes, time-dependent growth, and characteristic cluster shapes to gain mechanistic insight into how molecular interactions could stabilize the observed protein crystals.

BP 14.60 Tue 18:00 P2

Refining Coarse-Grained Models for Accurate Protein Folding and Mechanics — •Yi-Chen Tsai and Chi-cheng Chiu — National Cheng Kung University, Tainan, Taiwan

Accurately modeling protein folding and mechanical behavior in coarse-grained (CG) simulations requires balancing structural fidelity with physical realism. We develop a mesoscale modeling framework that advances CG protein simulations by integrating refined structure-based and hybrid physics-based approaches. The Gō-type structure-based model is refined by incorporating overlaid native-specific potentials, backbone dihedrals, improper torsions, and sidechain interactions. These additions improve folding accuracy, suppress chiral inversion, and yield more realistic mechanical responses across diverse proteins[1]. Building on this, a hybrid CG approach denoted as GōSPICA is developed by combining native-contact potentials with the physics-based SPICA CG force field. The hybrid model enables spontaneous folding, reproduces native fluctuation patterns and force-extension behavior, and remains fully compatible with membrane environments without relying on elastic network restraints. Together, these developments establish a versatile CG modeling framework for simulating protein behavior in biologically relevant environments.

[1] Y. Tsai *et al.*, Phys. Chem. Chem. Phys., Advance Article (2025).

BP 14.61 Tue 18:00 P2

PINNs based inference in reaction-diffusion systems — •Lukas Pöschl[1,2] and Vasily Zaburdaev[1,2] — [1]Friedrich-Alexander Universität Erlangen-Nürnberg — [2]Max Planck Zentrum für Physik und Medizin

Physics-informed neural networks (PINNs) promise to serve as universal function approximators that embed governing equations and biophysical constraints to operate under noisy, low data conditions. However, PINNs exhibit various training pathologies that limit broad practical application beyond simple benchmarking problems. We identify situations in biophysical models where PINNs fail, including stiff kinetics, sharp gradients and chaotic dynamics and map these to corresponding failure modes in the standard PINN formulation, together with the respective mitigations. We assess this improved formulation on four problems with synthetically generated experimental data. These tasks include the classical forward and inverse problems for parameter estimation and inference of experimentally inacessible species. Furthermore, we address the issue of discovering chaotic and pattern forming dynamics and thus the optimization of experimental parameters to explore these biophysically relevant regimes. Across selected problems, the modified PINNs suggest promising performance in handling the tested systems and the ability to operate with sparse measurements and noisy data.

BP 14.62 Tue 18:00 P2

Self-assembly of sarcomeres by pairwise interactions in muscle fibers — •Amirali Zandieh, Abhinav Kumar, Francine Kolley-Köchel, and Benjamin M. Friedrich — Cluster of Excellence "Physics of Life", Dresden University of Technology

Walking, flying, and heartbeat are powered by the contraction of sarcomeres, the elementary contractile units of striated muscle, which are arranged in series into periodic myofibrils extending across the length of a muscle cell [1]. While the physical principles underlying sarcomere self-assembly remain unclear, recent work on Drosophila indirect flight muscle revealed that myosin motor filaments, Z-disk proteins, and titin/Sallimus form an initial periodic pattern, with actin filaments becoming polarity-sorted only later, motivating 1D minimal models [2].

To develop more realistic 3D descriptions of myofibrillogenesis and capture their cross-sectional organization, we employ ESPResSo [3] for agent-based simulations. With only pairwise interactions, sarcomere-like periodic patterns emerge and become registered in-phase along the transverse direction, as quantified by Kuramoto order parameters. Additionally, the catch-bond behavior of actin crosslinkers enhances and stabilizes this order. Together, these results show that pairwise interactions between sarcomeric components are sufficient to drive the emergence of order, marking a key step toward understanding the physical basis of sarcomere self-assembly.

[1] F. Kolley, et al. PRX Life (2024) [2] F. Kolley-Köchel, et al. Biophysical Reviews, in press [3] Weik, Florian, et al. The European Physical Journal (2019)

BP 14.63 Tue 18:00 P2

Assessing the performance of quantum-mechanical descriptorsin physicochemical and biological property prediction — •Alejandra Hinostroza Caldas[1], Artem Kokorin[2], Alexandre Tkatchenko[2], and Leonardo Medrano Sandonas[1] — [1]TUD Dresden University of Technology, 01069 Dresden, Germany — [2]University of Luxembourg, L-1511 Luxembourg City, Luxembourg

Understanding how molecular structure relates to physicochemical and biological properties is essential for computer-aided drug design. A major challenge in applying machine learning (ML) to this problem is defining numerical representations that capture both geometric and electronic information. We introduce the QUantum Electronic Descriptor (QUED) framework [ChemRxiv, doi:10.26434/chemrxiv-2025-hj4dc], which integrates geometric descriptors (BOB, SLATM) with a quantum-mechanical descriptor (D_{QM}) that encodes global and local electronic properties computed efficiently with the DFTB method. We validate QUED on the QM7-X dataset of small drug-like molecules and show that incorporating electronic structure information substantially improves ML predictions of physicochemical properties. For biological endpoints, QUED also demonstrates predictive value for acute toxicity (LD50) in TDCommons-LD50 and for lipophilicity in the MoleculeNet benchmark. Our findings underscore the benefits of integrating electronic structure information with geometric descriptors and highlight the role of conformational diversity in improving the robustness of molecular property prediction.

BP 14.64 Tue 18:00 P2

Modelling neuron growth dynamics and role of extra-cellular matrix — •Mathar Kravikass, Federica Furlanetto, Lars Bischof, Pritha Dolay, Ben Fabry, Sven Falk, Marisa Karow, and Vasily Zaburdaev — Friedrich-Alexander-Universität (FAU)

Biological tissues are composed of cells embedded in extracellular matrix (ECM) and extracellular fluid. We study the role of cell-matrix interactions in the context of brain tissues and the mechanism of neurite growth through this matrix. We consider two modes for the neurite growth: linear growth by tip extension and growth by the traction force at the tip of the neurite with the modeled ECM particles. In a liquid-like ECM model, we demonstrate how growth is influenced by the ECM interactions when the matrix is freely deformable. These growth patterns were also shown to fit to a run-and-tumble process, which describes how the interaction parameters relate to the persistence and speed of the growth. Additionally, solid-like ECMs were considered in which the ECM particles are connected by springs, thus forming a lattice. In this scheme, we were able to study more closely how lattice stiffness affects neurite growth patterns. These simulations recapitulated growth patterns of neurites in organoids models of neurodevelopmental disease and neurite growth in artificial ECMs with controlled properties. Finally, we present how this model could be used in the future to describe more complex systems, such as neuronal network formation.

BP 14.65 Tue 18:00 P2

Motion or Player? Identifying Structural Drivers of Rare Transitions — •Ali Sharifian and Alexander Schug — Scientific Computing Centre, Karlsruhe Institute of Technology, Karlsruhe, Germany

Rare transitions in complex molecular and soft-matter systems are often described by low-dimensional collective variables (CVs) that track progress between long-lived states. Here we distinguish between the motion -pathway in high-dimensional space- and the players -specific atoms, residues, or coarse-grained units- that most strongly drive that motion. With accurate structure

prediction now routine for many proteins, the central challenge is to move from static models to a mechanistic view of functional dynamics based on full ensembles. We present an ensemble-based framework that takes high-dimensional structural data from simulations or experiments and, for any chosen CVs, identifies these structural players. From a structural ensemble and user-defined CVs, we construct the free-energy landscape, determine a minimum-barrier path between metastable states, and define a transition tube that isolates barrier-crossing configurations. Within this tube, a path-conditioned principal component analysis captures transition-specific fluctuations, while time-lagged independent component analysis resolves the associated slow modes. Combining each feature's contribution to variance and slowness into a single importance score yields a ranked map of transition hotspots. These hotspots can guide mutations, targeted coarse-graining, and allosteric drug design across biomolecular and synthetic systems.

BP 14.66 Tue 18:00 P2

Electronic and structural properties of (doped) bilayer systems of graphene and molybdenene — •Sabrina Smid — RWTH Aachen, Worringer Weg 3, 52074 Aachen

Two-dimensional (2D) materials have attracted intense interest since the discovery of semi-metallic graphene in 2004. Owing to its exceptional electronic, thermal, and mechanical properties, graphene has become a key platform for exploring van der Waals (vdW) heterostructures. Stacking different 2D crystals enables emergent phenomena absent in the isolated layers, as exemplified by graphene encapsulated in hexagonal boron nitride, where interfacial screening enhances carrier mobility. The introduction of twist angles in such heterostructures has further unlocked new electronic behavior, including flat-band correlated states in twisted bilayer graphene.

Recently, the emergence of metallic molybdenene, synthesized via microwave-assisted exfoliation of MoS_2, has further expanded the 2D materials landscape. Its intrinsic metallic character and tunable properties in vdW architectures suggest promising opportunities for heterostructure engineering. Motivated by this, we additionally perform density-functional theory calculations on a vdW bilayer composed of semi-metallic graphene and metallic molybdenene, examining how twist angle and carrier doping modify its structural and electronic properties.

BP 14.67 Tue 18:00 P2

Dynamic Generation of Rigidity and Curvature during Clathrin-mediated Endocytosis — •Johannes Dreckhoff, Leon Lettermann, and Ulrich Schwarz — University of Heidelberg, Germany

Clathrin-mediated endocytosis is a main transport pathway across cell membranes, yet the physical mechanisms by which the clathrin coat assembles to drive generation of membrane curvature are not understood well. In particular, it has been argued that bending would not be possible if the coat attained its high stiffness already at the initial stages. Here we address this crucial issue using agent-based kinetic Monte Carlo simulations for coat assembly in spherical geometries with variable curvature. By formulating a microscopic Hamiltonian governing individual clathrin legs, we elucidate the interplay between lattice growth, topological defects, effective membrane stiffness and macroscopic curvature generation. Our simulations reveal that the effective bending rigidity of the coat increases by approximately two orders of magnitude during assembly, driving the curvature generation. We also observed the growth curvature imprinting itself onto the system, resulting in a "curvature memory" effect. Crucially, our simulations capture the distinct dynamical regimes observed in experiments: we successfully reproduce the flat-to-curved transition, while also predicting stalled, flat growth events, potentially driven by premature lattice stiffening. This unifying description demonstrates that clathrin-mediated endocytosis is a multi-facetted process during which rigidity and curvature are generated in a cooperative manner.

BP 14.68 Tue 18:00 P2

Revealing Temporal Hierachy in Larval Zebrafish Behaviour and Its Neuronal Representation — •Leonard Constien[1], Gautam Sridhar[2], Joao C. Marques[3], Drew N. Robson[3], Jennifer M. Li[3], Antonio C. Costa[1], and Claire Wyart[1] — [1]Paris Brain Institute (Institut du Cerveau), Sorbonne University, INSERM U1127, CNRS UMR 7225, Paris, France — [2]Okinawa Institute of Science and Technology 1919-1 Tancha, Onna-son, Kunigami-gun Okinawa, Japan 904-0495 — [3]Max-Planck-Institut für biologische Kybernetik, Tubingen, Germany.

On a given timescale, animal behaviour can be structured into behavioural states, each defined by a similarity of kinematics, immediate goals and physiological states. Further, coarse behavioural state divide into substates, unfolding on faster timescales. How are these states represented in the brain and which structures control their dynamics across timescales? To address these questions, we apply a Markov chain analysis framework to a dataset of larval zebrafish behaviour with parallel recording of whole-brain activity at cellular resolution. The approach identifies behavioural states in a principled and unbiased manner and reveals a hierarchical organization of hunting behaviour from the seconds to minutes timescale. Further, by applying the framework independently on neuronal activity, we reveal a similar structure of the dynamics, identify representing brain regions and investigate the links to behaviour. This work will motivate further studies to determine the circuits and mechanisms behind the regulation of behavioural dynamics.

BP 14.69 Tue 18:00 P2

Dynamic Health Monitoring: Predicting COVID-19 with Wearable Sensor Data and catch22 Features — •Paul Buttkus and Dirk Brockmann — Technical University Dresden (SynoSys), Dresden, Germany

In the initial stages of a pandemic, when intervention leverage is highest, controlling infectious-disease spread hinges on timely detection of emerging cases. The rapid, global transmission of COVID-19 highlighted the need for scalable sensing tools that can pick up early physiological signatures of infection. Using data from the Corona Data Donation Project, which provides resting heart rate, step count, and sleep duration time series from over 120,000 voluntary participants in uncontrolled, real-world settings, we trained regression models to classify COVID-19 test results. Based solely on daily aggregated features, this model achieved an above random guessing success rate, revealing a non-trivial signal despite coarse temporal resolution and strong noise. To better highlight the underlying dynamics, we employ the catch22 (22 CAnonical Time-series Characteristics) feature set to map raw sensor data to a compact set of interpretable descriptors, and additionally extend our framework to higher-temporal-resolution data to incorporate periodicity metrics (e.g., circadian modulation of heart rate and activity) that are lost under daily aggregation. We show which dynamical features are most informative for distinguishing COVID-19-positive from negative individuals and discuss how this framework could turn large-scale wearable data into a real-time surveillance tool for public health.

BP 14.70 Tue 18:00 P2

A Computational Approach to Drug Screening for the Sphingosine-1-Phosphate Receptor Family for Therapeutic Use against Autoimmune Diseases — •Janos Hintze, Tim Bennet Hausmann, Jonathan Hungerland, and Ilia Solov'yov — Institute of Physics, Carl von Ossietzky Universität, Carl-von-Ossietzky-Str. 9-11, 26129 Oldenburg, Germany

Current drugs used in the treatment of multiple sclerosis (MS) often lead to a variety of unwanted side effects. Some of the target proteins in MS treatment are sphingosine-1-phosphate receptors (S1PRs), which form a family of five structurally similar G protein-coupled receptors (GPCRs) that are found in various tissues throughout the human body. In this work, a generative diffusion model was used to design a broad spectrum of novel ligand candidates. To account for receptor flexibility, molecular docking was performed on different protein conformations obtained through molecular dynamics (MD) simulations. Analysis of the generated ligand candidates showed a consistently low similarity to existing S1PR-targeting drugs. Approximately 2000 candidates show a favorable binding affinity and subtype-specific selectivity based on their docking scores. This dataset can be further investigated based on other criteria such as toxicity, synthesizability, and stability, aiming to identify selective ligands for S1PRs, relevant for MS therapy.

BP 14.71 Tue 18:00 P2

Applying a topology sensitive metric for RNA contact prediction — •Christian Faber[1], Utkarsh Upadhyay[1], Oskar Taubert[2], and Alexander Schug[1,2] — [1]Jülich Supercomputing Centre, Forschungszentrum Jülich, 52428, Jülich, — [2]Scientific Computing Centre, Karlsruhe Institute of Technology, 76344, Eggenstein-Leopoldshafen

Predicting the spatial structure of non-coding RNA (*ncRNA*) is an important task for understanding fundamental processes in living nature. Physical force fields are used to infer the structure from a sequence using simulations on high-performance computers. However, the best results are obtained by incorporating probable contacts as additional restraints. These can be derived from evolutionary data using statistical methods or from more recent artificial intelligence (AI) algorithms.

In the past, the focus was on achieving the highest possible proportion of correctly predicted contacts, while the distribution of these contacts on the contact map was overlooked. We have demonstrated the importance of this distribution for structure prediction and have therefore introduced a measure of it.

In our current work, we apply our new metric to a state-of-the-art algorithm *Barnacle*. To achieve this, the algorithms must undergo complete retraining and a new dataset must be generated that avoids data leakage. While our results demonstrate the practical application of such a procedure, they also underscore the challenges posed by the limited availability of data for RNA molecules, a problem which becomes particularly apparent when modelling AI networks.

BP 14.72 Tue 18:00 P2

Structure and Dynamics of Network-Forming Protein Solutions using SAXS and megahertz XPCS — •Adrian Maximilian Roda Lentz[1], Michael Paulus[1], Michelle Dargasz[2], Florian Wieland[3], and Christian Gutt[2] — [1]Department Physics/DELTA, TU Dortmund, Dortmund, Germany — [2]Department of Physics, University of Siegen, Siegen, Germany — [3]Institute of Metallic Biomaterials, Helmholtz-Zentrum Hereon, Geesthacht, Germany

This study explores the structure of networks formed by the biopolymer hyaluronic acid, together with the dynamics of embedded proteins, in this framework ferritin and apoferritin. Hyaluronic acid is a major constituent of synovial fluid and a key component in tissue dynamics and repair; therefore, characterization is essential for advancing biomedical applications. Static Small-Angle X-ray Scattering (SAXS) conducted at P10 (DESY) and BL2 (DELTA) was employed for structural characterization, complemented by megahertz Xray Photon Correlation Spectroscopy (XPCS) at MID (EuXFEL) to quantify the dynamics. First results indicate a pronounced impact of hyaluronic acid on the collective diffusion behavior of proteins.

BP 14.73 Tue 18:00 P2

Quantum mechanical/molecular mechanics (QM/MM) calculations for absorption spectra of photoactive proteins, including many-body screening contributions — •Jelena Schmitz[1,2], Maximilian Graml[1,2], Till Rudack[1,3], and Jan Wilhelm[1,2] — [1]Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, Germany — [2]Institute of Theoretical Physics, University of Regensburg, Germany — [3]Structural Bioinformatics, Regensburg Center for Biochemistry, University of Regensburg, Germany

The GW method and the Bethe-Salpeter equation (BSE) capture many-body screening effects, important for the full quantum mechanical description of excitations in large biological structures. Spectral shifts in photoactive proteins resulting from conformational changes can be described using a hybrid quantum mechanics/molecular mechanics (QM/MM) framework [1]. Our work investigates the impact of incorporating GW+BSE in QM/MM calculations, and examines how larger QM regions influence the accuracy of predicted shifts. We aim to compare to experimental results and QM/MM calculations using different ab initio approaches [1]. In order to perform calculations on larger, non-periodic systems, we are implementing RI-DFT as a pre-calculation method within the CP2K software package, prior to GW. This could provide us with access significantly larger system sizes, even full electrostatic protein surroundings, and therefore even higher accuracies.

[1] ChemBioChem 20, 1766 (2019)

BP 14.74 Tue 18:00 P2

Investigating molecular mechanisms of signaling in the multistep phosphorelay system of Magnaporthe oryzae via All-Atom Molecular Dynamics Simulations — •Jonas Paulus[1], Dennis Martin[1], Antonia Preuss[1], Milena Runge[2], Stefan Jacob[2], and Lukas Stelzl[1] — [1]Institut für molekulare Physiologie, Mainz, Germany — [2]Institut für Biotechnologie und Wirkstoff-Forschung, Mainz, Germany

Pathogenic fungi cause an annual loss of 15% of the world's major crops and the phenylpyrrole class of fungicides are upon the most successful to combat these pathogens, precisely because of their specificity and outstanding resistance management. The mode of action (MoA) takes place in a multistep phosphorelay system (MSP) thereby hyperactivating the high osmolarity glycerol (HOG) signaling pathway, but has not yet been clarified in detail on molecular level. Using all-atom molecular dynamics (MD) simulations, we investigate the structural and functional mechanisms of the cytosolic osmosensor MoHik1, its phosphotransfer signaling cascade, and nuclear import of downstream effectors. With this, we aim to design a multidimensional model of signal encryption and fungicide action in fungal MSP systems which will provide both, fundamental insights into fungal signal transduction and the chance to shed light on MSP systems as target for antifungal strategies.

BP 14.75 Tue 18:00 P2

Cryogenic Structural Stability of Human Serum Albumin in Aqueous Solution Studied by SAXS/WAXS — •Lukas Tepper, Michael Paulus, Jaqueline Savelkouls, and Metin Tolan — TU Dortmund, Maria-Goeppert-Mayer-Straße 2, 44227 Dortmund

The behavior of proteins during extreme temperature changes plays a crucial role in the development of stable biopharmaceutical formulations. Freezing and thawing processes are widely used in the production, processing, and long-term storage of protein-based drugs, but they can cause denaturation, aggregation, or loss of biological activity.

Cryoprotectants such as glycerol or other polyols are commonly used to mitigate these effects. They can stabilize proteins and prevent aggregation, among other things by changing the water structure and the hydration shell.

For structural characterization of these processes, Small- and Wide-Angle X-ray Scattering offer direct access to protein conformation, intermolecular distances, and mesoscale ordering phenomena, enabling analysis of proteins in solution without crystallization.

In this work, we use SAXS/WAXS at beamlines BL2 and BL9 at DELTA to study human serum albumin in aqueous and cryoprotective environments during cooling down to −100 °C and subsequent thawing. This allows us to analyze structural changes, stability, and possible reorganization processes across the entire cryogenic temperature range.

BP 14.76 Tue 18:00 P2

Coarse grained simulations for the peptide lge1 1-80 — Agaya Johnson[1], Anton Polyansky[2], Terpsichori Alexiou[1], Bojan Zagrovic[2], and •Sofia Kantorovich[1] — [1]Computational and Soft Matter Physics, University of Vienna, Kollingasse 14-16, 1090 Vienna — [2]Department of Structural and Computational Biology, Campus-Vienna-Bio Centre 5, 1030, Vienna

Due to the structural heterogeneity and fast dynamics of the bimolecular condensates, capturing their organization requires a coarse-grained modeling approach that bridges atomistic details with mesoscale properties. In this work, we develop a coarse-grained model based on atomistic potentials to study the formation of condensates of Lge1, a protein of interest in biomolecular phase separation. We implemented non-bonded interactions for these peptides derived from iterative Boltzmann inversion, with Martini force field parameters and votca tool kit into the espresso simulation package. We employ cluster analysis as a criterion to ensure that all these CG models retain key features of the self-assembly and phase separation comparatively, as it is observed in atomistic simulations. By leveraging CG modeling, we extend simulations to longer timescales and larger system sizes, enabling us to explore whether biomolecular condensates form through phase separation, self-assembly, or aggregation. Our approach provides insights into the structural transitions of Lge1 within condensates and the fundamental mechanisms governing these transitions. This work contributes to the development of predictive models for biomolecular organization in crowded cellular environments.

BP 14.77 Tue 18:00 P2

Investigating the binding of clients to small heat shock protein 16.5 using electrospray ion bean deposition and cryogenic electron microscopy — •Manami Imada, Noor Naseeb, and Stephan Rauschenbach — University of Oxford, Oxford, UK

Small heat shock proteins (sHSP) act as the first line of defence, preventing protein aggregation. sHSP do this by binding to the protein under stress to form a stable complex. We explore how these sHSPs bind to clients such as lysozymes using cryogenic electron microscopy (cryo-EM). However, sHSP are hard to image due to their dynamic nature and potential to form different oligomers.

Electrospray ion bean deposition (ES-IBD) is used to deposit the sample onto the cryo-EM grids. ES-IBD utilises native mass spectrometry (nMS), which transfers the complexes into the gas phase intactly and allows for mass filtration of the ion beam by a quadrupole. This allows specific complexes and binding stoichiometries to be deposited selectively onto the cryo-EM grids to be imaged.

BP 14.78 Tue 18:00 P2

Sparse sampling in single molecule spectroscopy — •Sebastian Stadler and Markus Lippitz — Universitätsstraße 30, 95447 Bayreuth

Single-molecule spectroscopy (SMS) is fundamentally limited by photobleaching, leaving only a short time window to record spectra from individual emitters. These constraints motivate measurement strategies that extract maximal information from minimal data. Sparse sampling provides a compelling alternative to traditional Fourier spectroscopy, which requires dense, uniformly spaced measurements to satisfy the Nyquist condition. In contrast to traditional Fourier spectroscopy, sparse or sub-Nyquist sampling enables accurate spectral reconstruction from substantially reduced datasets.

In this theoretical study, we explore optimized sparse sampling strategies using simulated single-molecule spectra. By systematically varying sampling patterns, we identify regimes and procedures in which sparse acquisition offers significant gains in efficiency without compromising spectral fidelity. As a conceptual example of such optimized strategies, we discuss the pathway toward sampling optimization based on ensemble spectra and adaptive sampling approaches that iteratively adjust measurement points based on previously obtained information.

Our results outline design principles for efficient measurement protocols and highlight the potential of sparse acquisition to push SMS beyond traditional limits imposed by photobleaching and limited interrogation time.

BP 14.79 Tue 18:00 P2

Single-molecule PIE-FRET and nsFCS Studies of Metal Ion-dependent Folding of an rRNA Tertiary Contact — •Mara Henschel[1], Vanessa Schumann[1], Andreas Hartmann[2], Michael Schlierf[2], and Richard Börner[1] — [1]Laserinstitut Hochschule Mittweida, Mittweida, Germany — [2]Technische Universität Dresden, Dresden, Germany

Tertiary interactions in ribosomal RNA are crucial for shaping the folding landscape. However, the dynamics of these interactions across different timescales are not well understood. We investigate the tertiary contact of a double fluorescent-labelled ribosomal RNA from Saccharomyces cerevisiae at the single-molecule level in vitro. We quantify metal-ion-dependent folding and dy-

namics during K(I) and Mg(II) titrations using single-molecule PIE-FRET as a nanometre-distance readout combined with nanosecond fluorescence correlation spectroscopy (nsFCS). FRET-histograms reveals ion-dependent broadening beyond shot noise, indicating structural dynamics on the microsecond to millisecond timescale. Furthermore, nsFCS measurements show fast domain motions ranging from nanoseconds to microseconds. By employing two complementary labeling schemes, we distinguish local folding of the kissing loop from formation of the long-range tertiary contact, resolving distinct folding trajectories within the same RNA construct. Our results provide a dynamic insight of rRNA tertiary-contact formation and lay the foundation for a quantitative, mechanistic model of metal-ion-regulated folding of ribosomal RNA.

BP 14.80 Tue 18:00 P2

Multiplexed magnetic tweezers for high-throughput measurements — •Leonhard Schatt, Stefanie D. Pritzl, Alptuğ Ulugöl, and Jan Lipfert — University of Augsburg, Augsburg, Germany

Single-molecule techniques, such as magnetic tweezers, are powerful tools for studying forces and torques on the nanoscale. However, throughput in single-molecule measurements can still be limiting. To solve this problem, we present a multiplexed magnetic tweezer setup that can perform real-time high-throughput force and torque measurements. In addition, our setup enables controlled excitation in the UV and visible range, to study the response to photo-triggers and photo-excitation.

BP 14.81 Tue 18:00 P2

Pulling Geometry as a Design Parameter for Coiled Coil-Based Molecular Force Sensors — •Laura M. Wolfthaler[1], Zeynep Atris[2], Angelo Valleriani[2], Russell J. Wilson[1,2], and Kerstin G. Blank[1,2] — [1]Johannes Kepler Universität, Linz, Austria — [2]Max Planck Institute of Colloids and Interfaces, Potsdam, Germany

Molecular force sensors (MFSs) measure piconewton-scale forces central to cell adhesion, migration and differentiation. While DNA-based MFSs are well established, their functionalization requires multistep chemistry. We introduce a protein-based MFS building block derived from heterodimeric coiled coils (CCs). Building on our prior work showing how CC length, helix stability and core packing shape mechanics, we now identify pulling geometry as a powerful and versatile parameter for tuning CC mechanical stability without altering thermodynamic or kinetic properties. Using atomic force microscope-based single-molecule force spectroscopy, we applied force parallel and perpendicular to the CC superhelix and observed strongly geometry-dependent rupture forces, including distinct responses for the two shear modes of a 4-heptad heterodimer. These results highlight how local helix stability and structural anisotropy determine CC mechanical behavior. This work establishes a foundation for using MFSs across a wide range of cell culture applications. Their ability to report forces at molecular scales could transform how mechanical signaling is studied at cell-material interfaces.

BP 14.82 Tue 18:00 P2

Thermal noise particle tracking and interaction measurements at interfaces under minimal external force — •Nils le Coutre and Alexander Rohrbach — Bio- and Nano-Photonics, IMTEK, University of Freiburg, Germany

Forces play a vital role in experimental biophysics. From receptor-binding studies to flow-drag analysis, understanding the magnitude, direction, and origin of these forces is essential for uncovering underlying mechanisms. Optical tweezers are widely used in this context because they not only enable the measurement of biophysical interactions, but also deliberately manipulate a biological system to trigger and observe otherwise highly unlikely yet relevant interactions between the system's individuals.

To leverage this advantage for studying specific interaction processes, a robust understanding of the probe position distributions, defined by both the trapping and the surface potential and the interferometric tracking response is required, especially near interfaces and surfaces such as cell membranes. We discuss the question how far an optical trap has to approach an interface such that a natural interaction process between two binding partners is enabled (e.g. receptor on surface and ligand in optical trap).

In this presentation, I expound experiments by exploring the underlying theory and by conducting benchmark measurements in electrolyte-controlled systems, characterizing the behavior of trapped probes as their microscopic environment is altered.

BP 14.83 Tue 18:00 P2

Plasma elastic properties in cross microchannels — •Michelle Kron, Joséphine Van Hulle, and Christian Wagner — Experimental Physics Saarland University

Cross-slot microfluidic geometries produce planar extensional flows and are used to investigate flow instabilities in Newtonian and complex fluids. In Newtonian liquids, an inertial instability produces a steady vortex beyond a critical Reynolds number. In viscoelastic polymer solutions, elastic stresses near the stagnation point lower this threshold. Here we investigate human plasma, which is weakly elastic under extensional flow. Using cross-slot experiments, we quantify how plasma elasticity shifts the Reynolds number threshold for vortex onset and compare the impact of common anticoagulants on this response. We show that plasma reduces the Reynolds-number threshold for vortex onset, underscoring the importance of considering its weak elasticity for physiological studies.

BP 14.84 Tue 18:00 P2

Effective binary models of multicomponent phase separation — •Henri Schmidt and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Biological cells rely on biomolecular condensates for spatiotemporal organization. Condensates consist of many differently interacting biomolecules, which leads to a rich and complex configuration space.

Yet, only a few types of molecules can be measured in experiments, and the resulting phase behavior is typically explained using low-dimensional models. To understand the conditions under which such dimensionality reduction is feasible, we numerically explore multicomponent phase separation and ask when the behavior of a particular component can be explained by simple binary phase separation. This is surprisingly often the case, even when the unobserved components undergo phase separation on their own. However, the predicted interaction parameters and molecular volumes typically deviate from their true values, indicating that the reduction introduced systematic measurement errors.

Understanding the details of the dimensionality reduction will allow us to better probe multicomponent phase separation by observing a few components in the future.

BP 14.85 Tue 18:00 P2

Dynamics of tissue sampling of resident tissue macrophages — •Miriam Schnitzerlein[1,2], Eric Greto[3,4], Stefan Uderhardt[3,4], and Vasily Zaburdaev[1,2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Erlangen — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen — [3]FAU und Universitätsklinikum Erlangen — [4]Optical Imaging Competence Center Erlangen, FAU

Resident tissue macrophages (RTMs) are a type of immune cell present in essentially every tissue in the human body. One of their main functions is to keep the tissue in homeostasis by resolving lesions or removing dead cells, thereby preventing unnecessary inflammation and avoiding collateral damage to the tissue. To find such incidents, RTMs show continuous sampling behaviour by extending and retracting cell protrusions. This sampling behaviour needs to be tightly regulated - due to finite amounts of available cell cytoplasm and membrane - while still guarding the entirety of the tissue.

In this project, we have employed a high-resolution, intravital imaging protocol to generate dynamic data of murine RTMs in vivo in the peritoneum. Next we have built a custom image processing pipeline to segment RTM protrusions and their dynamic behaviour. We could then analyse the sampling range of protrusions and found correlations between outgrowth and shrinking of protrusions. Furthermore, the data hints at a division of labour approach protrusions employ when scanning the tissue.

BP 14.86 Tue 18:00 P2

Bottom-up emergence of a primitive replicator — •Magdalena Häupl, Ivar Haugerud, and Christoph Weber — Faculty of Mathematics, Natural Sciences, and Materials Engineering: Institute of Physics, University of Augsburg, Universitätsstraße 1, 86159 Augsburg, Germany

Non-equilibrium selection pressures were proposed as a mechanism of forming oligonucleotides whose sequences encode rich functionalities, including catalysis. Since phase separation was shown to direct various chemical processes, we ask whether condensed phases can provide mechanisms for sequence selection.

To answer this question, we develop a non-equilibrium thermodynamic theory to describe oligomerization, templated ligation, and sequence fragmentation away from equilibrium and under non-dilute conditions prone to phase separation.

We show the emergence of a strong selection mechanism. Most strikingly, a primitive replicator arises that is solely based on the inter-sequence interactions that drive sequence condensation. These results highlight that out-of-equilibrium condensed phases may provide versatile hubs for Darwinian-like evolution toward functional sequences, both relevant for the molecular origin of life and de novo life.

BP 14.87 Tue 18:00 P2

Wetting of Chemically Active Condensates on Membranes — •Mengmeng Wu and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany

Droplets undergo partial spreading, division, merging, engulfment, and exocytosis in cellular environments. When these droplets are chemically active, as is common for many condensates in cells, the resulting long-range fluxes further enrich and modify these behaviors. To analyze the interplay between chemically active droplets and membranes, we develop a coarse-grained molecular dynamics model together with a continuum theory based on Cahn-Hilliard

reaction-diffusion dynamics coupled to membrane curvature elasticity. Our approach demonstrates how chemical reactions and the resulting fluxes control both droplet morphology and membrane deformation, providing physical insight for cellular condensates as well as for the design of synthetic responsive membrane-droplet systems.

BP 14.88 Tue 18:00 P2

staged self-organized attack mechanisms of camponotus japonicus against intruders — •YIFAN ZHANG and ZHANGANG HAN — School of Systems Science, Beijing Normal University, Beijing, China

Social insect colonies display complex collective behaviors that emerge from local interactions, enabling decentralized strategies to counter external threats. Although ant collective activities such as foraging and nest construction are well studied, the self-organized attack mechanisms ants employ against specific intruders remain poorly understood. Using the camponotus japonicus and earwigs as research subjects, we show that ants exhibit a staged escalation pattern when confronting an invader: from individual probing, to small-group containment, and ultimately large-scale coordinated assaults. Building on a master-equation framework, we establish continuous-space dynamical equations and propose an ant attack behavior model to characterize these processes. Notably, the collective attack displays strong nonlinear synergy*six ants generate an attack intensity far exceeding a simple tripling of that from two ants. These findings highlight the adaptive advantages of coordinated aggression, demonstrating how cooperative interactions among individuals greatly amplify group-level defensive efficiency. Our study offers new insights into how decentralized biological systems achieve swarm intelligence and produce emergent combat behavior, and clarifies the role of self-organization in shaping effective group decision-making.

BP 14.89 Tue 18:00 P2

Protein self-assembly, infinitely complex yet simple? — •LUKAS KALVODA[1] and MARTIN LENZ[1,2] — [1]LPTMS, CNRS, Université Paris-Saclay — [2]PMMH, CNRS, ESPCI Paris, PSL University

Cells rely on protein self-assembly to form functional complexes, but a lack of regulation gives rise to pathological fibers in diseases like Alzheimer's and sickle cell anemia. Why proteins robustly form these well-defined morphologies is largely unknown.

Beyond the molecular details, the complexity of proteins in shape and interactions suggests that their self-assembly may be governed by the laws of statistical physics. We introduce an analytical lattice model of anisotropic self-assembling particles to study what we term the "infinite complexity limit". Therein the number of distinct interactions grows to infinity. Strikingly, in this limit, the "molecular" details of the interactions do not matter anymore. Instead their distribution and extreme value statistics determine the self-assembly outcome.

BP 14.90 Tue 18:00 P2

From Individuals to Waves: Mechanisms Shaping Collective Responses in Sulphur Mollies — •BIANCA PACINI[1], YUNUS SEVINCHAN[1,3], DAVID BIERBACH[2,3], KORBINIAN PACHER[2,3], JENS KRAUSE[2,3], and PAWEL ROMANCZUK[1,3] — [1]Institute for Theoretical Biology, HU Berlin, Berlin, Germany — [2]Leibniz-Institute of Freshwater Ecology and Inland Fisheries, Berlin, Germany — [3]Science of Intelligence, TU Berlin, Berlin, Germany

Collective biological systems, from neuronal networks to animal groups, exhibit the remarkable ability to rapidly modify their collective behaviour in response to changing environmental cues. By integrating local interactions with external information, they achieve flexible and coordinated group-level responses.

We investigated large fish shoals of sulphur mollies (*Poecilia sulphuraria*) in Southern Mexico, which perform collective diving cascades as a response to predation, producing wave-like patterns on the water surface. Interestingly, as a form of collective perception, we found that the group responds as a unified entity, showing a gradual stimulus-response pattern in their initial reaction.

Informed by empirical patterns extracted from a large video dataset of surface waves triggered by synthetic stimuli or bird attacks, we developed an agent-based model which captures the system's essential features. Systematic exploration of the model identifies the key individual-level mechanisms driving collective dynamics and shows how changes in local behaviour can drive collective adaptations across ecological contexts.

BP 14.91 Tue 18:00 P2

Confirmation of Jarzynski's equality based on single molecular and macroscopic interaction force measurements — •IAGO PETERS, LAURA MEARS, STEFAN SZOKOLL, and MARKUS VALTINER — TU Wien, Wien, Austria

Knowledge about the free energy landscape of biomolecular reactions is necessary to understand how life works on the smallest scale. Unfortunately, obtaining experimental values of the free energy difference between two states like an unbound and a bound state of two molecules is rather difficult. Jarzynski proposed an equality that connects the free energy difference between two states with the irreversible work that leads from one state to the other. Precisely, an average of all possible realizations of a process that moves the system from an equilibrium state to another state in equilibrium. Here, we test this hypothesis with experimental values. Using a simple model system, the different nucleobase-pair interactions are measured using three different techniques that are able to measure the interaction forces between two single molecules and up to several million interactions in a single experiment run. Using the Atomic Force Microscope (AFM), Optical Tweezers and the Surface Force Apparatus allows us to additionally investigate the scaling of biological single molecule interactions. Together with molecular dynamics simulations a strong foundation is laid to confirm Jarzynskis equality and investigate the scaling of single-molecule interactions.

BP 14.92 Tue 18:00 P2

Phase separation in chemically reacting systems controls cross-phase pH difference — •LINGE LI, OMAR ADAME-ARANA, and FRANK JÜLICHER — Max Planck Institute for the Physics of Com- plex Systems, Nöthnitzer Str. 38, 01187, Dresden

Biomolecular condensates are increasingly recognized as dynamic chemical environments whose properties are strongly modulated by their pH environment. Recent experiments have focused on the pH differences between the coexisting liquid phases, but a minimal theoretical framework that can account for these observations and elucidating their physical principles is still lacking. Here, we develop a minimal thermodynamic model that integrates charge-regulated macromolecules and their counterions. By identifying the conjugate thermodynamic variables constrained by chemical equilibrium and charge neutrality, we construct the thermodynamics at equilibrium and uncover a variety of phase behaviors. We show that asymmetric partitioning of ions in phase separated compartments naturally generates electric potential and pH differences, with the dense-phase pH consistently buffered toward the macromolecular isoelectric point. We further demonstrate that these pH differences are governed by macromolecular interactions and molecular properties. Together, our results suggest that phase separation provides a robust mechanism for buffering dilute-phase pH variations and enabling controlled modulation of pH in the presence of condensates. The framework uncovers general physical principles of how pH regulation can be achieved phase-separated environments.

BP 14.93 Tue 18:00 P2

Phase separation in chemically reacting systems controls cross-phase pH difference — LINGE LI, •OMAR ADAME-ARANA, and FRANK JÜLICHER — Max Planck Institute for the Physics of Com- plex Systems, Nöthnitzer Str. 38, 01187, Dresden

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BP 14.94 Tue 18:00 P2

Statistical mechanics of disordered buckling instabilities — •TANGDI LUAN[1,2,3] and PIERRE A. HAAS[1,2,3] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Max Planck Institute of Molecular Cell Biology and Genetics — [3]Center for Systems Biology Dresden

Buckling instabilities drive the emergence of biological shape during morphogenesis, but the effect of the large variability of these systems at the microscopic cell scale on these instabilities at the macroscopic scale of tissues is largely unknown. The buckling of a rod with disordered growth [1] is perhaps the simplest setup of this problem. Numerical simulations [1] reveal that even in this minimal setup, the distribution of growth disorder has complex effects on the buckling threshold.

Here, we provide the theoretical underpinnings for these observations: we develop the statistical theory that explains how the spatial distributions of disorder of growth and material properties conspire to determine the threshold for the instability. Our results thus indicate how correlations and hence feedbacks between stress and growth can control mechanical instabilities and, by extension, the emergence of biological shape in development.

[1] Ramachandran *et al.*, Phys. Rev. E **110** (2024)

BP 14.95 Tue 18:00 P2

Exchange controls coarsening of surface condensates — •Riccardo Rossetto[1,2], Marcel Ernst[1,2], Gerrit Wellecke[1,2], and David Zwicker[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany — [2]University of Göttingen, Institute for the Dynamics of Complex Systems, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Biological membranes often exhibit heterogeneous protein patterns, which cells control. Strong patterns, like the polarity spot in budding yeast, can be described as surface condensates formed by physical interactions between constituents. However, it is unclear how these interactions affect the material exchange with the bulk. To study this, we analyze a thermodynamically consistent model which reveals that passive exchange leads to new equilibrium phenomena, such as reentrant phase transitions, and generally accelerates the coarsening of surface condensates. Active exchange can further accelerate coarsening, although it can also fully arrest it and induce complex patterns involving various length scales. We reveal how these behaviors are related to non-local transport via diffusion through the bulk, rationalizing the various scaling laws we observe and allowing us to interpret biologically relevant scenarios.

BP 14.96 Tue 18:00 P2

Noisy mixtures at the mesoscale: Vacuoles dancing in chemically active droplets — •Estéban Araspin, Leonardo Silva Dias, and Christoph A. Weber — Faculty of Mathematics, Natural Sciences, and Materials Engineering: Institute of Physics, University of Augsburg, Universitätsstrasse 1, 86159 Augsburg, Germany.

Understanding biological mixtures at the mesoscale calls for models that connect microscopic reactions with emergent continuum behavior in a thermodynamically consistent way. At such coarse-grained scales, noise, generally of multiplicative nature, is essential to capture phenomena like nucleation or stochastic switching between non-equilibrium steady states.

We developed a theoretical framework based on effective mesoscopic reaction-diffusion master equations that is applicable to both passive systems and non-equilibrium scenarios in which chemostatted fluxes make the mixture active. The framework connects to the macroscopic limit, recovering reactive Cahn-Hilliard-Cook dynamics.

As an application, we explore chemically active droplets in which a chemostatted ATP concentration leads to striking morphological dynamics. We find dilute-phase vacuoles that form and dissolve, reminiscent of bubbly phase separation in Model B+. We observe growth of small vacuoles at the expense of larger ones, dynamics that can be considered an inverse-ripening process.

Our results highlight the value of mesoscopic stochastic frameworks for understanding active phase separation and other soft-matter systems maintained away from equilibrium.

BP 15: Computational Biophysics III

Time: Wednesday 9:30–12:45 Location: BAR/SCHÖ

BP 15.1 Wed 9:30 BAR/SCHÖ

Local chain stiffening regulates non-equilibrium maturation and clustering in biomolecular condensates — •Subhadip Biswas[1] and Davit A Potoyan[2] — [1]Iowa State University, Ames, Iowa, USA — [2]Iowa State University, Ames, Iowa, USA

Biomolecular condensates formed through liquid-liquid phase separation display complex structural and dynamical features that are essential for cellular organization, signaling, and aging. Using coarse-grained molecular dynamics simulations based on a polymer model with tunable local semiflexibility and sticker stickiness, we systematically examine how angular rigidity modulates aging and clustering within condensates. We investigate four regimes involving coupled variations of sticker/spacer stiffness and interaction strength. By quantifying structural heterogeneity, orientational ordering, and rheological responses, including oscillatory shear, Green-Kubo viscosity, and uniaxial deformation, we uncover distinct non-equilibrium behaviors and maturation pathways that emerge from local chain stiffening. These results highlight angular rigidity as a key regulator of condensate stability and internal organization, with implications for understanding condensate aging in cells and for designing programmable biomaterials.

BP 15.2 Wed 9:45 BAR/SCHÖ

Uncovering the thermodynamic principles of enzymatic regulation in biomolecular condensates with reactive simulations — •Enrico Lavagna[1], Francesco Delfino[1], Georgii Koniukov[1], Matteo Paloni[1,2], Luca Ciandrini[1,3], and Alessandro Barducci[1] — [1]Centre de Biologie Structurale (CBS), Montpellier, France — [2]Department of Chemical Engineering, Thomas Young Centre, University College London, London WC1E 7JE, United Kingdom — [3]Institut Universitaire de France (IUF)

Biomolecular condensates are dynamic cellular assemblies often regulated by energy-consuming processes such as post-translational modifications (PTMs). Nevertheless, the coupling between reaction dynamics and cellular spatial organization remains poorly understood at the molecular scale. Using a minimal, particle-based model, we investigate how phosphorylation controls condensate steady-state behavior. We find that condensate formation is regulated by the steady-state fraction of phosphorylated scaffold proteins, which increases with enzyme activity. This chemical regulation exhibits a non-linear, non-trivial dependence on the phosphorylation strength. Furthermore, reaction fluxes are spatially heterogeneous, with phosphorylation activity sharply peaking at the condensate interface. Our findings highlight novel, general features of chemically active biomolecular condensates. Moreover, we observe that incorporating local detailed balance is essential for understanding how energy-consuming reactions shape the steady-state properties of phase-separated systems.

BP 15.3 Wed 10:00 BAR/SCHÖ

Multiscale Simulation of Phosphofructokinase-1 Assemblies: From Transient Interactions to Large-Scale Assembly Formation — Mehrnoosh Khodam Hazrati, Tom Miclot, and •Stepan Timr — J. Heyrovsky Institute of Physical Chemistry, Czech Academy of Sciences, Prague, Czech Republic

Human phosphofructokinase-1 (PFK1)—a key glycolytic enzyme—forms filaments and localizes into large-scale assemblies that are thought to play a major role in the regulation of glycolysis. However, the molecular interactions driving this assembly and the precise mechanisms by which it regulates the pathway remain poorly understood. In this work, we combine three levels of description—atomistic, residue-level coarse-grained, and highly coarse-grained—to characterize interactions between PFK1 tetramers and to elucidate factors governing PFK1 assembly formation. Atomistic molecular dynamics simulations of PFK1 filament interfaces reveal specific side-chain interactions that are critical for filament stability. These insights enable us to improve the description of filament formation in residue-level coarse-grained models. Using the Martini 3 and OPEPv7 coarse-grained models, we further identify key regions mediating transient PFK1–PFK1 interactions and show that these include filament-forming interfaces. Finally, we construct a highly coarse-grained model that integrates information from the more detailed simulations. Using this model, we investigate the role of membranes in PFK1 filament formation and describe how filaments may affect the recruitment of other constituents into large-scale glycolytic assemblies.

BP 15.4 Wed 10:15 BAR/SCHÖ

Multiscale Approaches to Phase Behaviour and Mechanical Properties of Synthetic DNA Networks — •Aaron Gadzekpo[1], Xenia Schneider[1], and Lennart Hilbert[1,2] — [1]Karlsruhe Institute of Technology, Institute of Biological and Chemical Systems — [2]Karlsruhe Institute of Technology, Zoological Institute

DNA can be used as a programmable material whose sequence-level design governs emergent properties. However, approaches that link sequences to the macroscopic behaviours needed in biotechnology remain limited. Here, we integrate coarse-grained simulations, Bayesian optimisation, and graph-based rheology to connect sequence-encoded, molecular-scale parameters to network-level properties. We apply our methods to DNA nanomotifs, which are nanometre-sized, multi-armed molecules assembled from single strands. Network formation among nanomotifs via sticky-end overhangs enables phase separation into liquid-like condensates or the assembly of viscoelastic hydrogels. Our multiscale approaches reveal how nanomotif flexibility, affinity, and concentration govern network formation, phase behaviour, and viscoelasticity. By combining our approaches, we propose inverse design strategies to select sequences that yield targeted emergent properties.

BP 15.5 Wed 10:30 BAR/SCHÖ

Self-Assembly of KAHRP Spirals in Malaria-Infected Red Blood Cells — Devika Magan[1], Michael Lanzer[2], and •Ulrich S. Schwarz[1] — [1]Institute for Theoretical Physics, Heidelberg University — [2]Center for Infectious Diseases, University Hospital Heidelberg

Malaria infections alter the mechanical and adhesive properties of red blood cells (RBCs). To avoid clearance by the spleen, infected RBCs develop thousands of nanoscale protrusions called knobs, which stiffen the RBC and mediate cytoadhesion to the endothelium. A central player in this process is the exported para-

site protein KAHRP. The parasite sends KAHRP to the RBC membrane skeleton, where it interacts with spectrin and actin to reorganize the local architecture. Strikingly, KAHRP also forms prominently sized spirals underneath the knobs, yet the physical principles governing their formation and how such structures might influence membrane mechanics are still not understood. In this talk, I present a coarse-grained, patchy-particle framework designed to explore how simple interaction rules can give rise to spiral formation. By tuning local binding geometry and torsional preferences, the model produces a rich variety of self-organized states, ranging from compact rings to extended curved chains. These simulations provide a starting point for connecting protein-level organization to cell-level mechanics. I will outline how this approach can be extended toward membrane-associated scenarios to investigate whether KAHRP assemblies can generate spontaneous curvature or store elastic energy - providing a path toward understanding their potential function during parasite cytoadhesion and egress.

30 min. break

BP 15.6 Wed 11:15 BAR/SCHÖ

From Data to Discovery: Machine Learning Force Fields for Fast and Accurate Ligand-Protein Screening — •Sergio Suárez-Dou[1], Miguel Gallegos[1], Hamza Ibrahim[2], Joshua T. Berryman[1], Andrea Volkamer[2], and Alexandre Tkatchenko[1] — [1]Department of Physics and Materials Science, University of Luxembourg, Luxembourg — [2]Data Driven Drug Design, Center for Bioinformatics, Saarland University, Germany

Pretrained Machine Learning Force Fields (MLFF) are transforming computational chemistry by combining speed and accuracy. In drug discovery, predicting binding energies and affinities is key to identifying viable candidates. Among MLFFs, SO3LR excels in both performance and efficiency, enabling accurate ligand and binding predictions at low computational cost, surpassing semiempirical methods.

However, data coverage remains a challenge. While datasets like OMol25 and QCell offer broad molecular diversity, drug-like chemical space requires more targeted representation. To address this, we are developing a dataset optimised for docking evaluations, covering key regions of drug-like space. Our goal is a pretrained model capable of predicting drug-ligand affinities with PBE0+MBD DFT-level accuracy, bridging quantum precision with high-throughput screening and accelerating drug discovery.

BP 15.7 Wed 11:30 BAR/SCHÖ

Modelling Protein Dynamics with Machine Learned Coarse-Grained Models — •Klara Bonneau — Freie Universität Berlin, Germany

The most popular and universally predictive protein simulation models employ all-atom molecular dynamics (MD). However, understanding dynamical processes like protein folding, interactions, and aggregation requires accessing timescales beyond conventional MD capabilities. Coarse-graining (CG) accelerates simulations by focusing on essential degrees of freedom, but a universally predictive CG model for proteins remains elusive. Our work introduces the first thermodynamically consistent CG model that extrapolates to unseen protein sequences. By leveraging state-of-the-art machine learning techniques, we simulate the folding of unknown proteins, protein-protein interactions, intrinsically disordered proteins, and mutation effects. Current extensions include larger proteins and protein-ion/small molecule interactions, surpassing conventional MD timescale limitations. Additionally, explainable AI techniques enable us to interpret results and demonstrate that deep learning models capture physically consistent interactions.

BP 15.8 Wed 11:45 BAR/SCHÖ

Gradient-Estimating Gillespie Simulators for Parameter Inference in Stochastic Models — •Ludwig Burger[1], Annalena Kofler[2], Lukas Heinrich[3], and Ulrich Gerland[1] — [1]Physics of Complex Biosystems, School of Natural Sciences, Technical University Munich — [2]Max Planck Institute for Intelligent Systems, Tübingen — [3]Data Science in Physics, School of Natural Sciences, Technical University Munich

Stochastic models are ubiquitous in (biological) physics, yet fitting such parameterized models to experimental data remains challenging. While gradients in deterministic systems can be obtained efficiently through numerical or automatic differentiation, these tools cannot be directly applied to stochastic simulation algorithms such as the Gillespie algorithm, where sampling from a discrete set of reactions introduces non-differentiable operations. In this work, we adapt three gradient estimators from machine learning for use in Gillespie simulations: the Gumbel-Softmax Straight-Through estimator, the Score Function estimator, and the Alternative Path estimator. We extend all three estimators to address the specific requirements of gradient estimation in Gillespie simulations. We analyze the statistical properties of the estimators and highlight practical advantages and limitations in two representative systems: a minimal bimolecular association-dissociation model and the repressilator. Our results demonstrate that gradient estimators can be effectively integrated into the Gillespie algorithm, providing a systematic approach for gradient-based parameter inference in stochastic models.

BP 15.9 Wed 12:00 BAR/SCHÖ

Deep-Pose-Tracker: a unified model for behavioural analysis of *Caenorhabditis elegans* — •Debasish Saha[1], Shivam Chaudhary[1], Dhyey Vyas[2], Anindya Ghosh Roy[2], and Rati Sharma[1] — [1]Indian Institute of Science Education and Research Bhopal, Bhopal, India — [2]BRIC-National Brain Research Centre, Gurugram, India

The ability to respond to environmental stimuli by living organisms is essential for survival and adaptation. Locomotion and posture-based analyses of animals are commonly performed; however, manually performing these tasks is effort-intensive, time-consuming, and error-prone. Automation of this process is therefore crucial for accurate and fast detection. To this end, in this work, we report the development of Deep Pose Tracker (DPT), an end-to-end deep learning model to automate the study of posture dynamics and locomotion behaviour of *C. elegans*, a model organism useful to study neuroscience, genetics, drug design, *etc*. The DPT model enables automatic detection and tracking of these animals while measuring essential behavioural features like locomotion speed, orientation, forward or reverse locomotion, complex body bends as omega turns, and eigenworms (representing the overall posture dynamics in a low-dimensional space). Our DPT model can generate highly accurate data, with very high inference speed, while being user-friendly and robust to experimental variabilities. DPT, therefore, can be a valuable toolkit for researchers studying behaviour under different environmental stimuli.

BP 15.10 Wed 12:15 BAR/SCHÖ

Adaptive Determination of Cluster Number in Single-Cell RNA-seq — •Cornelius Miller, Felix Wehrenberg, Dominik Egger, and Sophia Rudorf — Institute of Cell Biology and Biophysics, Leibniz University Hannover, Hannover, Germany

Single-cell RNA sequencing (scRNA-seq) has transformed transcriptomic research by enabling gene expression profiling at the resolution of individual cells. The complexity and high dimensionality of scRNA-seq data pose substantial challenges for effective data interpretation. Current analysis pipelines often struggle with computational scalability and the subjective nature of parameter selection. Here, we introduce a comprehensive Python-based framework that automates key analytical stages while maintaining user flexibility. A critical innovation of this framework is the implementation of an adaptive clustering algorithm designed to estimate cluster count without prior knowledge. This method was specifically developed to define the number of distinct subpopulations in Mesenchymal Stem Cell (MSC) datasets, where cellular heterogeneity is often ambiguous. Furthermore, by leveraging parallelization, the proposed architecture handles high-dimensional datasets with improved latency compared to sequential execution. This approach resolves common ambiguities in defining cell types, offering a robust tool for unbiased exploratory data analysis.

BP 15.11 Wed 12:30 BAR/SCHÖ

AI-Guided Transition Path Sampling of Lipid Flip-Flop and Membrane Nanoporation — •Matthias Post and Gerhard Hummer — Max Planck Institute of Biophysics, Frankfurt, Germany

We studied lipid translocation (or *"flip-flop"*) between leaflets of a bio-membrane and the possible involvement of water nanopores via molecular dynamics simulation.[1] We used transition path sampling[2] within the AIMMD[3] framework to efficiently sample unbiased lipid flip-flops and pore formation. A neuronal network model was trained to predict the *"committor"*, that is the probability of a successful transition from a given microscopic conformational state. While coarse-grained DMPC lipids flip via tunneling through the intact membrane, atomistic (CHARMM36) simulations reveal that flip-flop requires the formation of metastable water pores. DSPC bilayers and plasma membrane mimetics[4] facilitate flip-flop via transient water threads or nanodroplets to cross a locally thinned membrane. Deep neural networks map the transition mechanism from a high-dimensional (660d) feature space to a nearly linear committor model, consistent with Cover's theorem[5] and the concept of dominant reaction tubes.[6]

[1] Post, Hummer, *arXiv*.2502.11894 (2025) [2] Bolhuis et al., *Annu. Rev. Phys. Chem.* **53**, 291-318 (2002) [3] Jung et al., *Nat. Comput. Sci.* **3**, 334-345 (2023) [4] Pogozheva et al., *J. Chem. Inf. Model.* **62**, 1036-1051 (2022) [5] Cover, *IEEE Trans.Electron. Comput.* **EC-14**, 326-334 (1965) [6] E, Vanden-Eijnden, *J. Stat. Phys.* **123**, 503-523 (2006).

BP 16: Membranes, Vesicles and Synthetic Life-like Systems II

Time: Wednesday 9:30–12:45 Location: BAR/0205

Invited Talk BP 16.1 Wed 9:30 BAR/0205

Illuminating mitochondrial permeabilisation in apoptosis — •Ana J. Garcia Saez — Max Planck Institute of Biophysics, Frankfurt am Main, Germany

Mitochondrial permeabilization is a key step in the signaling pathway of apoptosis and in the cell*s commitment to death. It affects the outer and subsequently the inner mitochondrial membranes through the opening of membrane pores via mechanisms that are not fully clear. This releases cytochrome c and SMAC into the cytosol, leading to the activation of caspases, a set of proteases that accelerate cell death and that block inflammation by inactivating intracellular innate immunity effectors. Mitochondrial inner membrane permeabilization additionally releases mtDNA into the cytosol, which in turn activates intracellular innate immunity pathways unless counterbalanced by caspases. Here, I will discuss our work using advanced microscopy methods to advance our understanding of the molecular mechanisms of mitochondrial pores in apoptosis and how they function in the regulation of cell death and of inflammatory signaling outcomes.

BP 16.2 Wed 10:00 BAR/0205

Phase separation driven by membrane binding of receptor proteins of different size — •Samuel S. Gomez[1], Lennart Kleinschmidt[2], Daxiao Sun[2], Alf Honigmann[2], and Christoph Weber[1] — [1]Faculty of Mathematics, Natural Sciences, and Materials Engineering, Institute of Physics, University of Augsburg, Augsburg, Germany — [2]Technische Universität Dresden, Biotechnologisches Zentrum, Center for Molecular and Cellular Bioengineering (CMCB), Dresden, Germany

We aim to understand the physical mechanisms governing the spatial organisation and assembly of adherens junctions (AJs). A key open question is how size differences in the extracellular domains of AJ receptor proteins contribute to their segregation during junction formation. To address this, we develop a theoretical model of receptor-mediated adhesion between a GUV and a SLB, using both simulations and an experimental in-vitro setup to test and refine our model. Our model suggests that differences in receptor length are sufficient to drive spatial segregation, even in the absence of cis-interactions with similar adhesion affinities. We extend our model to understand the link between spatial organisation at the mesoscopic level of receptor segregation at membrane adhesion contact sites to the macroscopic heterogenous organisation of receptor proteins on the GUV. Our model aims to provide new insights into the physical principles underlying AJ assembly, in particular spatial organisation of receptor proteins on the mesoscopic and macroscopic level of the membrane within the AJ complex.

BP 16.3 Wed 10:15 BAR/0205

Selective information processing by particle distributions at living interfaces — •Jenna Elliott[1,2] and Anna Erzberger[1,2] — [1]European Molecular Biology Laboratory (EMBL), Heidelberg, Germany — [2]University of Heidelberg, Heidelberg, Germany

Living cells are capable of responding to environmental cues under noisy conditions, even in the absence of a centralised control unit or brain. Such systems therefore provide an ideal platform for uncovering the physical principles behind robust, decentralised information processing in soft materials. Motivated by the role interfaces play in relaying signals across cell boundaries, we investigate how spatially-varying particle distributions on interfaces facilitate information transmission in living cells. Starting from a statistical description of particle dynamics, we show that these distributions act as signal filters that non-linearly amplify heterogeneities in their environment. This mechanism permits a form of pattern recognition, with inter-particle interactions tuning the response function of the filter. We explicitly identify both thresholding and edge-detecting regimes and, accounting for thermal noise in the filters, quantify the flow of information across the interface. We find that, when suitably tuned, the noisy filters selectively compress input signals, resulting in the efficient encoding of information relevant to downstream tasks. Overall, our results indicate that the noisy patterning of membranes may be used to selectively sense environmental cues in biologically inspired systems, suggesting exciting implications for how physical interactions may encode computational logic in soft materials.

BP 16.4 Wed 10:30 BAR/0205

Synthetic cell-based artificial tissues to study T cell activation — Anna Burgstaller[1] and •Oskar Staufer[1,2,3] — [1]INM - Leibniz Institute for New Materials, Saarbrücken, Germany — [2]Campus D2 2 — [3]Max Planck Bristol Center for Minimal Biology, Bristol, United Kingdom

T cells integrate biochemical and biophysical cues within lymph nodes, collectively determining activation of adaptive immunity. Quantitatively understanding how mechanical and biochemical signals converge at the single-cell and tissue level requires new model systems. To address this, we developed millimeter-sized artificial lymph nodes assembled from synthetic cells. The mechanical properties of the synthetic cells, specifically their Young*s modulus, can be precisely tuned, while their surfaces can be functionalized with biochemical stimuli. This allows to independently tune their biomechanics and biochemistry. The resulting tissue architecture, including its anisotropy and stiffness, can be engineered to probe emergent, tissue-scale phenomena. Performing live cell microscopy of migrating T-cells within synthetic lymph nodes, we validate that they reproduce in vivo T-cell motility. Statistical modeling of migration trajectories reveals that tissues must support search strategies for effective signal integration and that confinement degree promotes regulatory phenotypes of the T cells. Our synthetic cell-based tissues recapitulate architectural features of lymphatic organs, providing a platform to dissect how mechano-signaling interacts with biochemical cues to shape T-cell immunity

BP 16.5 Wed 10:45 BAR/0205

Excitable lipid nanotubes as a model system of neuron signaling and for neuromorphic systems — •Jan Steinkühler — CAU Kiel University, Germany

Voltage-sensitive ion channels stand at the centre in the study of cellular excitability in neuronal networks. However, the spatial propagation of electrical waves along nerve fibres is not a property inherent to an individual ion channel but rather emerges from the arrangement of ion channels along a tubular lipid membrane. While the *in vitro* study of functional ion channels in model membranes is well established, the propagation of an action potential along a lipid-bilayer nanotube has not yet been investigated. Here we present our experimental work examining these phenomena with electro-optical measurements on force-induced lipid nanotubes and demonstrate the cable-like properties of such nanotubes. Furthermore, we study memory effects arising from the interplay between electrical-field-induced lipid migration and ionic nanofluidic conductance. Finally, we show our lab's efforts toward automated cell-free expression of ion channels and data-driven modeling of membrane excitability. More broadly, our results help establish the interplay between membrane phase, shape, and electrical properties in a controlled experimental setup.

15 min. break

BP 16.6 Wed 11:15 BAR/0205

Membrane reshaping across the tree of life — •Felix Frey — Institute of Science and Technology Austria, Klosterneuburg, Austria — Eindhoven University of Technology, Eindhoven, The Netherlands

Across the tree of life, different designs of cellular membranes have evolved that are both stable and flexible. In bacteria and eukaryotes single-headed lipids self-assemble into flexible bilayer membranes. By contrast, archaea have distinct membranes that typically contain mixtures of single-headed bilayer lipids and double-headed bolalipids. While this composition is believed to enable extremophile archaea to survive harsh environments, the physical mechanisms underlying the reshaping of archaeal membranes are often unknown. Here, through the development of coarse-grained molecular dynamics simulations, we systematically compare the different membrane designs [1]. We explore the physical properties of archaeal membranes and explain how their stability and response to reshaping depends on the flexibility of single bolalipids and the amount of bilayer lipids they contain.

[1] M. Amaral*, F. Frey*, X. Jiang, B. Baum, A. Šarić (2025) Balancing stability and flexibility when reshaping archaeal membranes, eLife 14:RP105432, *Equal contributions.

BP 16.7 Wed 11:30 BAR/0205

Fluctuating triply periodic membranes: a phase-field study of diffusion in dynamic, confining environments — •Jakob Mihatsch and Andreas M. Menzel — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Understanding how individual entities move through interconnected structures is crucial for applications in biology and technology. A key example is the diffusive motion of molecules in porous networks. This porous environment is usually not static, but subject to thermal fluctuations and interactions with the object that is transported through it. Focusing on the situation of a spherical diffusive particle confined by fluctuating triply periodic membrane structures, we investigate numerically the effect of such a dynamic environment on the motion of a confined object [1]. We employ a phase-field approach to model the membrane surface, which allows us to apply dynamic perturbations to the shape of the membrane, without having to track its location explicitly. Triply periodic membranes can form channels with narrow pores, which lead to transient trapping. We find that thermal fluctuations can widen these pores, which speeds up diffusive transport and allows larger particles to pass through the pores than one would expect for an unperturbed membrane. Our work also shows that deformation of the membrane induced by the particle plays an important role in enhancing diffusion. Our results should be directly observable, for example, during protein diffusion through biological environments.

[1] J. Mihatsch, A. M. Menzel, arXiv:2511.23192 (2025).

BP 16.8 Wed 11:45 BAR/0205

Optimizing Dynamin for Membrane Fission — •Russell Spencer and Marcus Muller — Georg-August University Göttingen, Göttingen, Germany

Membrane tube fission is a fundamental cellular process, facilitated by the dynamin protein family. The primary energetic barrier to fission arises from the (constriction-catalyzed) collapse of the tube into a hemifused intermediate. We previously developed a self-consistent field theory (SCFT) framework to systematically study this process, and validated it against experiments. The precise mechanisms by which dynamin promotes this transition, however, remain unclear. We now model membrane tubes in the presence of dynamin-like proteins, incorporating both steric constriction and surface interactions. We explore the effect of different protein-membrane coupling mechanisms on the fission barrier, including excluded volume, head-group adhesion, and leaflet splay. While membrane attraction is necessary for protein assembly and induces curvature, it also opposes local constriction, inhibiting tube collapse. In contrast, insertion of the PH domain into the head groups leads to their splaying and produces a localized chevron-shaped membrane deformation. This facilitates tube collapse without opposing local constriction, thus promoting fission.

BP 16.9 Wed 12:00 BAR/0205

Interferometric and Fluorescence Nanoparticle Tracking for Analysis of Extracellular Vesicles — •Shuhan Jiang[1,2], Anna Kashkanova[4], Morgan Miller[1,2], Hannarae Lee[1,2,3], Hamed Qazvini[1,2], and Vahid Sandoghdar[1,2,3] — [1]Max Planck Institute for the Science of Light, Erlangen, Germany — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany — [3]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [4]AE Eindhoven, Groene Loper 19, Flux, Netherlands

Extracellular vesicles (EVs) are considered to be important disease markers. However, their inherent heterogeneity poses a major challenge for the characterization of their physical properties and biochemical content. We combine interferometric nanoparticle tracking analysis (iNTA) with fluorescence detection to measure particle size, refractive index, and fluorescence intensity with single-molecule sensitivity. We verify that the fluorescence signal increases with particle size for dye-labeled liposomes, and that count rates shift as one changes the labeling density. In an exemplary case study applied to HEK293-derived EVs, we show that the method resolves CD9/CD81-positive subpopulations, while marker-negative particles appear more heterogeneous, suggesting contaminants or altered composition. We discuss the potential of this multimodal approach for precise differentiation of heterogeneous nanoparticles and quantitative biomarker analysis.

BP 16.10 Wed 12:15 BAR/0205

Active and Brownian Colloids interacting with Lipid Vesicles — •Antonio Stocco, Clément Marque, and Florent Fessler — Institut Charles Sadron, CNRS, Strasbourg, France

Motion of active and passive Brownian particles is strongly affected by confinement effects, which impact the persistence of the ballistic dynamics and can guide transitions and instabilities when dealing with deformable interfaces. Here, I will present some experimental results describing the dynamics of active and passive colloids interacting with soft fluctuating membranes. Our experimental systems are composed of Giant unilamellar vesicles (GUVs) with tunable membrane tension and bare or Janus self-propelled colloids showing different hydrodynamic and particle-membrane interactions. We were able to observe emerging dynamics such as autonomous particle engulfment by the vesicle membrane, hysteresis of the particle wrapping dynamics and membrane tension dependent particle drag [1,2,3]. References: [1] F Fessler, M Wittmann, J Simmchen, A Stocco. Dynamics of Active Colloid Engulfment by Giant Lipid Vesicles, Soft Matter 2024, 20, 5904. [2] F Fessler, P Muller, A Stocco, Energetics and dynamics of membrane necks in particle wrapping, Journal of Colloid and Interface Science 2025, 700, 138524 [3] C Marque, G d'Avino, D Larobina, A Michel, A Abou-Hassan, A Stocco Diffusion of a single colloid on the surface of a giant vesicle and a droplet Physical Review E2025, 111 (2), 025411

BP 16.11 Wed 12:30 BAR/0205

pH Dependence of the Structure of Drug-Free Lipid Nanoparticle Dispersions — •Marta Gallo[1], Klaus Götz[1], Bishoy Hakim[1], Carola Vogel[1], Christian Bär[1], Lionel Porcar[2], and Tobias Unruh[1] — [1]Institute for Crystallography and Structural Physics, Friedrich Alexander University Erlangen Nürnberg — [2]Institut Laue-Langevin, 71 Avenue des Martyrs, Grenoble 38042, France

Lipid nanoparticle (LNP) dispersions are promising drug-delivery systems due to their ability to encapsulate diverse therapeutics and release them in controlled ways. A key advantage of many LNPs is their sensitivity to environmental pH, enabling drug release in acidic endosomal conditions through lipid conformational changes that destabilize the particles. To clarify these mechanisms, we synthesized drug-free LNPs mimicking the Comirnaty formulation and examined how pH affects their structure. Using simultaneous small angle X-ray and neutron scattering (SAXS/SANS) at the ILL D22 instrument, we monitored particle swelling and ordered-structure formation across different pH levels. Dialysis experiments, transitioning samples between pH 3.3 and 7, demonstrated fully reversible structural changes, as confirmed by cryo-TEM. Coupling SAXS/SANS with photon correlation spectroscopy (PCS) revealed a complex particle size distribution and deeper insight into LNP dynamics under different contrasts and pH conditions. The results clarify how pH-triggered structural transitions govern LNP behavior, supporting the design of next-generation delivery systems with enhanced release control and targeting.

BP 17: Statistical Physics of Biological Systems I (joint session DY/BP)

Time: Wednesday 9:30–12:45 Location: ZEU/0114

See DY 33 for details of this session.

BP 18: Focus session: Integrative Structural Modeling

Modern biological questions - and the growing recognition that biomolecular dynamics are central to molecular function - demand increasingly integrated technological strategies to probe the structure and behavior of biomolecules. Yet bringing insights from diverse experimental techniques together in a rigorous, quantitative way remains a formidable challenge, requiring deep expertise across methods as well as sophisticated modeling approaches. This focus session aims to ignite collaboration at this interface. By gathering experimentalists with complementary skill sets and researchers specializing in computational and theoretical modeling, we will create a space for vibrant exchange, cross-disciplinary learning, to lead to the development of well-informed, predictive models of complex biological systems.

Organized by Richard Börner (HS Mittweida) and Sigrid Milles (FMP Berlin)

Time: Wednesday 10:30–12:45 Location: BAR/0106

Invited Talk BP 18.1 Wed 10:30 BAR/0106

Protein complex structure prediction, state-of-the-art and challenges — •Ezgi Karaca — Izmir Biomedicine and Genome Center — Dokuz Eylul University, Izmir, TR

The advent of artificial intelligence has reshaped structural biology, enabling unprecedented accuracy in protein modeling. As the assessor for CASP14 and CASP15, I witnessed remarkable progress facilitated by AlphaFold. While CASP14 participants struggled with intersubunit contacts, CASP15 saw prediction success rates rise from 31-percent to 90-percent by incorporating AlphaFold2 (AF2) into customized pipelines. This improvement was driven by curated multiple sequence alignments (MSAs), though complexes with shallow MSAs remained challenging. Addressing this, we developed MinnieFold, an efficient protocol achieving a 50-fold reduction in GPU usage while maintaining accuracy in antibody-antigen complexes. Further investigating AF's performance,

we analyzed 276 human-parasite interactions across 15 species. Comparing AF2 and AlphaFold3 (AF3), we observed striking differences in predicted structures. This presentation highlights these advances, challenges, and our contributions to AI-driven structural biology.

BP 18.2 Wed 11:00 BAR/0106

Extending the Fluorophore Dye Library for FRET-guided Modeling — •Isolde Kirk[1], Felix Erichson[1], Josephine Meitzner[1], Patrick K. Quoika[2], and Richard Börner[1] — [1]Laserinstitut Hochschule Mittweida, Mittweida, Germany — [2]Technische Universität München, Munich, Germany

Integrative structural modeling combines experimental observables with computational methods to obtain realistic descriptions of biomolecular structures and their dynamics. One such approach integrates Förster Resonance Energy Transfer (FRET) and dynamic fluorescence anisotropy with molecular dynamics (MD) simulations. Ensuring comparability between experiment and simulation requires realistic modeling of fluorescent dyes in silico. In practice, existing dye libraries do not cover the full range of available fluorophores, including phosphate-backbone-linked carbocyanine (Cy) dyes. We therefore modeled and parametrized a FRET dye pair of Cy3 and 5 with a backbone-linked Cy3 fragment for MD simulations. We used Gaussian to assign partial charges with the restrained electrostatic potential method, as implemented in Antechamber, yielding several parametrization variants. The dye fragments were then incorporated into a DNA hairpin model and characterized using MD simulations with GROMACS. Depending on the parametrization, the DNA hairpin showed different structural responses, ranging from stable dye intercalation to partial helix destabilization. One parametrization showed agreement with the experimental data and therefore provides a validated extension for future FRET-guided modeling.

BP 18.3 Wed 11:15 BAR/0106

Structural dynamics and long-range interactions controlling timing of the Neurospora circadian clock — •Muriel Hartsch[1], Ida Marie Vedel[1], Kathrin Motzny[1], Michael Brunner[2], and Sigrid Milles[1] — [1]Leibniz-FMP Berlin, Robert-Roessle-Str. 10, 13125 Berlin — [2]Heidelberg University, Biochemistry Center (BZH), Im Neuenheimer Feld 328, 69120 Heidelberg

The function and maintenance of the circadian clock in Neurospora crassa are governed by a feedback loop involving both negative and positive regulatory elements, which together drive the oscillating circadian rhythm with a period of approximately 24 hours. The dimeric, intrinsically disordered protein FREQUENCY (FRQ) is a key component of the negative feedback complex and subject to post-transcriptional hyperphosphorylation by casein kinase 1a (CK1a). Phosphorylation of clock proteins is highly conserved across species, from fungi to mammals, with the human PERIOD (PER) protein being a notable example. However, the precise functions associated with hyperphosphorylation remain poorly understood. We hypothesize that time-dependent hyperphosphorylation of FRQ at multiple sites facilitates a transition from closed to open conformation, regulating interactions with its partners. Using nuclear magnetic resonance (NMR) and single-molecule fluorescence resonance energy transfer (smFRET), we investigate the conformational dynamics going along with FRQ phosphorylation by recombinant CK1a. This will allow, combined with structural modeling of the intrinsically disordered protein, to understand how phosphorylation alters the conformation and triggers a switch in FRQ.

15 min. break

Invited Talk BP 18.4 Wed 11:45 BAR/0106

From Sparse Restraints to All-Atom Models: Integrative Reconstruction of Hidden GPCR Conformations — •Matthias Elgeti — Institute for Drug Discovery, Leipzig University Medical School, Leipzig, Germany

Transmembrane proteins such as G protein coupled receptors (GPCRs) play central roles in cellular signal transduction and constitute major targets for therapeutic intervention. Their intrinsic conformational flexibility, however, leads to the coexistence of multiple interconverting states, which complicates structural characterization by high-resolution methods. Site-directed spin labeling (SDSL) EPR spectroscopy is uniquely suited to probe such flexible systems independent of molecular size, but it provides only sparse structural restraints. To bridge this gap, we integrate SDSL-EPR distance data with deep-learning-based structure prediction and molecular dynamics simulations. Using the angiotensin receptor (AT1R), a key regulator of cardiovascular function, we demonstrate how this integrative approach reveals a ligand-stabilized conformational state with distinct functional properties. We further present a computational pipeline that reconstructs corresponding all-atom models from sparse spectroscopic restraints and enables systematic exploration of hidden conformational states, providing a general framework for structure-guided analysis of signaling mechanisms and future drug discovery.

BP 18.5 Wed 12:15 BAR/0106

RNA 3D Folding Using Diffusion Models and Agentic Tree Search — •Arunodhayan Sampathkumar and Danny Kowerko — Professorship of Media Informatics, Technische Universität Chemnitz

Accurate prediction of RNA three-dimensional structure is essential for understanding RNA function and guiding RNA-based therapeutics. However, RNA folding remains challenging due to complex tertiary interactions, context-dependent base pairing and limited structural data, especially for short sequences with fewer than 80 nucleotides. To address this, we introduce a multi-model RNA structure prediction framework that combines an RNA-adapted Protenix model, a Boltz diffusion sampler and a template-based modeling (TBM) baseline together with GAN-augmented training for underrepresented short RNAs. Protenix offers accurate local geometry, Boltz supplies diverse global conformations and TBM contributes strong constraints when templates exist. All models are evaluated on the Kaggle RNA 3D public and private test sets. Protenix reaches TM-scores of 0.48/0.46, Boltz 0.41/0.40 and TBM 0.61/0.57. We further introduce an agentic tree-search ensemble that selects and refines conformations using consensus scoring and RMSD-based diversity. This ensemble significantly improves performance, achieving TM-scores of 0.68 (public) and 0.63 (private). Our results demonstrate that integrating generative models, template signals and agentic search yields more accurate RNA structures and improves robustness for novel RNA families.

BP 18.6 Wed 12:30 BAR/0106

RNA adsorption in confinement, from electrostatic properties to spatial organization — •Horacio V. Guzman, Willy Menacho, and Ian Addison-Smith — Biophysics & Intelligent Matter Lab, Material Science Institute of Barcelona, CSIC, 08193 Barcelona, Spain

Electrostatic interactions are the main driving force of the RNA-protein association during viral assembly and disassembly processes. However, the properties of confined single stranded ss-RNA inside diverse proteinaceous viral geometries remain largely unexplored due to challenges associated with their high-resolution characterization. Electrostatics and mechanical properties at the RNA-proteins interface are also the origin of ss-RNA stability in confinement. Combining archetypical RNA fragments and diverse confined symmetries, we present multiple-solvent molecular models to explore the most favorable initial spatial organization as a function of the type of confinement. Our method shows that electrostatic interactions drive the 3D RNA structure path towards possible initial conformations. In particular for small RNAs, which are frequently interacting with the proteinaceous subunits during the virus assembly process, also known as packaging signals. We compared our results to X-ray structures of small plant viruses validating the most favorable initial conformations with our method and the virus folding symmetry. Our findings start a quantitative route to elucidate the electrostatic character of RNA-protein interfaces, and a complementary understanding to RNA packaging, assembly and disassembly processes.

BP 19: Round Table Discussion: The Future of Neutrons in France and Germany (joint session CPP/BP)

Organized by Benoit Coasne and Christine M. Papadakis.

Time: Wednesday 11:45–12:45 Location: ZEU/LICH

See CPP 36 for details of this session.

BP 20: Protein Structure and Dynamics

Time: Wednesday 15:00–17:45 Location: BAR/0106

BP 20.1 Wed 15:00 BAR/0106

Enhanced Conformational Dynamics of Biomolecules with Quantum-Accurate Machine Learning Force Fields — •Naziha Tarannam — University of Luxembourg, Luxembourg

Machine Learning Force Fields (MLFFs) address a long-standing challenge in computational biophysics: lifting quantum accuracy in the treatment of biomolecules to the large scales, above nanometres and nanoseconds, normally available only to classical-like molecular mechanics force fields (MMFFs). Our recently developed SO3LR model was trained on a diverse set of over four million configurations and achieves ab initio-level accuracy while remaining computationally efficient for large systems in explicit solvent. We explore the dynamics of several globular proteins in aqueous systems comprising up to 35,000 atoms using SO3LR, and compare its performance against a set of widely used MMFFs. While SO3LR faithfully reproduces the static structural properties of proteins, it exhibits enhanced exploration of conformational space during molecular dynamics simulations compared to MMFFs, showing qualitatively different properties of sampling and convergence. This stems from its relatively accurate treatment of quantum many-body forces. Notably, SO3LR enables proteins to explore a broader spectrum of dihedral angles (ψ/ϕ distributions) that are inaccessible to conventional force fields, leading to higher configurational entropy over comparable simulation timescales. These results imply that classical treatments of biomolecules, even if they reach an adequate thermodynamic accuracy, may often do so for the wrong reasons.

BP 20.2 Wed 15:15 BAR/0106

Molecular dynamics simulations of native state collagen fibrils — Konstantinos Steiakakis[1], Alan Pichard[2], and •Maxime Vassaux[2] — [1]Processing and Performance of Materials, Department of Mechanical Engineering, Eindhoven University of Technology, Eindhoven, 5600 MB, The Netherlands — [2]Univ. Rennes, CNRS, IPR - UMR 6251, Rennes, 35000, France

Collagen fibrils are the building block of many biological tissues, which viability depend on the fibrils properties. Altered properties of collagen fibrils are central to the appearance of many diseases, and physiological or native properties must be reproduced for tissue engineering. Yet, the self-assembly, the structure, and therefore the properties of collagen fibrils remain elusive. One main reason is the extreme sensitivity of the fibrils to their environmental conditions, and in particular hydration which is only loosely bound by experimental measurements. Furthermore, mechanics are an integral part of the self-assembly process and may result in internal stresses in collagen fibrils in native conditions. Here, we investigate hydradtion, structure and internal stresses in collagen fibrils by means of molecular dynamics simulations of the collagen microfibril model. Overall, our findings provide insights into the native properties of collagen fibrils such as longitudinal pre-strain and water content. More than ever, collagen fibrils appear to be assembled via an out-of-equilibrium process key for the synthesis of viable tissues.

BP 20.3 Wed 15:30 BAR/0106

Atomic-Level Insights into Amyloid Resistance Gained from Molecular Dynamics Simulations — •Adrian Felix Schnell[1], Tim Moderer[2], Marcus Fändrich[2], and Nadine Schwierz[1] — [1]Institute of Physics, Computational Biology, University of Augsburg, Universitätsstraße 1b, 86159 Augsburg, Germany — [2]Institute of Protein Biochemistry, Ulm University, 89081 Ulm, Germany

Systemic AA amyloidosis arises from the misfolding and aggregation of normally soluble serum amyloid A1 (SAA1) protein into pathogenic fibrils. Despite extensive experimental efforts, the molecular driving forces that govern fibril formation and resistance remain only partly understood.

Using atomistic molecular dynamics (MD) simulations of experimentally resolved structures in both the fibrillar and native states, we investigated sequence-specific features that modulate amyloid stability and resistance. Simulations of wild-type SAA1 and two naturally occurring variants known to display amyloid resistance reveal how single-point mutations can markedly influence fibril stability and impede fibril growth. Specifically, the atomistic MD trajectories show that the resistant variants fail to stably adopt the pathogenic fibril conformation, pointing to distinct structural and dynamical mechanisms underlying their protective effect.

Invited Talk BP 20.4 Wed 15:45 BAR/0106

Solution scattering and MD simulation as quantitative probes of protein-specific and temperature-dependent hydration — •Jochen S Hub — Saarland University, Saarbrücken, Germany

The hydration shell is an integral part of proteins since it plays key roles for confor- mational transitions, molecular recognition, and enzymatic activity. While the dynam- ics of the hydration shell have been described in detail by spectroscopic techniques, the structure of the hydration shell remain less understood due to the lack of hydration shell-sensitive structural probes with high spatial resolution. Whether MD simulations correctly reproduce the hydration shell structure is not known. Small-angle scattering (SAS) with X-rays or neutrons (SAXS/SANS) is sensitive to the hydration shell; however, the hydration shell effects on SAS data has traditionally been considered as a problem, which had to be absorbed into free fitting parameters, rather than a chance to learn the hydration shell structure. We combine SAS data with MD simulations and explicit-solvent SAS predictions to reveal how factors such as surface properties, temperature, and force fields influence protein hydration. We find that (i) MD simulations with certain (but not all) force fields yield excellent agreement with the SAS data; (ii) chemical characteristics of surface-exposed moieties strongly modulate the hydration shell contrast and structure; (iii) temprature-ramp SAXS and MD show consistently that the protein hydration shell is remarkably temperature-sensitive. Our studies demonstrate the combination of SAS and explicit-solvent MD simulations as quantitative structural probes of protein hydation.

15 min. break

BP 20.5 Wed 16:30 BAR/0106

Microscopic Insights into the Solvation of Stapled Peptides A Case Study of p53-MDM2 — Vikram Gaikwad, •Asha Rani Choudhury, and Rajarshi Chakrabarti — Indian Institute of Technology Bombay, Mumbai, India

Water often termed the universal solvent, plays a vital role in numerous biomolecular processes, including protein-protein interactions. One such critical complex is p53-MDM2, which is central to cellular regulation. Inhibiting the p53-MDM2 interaction remains a therapeutic challenge, and stapled peptides have emerged as promising candidates in this context.The stapled peptides are peptidomimetics in which the side chains of two suitably positioned amino acids are covalently linked using an appropriate chemical moiety. In this study, we investigate the role of water in the binding of stapled p53 peptides to MDM2 using molecular dynamics simulations. Our aim is to understand how variations in the chemical nature and stapling position of the hydrocarbon cross-linker influence the behavior of water molecules surrounding the p53 peptide. Using rigorous entropy calculations, we rationalize the enhanced binding affinity of stapled p53 peptides compared to that of their unstapled counterparts from a solvent-centric perspective. Specifically, the entropy gain of water molecules around the stapled peptides, combined with the conformational entropy loss of the peptide, contributes favorably to binding. These findings offer valuable insights into the rational design of stapled peptides and support the development of improved therapeutic inhibitors targeting the p53-MDM2 interaction.

BP 20.6 Wed 16:45 BAR/0106

What is the structure of biomolecular condensates? — •Charlotta Lorenz[1,2], Nathaniel Hess[3], Sully Bailey-Darland[1], Teagan Bate[1], Takumi Matsuzawa[1], Tong Wang[1], Kaarthik Varma[1], Dana Matthias[1], Harsha Koganti[1], Lois Pollack[1], Benjamin Schuler[2], Jerelle Joseph[3], and Eric Dufresne[1] — [1]Cornell University, Ithaca, NY, USA — [2]University of Zurich, Zurich, Switzerland — [3]Princeton University, Princeton, NJ, USA

Biomolecular condensates are important for a variety of cellular functions, such as biochemical regulation, structural organization, and RNA metabolism. While the properties and physiology of these condensates depend on their structure, this important aspect has received little experimental consideration. We expect a structure-function relationship determined by protein-protein interactions. Recent simulations of disordered proteins with interactions based on the sticker-and-spacer suggest fascinating structures in the bulk and surface of condensates. We reveal the structure of biomolecular condensates using small-angle X-ray scattering. We show that condensates made from a simple model system of bovine serum albumin (BSA) and polyethylene glycol (PEG) behave like a classical liquid. We extend our approach to the structure of condensates made of disordered proteins such as fused in sarcoma (FUS) and we find that FUS inside condensates structurally behaves like a gas. Our approach is applicable to a variety of different condensates and shows that diverse condensates have diverse structures.

BP 20.7 Wed 17:00 BAR/0106

Dynamics and (self-)interactions of the endocytic protein Eps15 — •Andromachi Papagiannoula, Ida M Vedel, Arbesa Saiti, Kathrin Motzny, and Sigrid Milles — Leibniz-Forschungsinstitut für Molekulare Pharmakologie im Forschungsverbund, Berlin

Eps15 is one of the earliest initiators of clathrin-mediated endocytosis (CME). The dimeric protein carries three EH domains per monomer, which are known to recognize Asn-Pro-Phe (NPF) motifs in intrinsically disordered regions (IDRs). Using nuclear magnetic resonance (NMR) spectroscopy, we examined interactions between EH domains and the IDR of the endocytic partner Dab2. In ad-

dition to canonical NPF recognition, we detect a high level of binding promiscuity leading to interaction with other phenylalanine-rich regions. This behavior enables EH domains to also engage with Eps15's own IDR, creating partial competition with Dab2. Nevertheless, Dab2 and the Eps15 IDR can bind EH domains simultaneously, leading to recruitment of Dab2 into Eps15 condensates. When EH domains are expressed in row, as they naturally occur in the wild type full length protein, EH2 and EH3 tumble together as one entity, while EH1 moves independently. Using single molecule Forster resonance energy transfer (smFRET), we assess the three dimensional organization of the three EH domains with respect to each other and assess binding with both Dab2 and Eps15 IDRs.

BP 20.8 Wed 17:15 BAR/0106

ASAXS Based Absolute Intra-Molecular Distance Measurements for Proteins — •Samuel Stubhan[1], Anna Baptist[1], Caroline Körösy[1], Alessandra Narducci[2], Gustavo Gabriel Moya Munoz[2], Nicolas Wendler[2], Aidin Lak[1], Michael Sztucki[3], Thorben Cordes[2], and Jan Lipfert[1] — [1]Department of Physics and Center for NanoScience, LMU Munich, Amalienstr. 54, 80799 Munich, Germany — [2]Physical and Synthetic Biology, Faculty of Biology, LMU Munich, Großhadernerstr. 2-4, 82152 Planegg-Martinsried, Germany — [3]ESRF, 71 Avenue des Martyrs, 38043 Grenoble, France

Intramolecular distance measurements are key to understanding macromolecular structure and dynamics. Anomalous Small-Angle X-ray Scattering (ASAXS) interferometry enables such measurements by attaching small (~1 nm) gold nanoparticles to target molecules and using X-ray scattering to extract distance distributions. ASAXS provides absolute distances over >10 nm, full ensemble distributions, and minimal sensitivity to label orientation, offering advantages over FRET and NMR.

We demonstrate ASAXS on proteins for the first time using two cysteine variants of maltose binding protein in apo and holo states, directly revealing ligand-induced conformational changes. The resulting distance distributions agree with single-molecule FRET measurements. Requiring only a double-labeled sample and accommodating diverse solution conditions, ASAXS offers a robust, broadly applicable tool for probing protein conformational ensembles.

BP 20.9 Wed 17:30 BAR/0106

Probing membrane protein dynamics on lipid-functionalized graphene transistors through low-frequency noise — •Florian Steinbach[1], Mykola Fomin[1], Eduard Haar[2], Svetlana Vitusevich[3], Mykhaylo Petrychuk[3], Christian Ungermann[2], and Carola Meyer[1] — [1]Institute of Physics, University of Osnabrück — [2]Department of Biology/Chemistry and Center for Cellular Nanoanalytics, University of Osnabrück — [3]Institute of Biological Information Processing (IBI-3), Forschungszentrum Jülich

Graphene field-effect transistors (GFETs) functionalized with lipid monolayers provide a controlled and label-free platform for studying membrane-associated proteins [1]. Here, we present electronic transport experiments where the Rab7-like GTPase Ypt7 is immobilized within a lipid monolayer. While there is not electrostatic gating effect observed, the addition of the protein causes a pronounced increase in low-frequency 1/f noise. This noise signal is diminished upon binding of the membrane tethering HOPS complex [2]. The persistence of distinct noise signatures despite strong screening indicates a transduction mechanism that may circumvent the screening within the Debye length.

[1] M. Fomin, L. Jorde, F. Steinbach, C. You, C. Meyer, Phys. Status Solidi B 2300324 (2023).

[2] M. Fomin et al, accepted for publication in Fluctuation and Noise Letters (2025).

BP 21: Focus Session: Sequence Spaces, Populations and Evolution

Evolutionary processes are central in the living world: they leave patterns in sequence databases and underlie phenomena such as cancer progression and antibiotic resistance. Achieving a quantitative understanding of evolution relies on two key components: variation and selection. The first component - variation - arises from random mutations in genotypic sequences that lead to selectable changes in phenotype and fitness. Thus, variation depends on how phenotype and fitness are distributed in biological sequence spaces. The second component - selection * shapes the composition of future generations and thus acts at the population level. Since these components jointly shape evolutionary processes, this focus session will encompass both: variation in sequence spaces and selection on the population level.

Organized by Nora Martin (Centre for Genomic Regulation, Barcelona) and Paula Garcia Galindo (University of Cambridge)

Time: Wednesday 15:00–17:30 Location: HÜL/S386

Invited Talk BP 21.1 Wed 15:00 HÜL/S386

Microbial Behavior in Context — •Fernanda Pinheiro — Human Technopole, Milan, Italy

Predicting microbial responses to antibiotics, nutrient shifts, or invading species requires models linked to metabolic pathways and cellular functions. In this talk, I present quantitative approaches for characterizing microbial behavior, from growth kinetics to coarse-grained models of cell metabolism and empirical growth laws. I will connect growth parameters to resource allocation and physiological constraints, and I will show how growth perturbations reveal layers of organization, from cellular physiology to ecological interactions and evolutionary change. In a broader context, I will discuss how metabolic models linking systems biology, ecology, and evolution can become tools for prediction.

BP 21.2 Wed 15:30 HÜL/S386

Insertions and Deletions make important contributions to the arrival of phenotypic variation — •Manuela Giraud[1,2] and Nora Martin[1] — [1]CRG (Barcelona Collaboratorium for Modelling and Predictive Biology), Dr. Aiguader 88, Barcelona 08003, Spain — [2]Universitat Pompeu Fabra (UPF), Barcelona, Spain.

In evolution, phenotypic variation is a prerequisite for selection and arises from random genotypic mutations. An extensive mapping of genotypes to their corresponding phenotype (GP map) provides us with a quantitative model for variation, thus informing evolutionary predictions. The features of GP maps and their relevance for evolutionary processes have been analyzed for different model systems, but these analyses have largely been limited to short substitutions. Insertions and deletions (InDels) of different lengths have been neglected despite their presence in natural sequence families. In this study, we analyze InDels in computational GP maps modelling RNA secondary structure, enzyme functionality, and a toy-model for protein quaternary structure self-assembly. We find that InDels are more likely to preserve the phenotype than expected from null models. These phenotype-conserving indels imply large sequence changes, affecting the effect of subsequent mutations: after a phenotype-conserving InDel, the distribution of accessible phenotypes shifts increasingly with the mutation size. Evolutionary simulations indicate that such phenotype-conserving indels can fix and strongly affect the number of encountered phenotypes. These results imply that InDels, even if rare, can make an important contribution to the arrival of phenotypic variation.

BP 21.3 Wed 15:45 HÜL/S386

Bias toward simplicity and symmetry in protein self-assembly — •Prarthana Agrawal — University of Oxford

Symmetry is ubiquitous in protein complexes and other biological assemblies and is often attributed to natural selection. Algorithmic information theory offers an alternative explanation: when structures are generated by simple local rules, outcomes that require less information to specify are intrinsically more likely [1]. Because symmetry enables reuse of the same assembly instructions, symmetric structures typically have low algorithmic (Kolmogorov) complexity and are therefore strongly favored.

We test this idea using a three-dimensional polycube self-assembly model as an abstract representation of protein quaternary structure. By sampling interaction rule spaces, we find a strong bias toward low-complexity assemblies, with symmetric structures occurring far more frequently than asymmetric ones. We further show that not all symmetries are equally accessible: some symmetry operations reduce assembly complexity more effectively than others and are therefore disproportionately likely.

These results indicate that biases toward simple and symmetric structures in self-assembly arise from intrinsic generative constraints rather than natural selection alone, suggesting that evolutionary outcomes are shaped not only by selection but also by how phenotypic variation is generated.

[1] Johnston et al., Proc. Natl. Acad. Sci. U.S.A. 119, e2113883119 (2022)

15 min. break

Invited Talk BP 21.4 Wed 16:15 HÜL/S386

The navigability of fitness landscapes shaped by global and universal epistasis — •Joachim Krug — Institute for Biological Physics, University of Cologne, Germany

Epistasis is the dependence of the effect of a mutation on the genetic context in which it occurs. Epistatic interactions shape the topography of the fitness landscape, the mapping from genotype to reproductive success. Global epistasis refers to interactions that arise when a nonlinear phenotype-fitness map acts on a lower-dimensional set of non-epistatic phenotypes, and has been argued to be a common occurrence at different scales of biological organization. It is therefore of interest to ask what features characterize fitness landscapes when epistasis is purely global. Here I show that, under certain conditions, global epistasis implies universal negative epistasis [1], an order relation on sequence space that is closely related to submodularity of set functions [2]. Universal epistasis makes fitness landscapes easily navigable, because any fitness peak is accessible through combinatorially many fitness-increasing mutational paths. I will discuss the theoretical results within the context of recent studies of large-scale empirical fitness landscapes that have found that rugged landscapes may also be highly navigable.

[1] Krug, J. & Oros, D.: Evolutionary accessibility of random and structured fitness landscapes. J. Stat. Mech. 034003:2024

[2] Pahujani, S. & Krug, J.: Complexity and accessibility of random landscapes. arXiv:2502.05896

BP 21.5 Wed 16:45 HÜL/S386

Adaptive Response of Quantitative Traits to a Moving Fitness Landscape — •Sakshi Pahujani, Yuna Zhang, Markus G. Stetter, and Joachim Krug — University of Cologne, Cologne, Germany

Phenotypic adaptation to long term persistent changes in the environment is typically studied using moving optimum models which consider a fitness landscape traversing the phenotypic space over time. Invoking the strong-selection-weak-mutation regime, we study adaptation as a walk towards the moving fitness optimum described by a continuous-state-discrete-time stochastic process. In this framework, at a critical speed of the optimum, we elucidate a transition, from a regime where the phenotypic gap of the adapting population from the optimum attains a stationary mean value to one where it increases indefinitely. Through a special case of the problem, we provide an alternative description of this transition in terms of a force that drives the adaptive process and a corresponding potential that switches from being confining to non-confining at the critical speed. Further analysis of this case suggests that adaptation is rather successfully carried out, until the population becomes limited by the maximum rate at which it can adapt. Remarkably, despite the simplicity of this special case, its predictions align well with observations from the original, more complex model [1].

[1] Sakshi Pahujani, Yuna Zhang, Markus G. Stetter, Joachim Krug, Adaptive Dynamics of Quantitative Traits in a Steadily Changing Environment, bioRxiv 2025.09.28.679017

BP 21.6 Wed 17:00 HÜL/S386

A simplified Rough Mount Fuji model clarifies how local adaptive walks can reach the highest peaks in rugged fitness landscapes — •Kye E Hunter[1,2] and Nora Martin[1] — [1]CRG (Barcelona Collaboratorium for Modelling and Predictive Biology) — [2]Facultat de Física, Universitat de Barcelona (UB)

Adaptive evolution selects random genotypic mutations according to their fitness. This can be modeled using a fitness landscape, a network of possible genotypes with a fitness value associated to each sequence. In the simplest models of adaptive evolution, populations move through this network in fitness-increasing steps until reaching a genotype whose fitness exceeds that of all its neighbors—a fitness peak. In evolutionary simulations on their empirical folA landscape, Papkou et al. (Science 2023) found that such fitness-increasing walks are likely to reach the globally-highest-ranked peaks among a large number of peaks, despite only being based on local rules. Similar results were found in a mathematical model of fitness landscapes, the Rough Mount Fuji model (Li & Zhang MBE 2025).

We use a simplified Rough Mount Fuji model to find simple analytical explanations for how a landscape can have both a large number of peaks and populations that reach the highest-ranked peaks. Our explanation proceeds by dividing the landscape into different regions, and considering the number of peaks relative to the total number of genotypes in each region. We then identify the degree to which those same arguments apply in the empirical folA landscape.

BP 21.7 Wed 17:15 HÜL/S386

Mean adaptive basin size for fitness peaks in the House of Cards landscape — •Daniel Oros and Joachim Krug — Institute for Biological Physics - University of Cologne

Fitness landscapes have been studied extensively in evolutionary theory. In a simple form, the fitness landscape maps the genotype of an organism to its reproductive success, denoted by fitness. While being a drastic simplification of biology, the concept is useful for understanding how evolution navigates such a landscape. When the time between mutations is much larger than the fixation time, one can think of a genetically homogeneous population moving one mutation at a time. The fitness value increases at each step and the population eventually reaches a fitness peak, a genotype having larger fitness than all its single mutant neighbors. The adaptive basin of a peak is composed of all genotypes which have a monotonically increasing fitness path to it.

Large scale fitness landscape measurements show that the basins of high fitness peaks contain a large fraction of all genotypes, a finding that has been argued to be inconsistent with existing fitness landscape models [1]. In House of Cards (HoC) landscapes fitness values are assigned independently at random, resulting in a maximally rugged landscape. Building on previous work on accessibility percolation [2] we show that typical peak adaptive basins in the HoC landscape contain a positive fraction of all genotypes, and derive an explicit expression for the mean basin size.

[1] Papkou A et al. 2023 *Science* **382** eadh3860

[2] Schmiegelt B and Krug J 2023 *J. Math. Biol.* **86** 46

BP 22: Statistical Physics of Biological Systems II (joint session DY/BP)

Time: Wednesday 15:00–16:30 Location: ZEU/0114

See DY 40 for details of this session.

BP 23: Biopolymers, Biomaterials and Bioinspired Functional Materials I (joint session CPP/BP)

Time: Wednesday 15:00–16:45 Location: ZEU/0255

See CPP 38 for details of this session.

BP 24: Biopolymers, Biomaterials and Bioinspired Functional Materials II (joint session CPP/BP)

Time: Wednesday 17:00–18:45 Location: ZEU/0255

See CPP 41 for details of this session.

BP 25: Members' Assembly

Time: Wednesday 18:30–20:00 Location: BAR/0205

All members of the Biological Physics Division are invited to participate.

BP 26: Biomaterials and Biopolymers (joint session BP/CPP)

Time: Thursday 9:30–12:45 Location: BAR/SCHÖ

BP 26.1 Thu 9:30 BAR/SCHÖ

Characterization and Application of Honey-PVA Electrospun Scaffolds in Tissue Engineering — •Catalina Navarrete-Vera[1], Karen Yáñez[2], Cristian Acevedo[2], and Tomas Corrales[1,2] — [1]Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso, Chile — [2]Centro de Biotecnología Daniel Alkalay Lowitt, Universidad Técnica Federico Santa María, Chile

Tissue engineering seeks to develop functional biomaterials that integrate seamlessly with biological systems. Electrospinning with static collectors enables the production of nanostructured scaffolds suitable for cell regeneration (10.1021/acsomega.3c06436). Incorporating natural components, such as honey, valued for its regenerative, anti-inflammatory, and antimicrobial properties, offers a route to bioactive wound-dressing alternatives (10.1016/j.carbpol.2019.05.004).

In this study, Manuka and Ulmo honeys were each combined with PVA to generate nanofibers and scaffolds via electrospinning. AFM force spectroscopy was used to assess individual fiber mechanics, and SEM and cell-culture assays were employed to evaluate morphology and biocompatibility. Both formulations produced fibers of similar diameter (100-300 nm) and nanomechanical stiffness (~200 MPa), while honey-containing scaffolds improved cell growth over controls. These results indicate that Ulmo honey is a promising alternative to Manuka honey for tissue-engineering applications.

BP 26.2 Thu 9:45 BAR/SCHÖ

Additive Manufacturing in Wound Care Innovation from Sugarcane Bagasse — •Ahmed El-Hussein Elnewishy[1], Muhammad Mounir[1], Mona Tarek[1], and Ita Junkar[2] — [1]Biotechnology Program, Faculty of Science, Galala University — [2]Department of Surface Engineering, Jožef Stephan Institute, Ljubljana, Slovenia

Three-dimensional (3D) printing technology is capable of creating highly complex, customizable objects, offering unique advantages for various biomedical applications through methods such as inkjet-based, extrusion-based, and light-assisted techniques. This study focuses on using direct ink writing for additive manufacturing to print antibacterial wound dressings, addressing a critical gap in the current wound care market. The management of chronic and acute wounds presents significant challenges facing human health and overall wellness. Current wound dressing fails to meet patients needs in terms of high adhesion, poor gas exchange, low moisture retention, and the use of systemic and synthetic antibiotics. Additionally, the presence of unused agricultural waste and weak waste management increase greenhouse gas emissions, thus contributing to global warming. To address these issues, we utilized agricultural waste, specifically sugarcane bagasse, to create biopolymer 3D printing ink for wound dressings. We extracted cellulose from sugarcane bagasse and antibacterial bioactive compounds from plant extracts. The synthesized ink was then printed and post treated to enhance mechanical properties. We evaluated the cytotoxicity, antibacterial activity, and morphological structure of the patches using scanning electron microscopy.

BP 26.3 Thu 10:00 BAR/SCHÖ

FCS-Based RNA Payload Quantification and FLIM Analysis of pH-Dependent Lipid Phase Transitions in Lipid Nanoparticless — •Bernhard Kirchmair[1], Judith Müller[1], Thomas Kellerer[2], Ekaterina Kostyurina[1], and Joachim Rädler[1] — [1]Ludwig-Maximilians-Universität München, Germany — [2]Max Planck-Institut für Biochemie, Martinsried, Germany

Lipid nanoparticles (LNPs) emerged as one of the most promising delivery systems for transfecting mammalian cells with synthetic messenger RNA (mRNA). However, LNPs show a substantial heterogeneity both in shape and cargo and the precise mRNA payload and stoichiometric ratios in multi-component nucleic acid delivery remain poorly quantified. In this project we investigate how mRNA payload depends on LNP size and surface composition using fluorescence correlation spectroscopy (FCS) supported by dynamic light scattering, enabling estimation of particle concentration and RNA copies per LNP. Fluorescence cross-correlation spectroscopy further allows measurement of siRNA/mRNA ratios in mixed cargos. To link payload properties to endosomal escape rates and hence delivery efficiency, we probed pH-dependent lipid phase transitions using fluorescence lifetime imaging (FLIM) and fluorescence anisotropy, capturing changes both in bulk lipid phases and in intact LNPs. These measurements build a framework to monitor structural changes relevant to endosomal escape and can be applied to other LNP formulations and cargo types. Quantitative knowledge about content and ratios will ultimately support the delivery of genetic programs for regulated gene expression.

BP 26.4 Thu 10:15 BAR/SCHÖ

pH-dependent phase transitions in ionizable lipid mesophases — •Ekaterina Kostyurina[1], Susanne Liese[2], Akhil Sudarsan[2], Julian Philipp[1], and Joachim Rädler[1] — [1]Faculty of Physics, Ludwig-Maximilians University, 80539 Munich, Germany — [2]Faculty of Mathematics, Natural Science, and Materials Engineering, Institute of Physics, University of Augsburg, 86159 Augsburg, Germany

Lipid Nanoparticles (LNPs) have proven valuable in modern medicine as a medium for RNA delivery. Nanoparticles containing cationic ionizable lipid (CIL), cholesterol and structural lipids complex with nucleic acids into size-controlled particles that transport nucleic acid molecules across cell membranes via the endocytic uptake pathway. The delivery efficiency of a drug or vaccine is directly related to the efficiency of the endosomal release. Here, we study pH-dependent structural transitions of the CIL core phase which are believed to play an essential role in this process. We use bulk phases of ionizable lipid/cholesterol as a model system of the LNP core which allows us to study the structure of the lipid phases with high precision using X-ray diffraction. We show that the commonly used ionizable lipids overcome the inverted micellar-inverted hexagonal phase transition within the pH range typical for endosomal life cycle, and connect structural properties of the phases with LNP efficacy. Furthermore, we are aiming to understand the thermodynamics of these phase transitions by combining experimental measurements with theoretical modeling. This will help to better understand the structure-activity relation of LNPs and to increase the delivery efficiency in clinically relevant LNP delivery systems.

BP 26.5 Thu 10:30 BAR/SCHÖ

To gel or not to gel? Assembly phase changes of engineered spidroin proteins induced by temperature and time — •Isabell Tunn[1,2,3], Dmitry Tolmachev[2,4], Adam L. Harmat[2,4], Nea B. Möttönen[1,2], Alberto Scacchi[2,4,5], Maria Sammalkorpi[2,4], and Markus B. Linder[1,4] — [1]Department of Bioproducts and Biosystems, Aalto University, Finland — [2]Academy of Finland Center of Excellence in Life-Inspired Hybrid Materials (LIBER), Aalto University, Finland — [3]Fraunhofer Institute for Applied Polymer Research (IAP), Germany — [4]Department of Chemistry and Materials Science, Aalto University, Finland — [5]Department of Mechanical and Materials Engineering, University of Turku, Finland

Bioinspired silk-like proteins offer exciting possibilities for developing the next generation of advanced materials - from medicine to food packaging. Here, we investigate the temperature- and time-dependent assembly behaviour of engineered silk-like proteins into hydrogels conducting experiments and molecular dynamics simulations.* Phase transitions are controlled by entropic changes in flexible glycine-rich regions and hydrophobic interactions of alanine-rich α-helical regions. High-temperature gelation proceeds through interactions between alanine-rich domains, leading to β-sheet formation while time-induced gelation occurs via protein percolation mainly driven by dimerization of terminal domains. These findings provide guidelines for engineering protein-based materials with tailored assembly properties and gel characteristics, advancing the rational design of biomimetic soft materials. *https://doi.org/10.1016/j.ijbiomac.2025.147712

BP 26.6 Thu 10:45 BAR/SCHÖ

Power-Law Analysis of Force Relaxation and Creep Compliance in Nanoindentation of Glassy Gelatin in Humid Air — Paul Zech, Martin Dehnert, Mario Zerson, and •Robert Magerle — Fakultät für Naturwissenschaften, TU Chemnitz

Gelatin-based materials are widely used in food technology, drug delivery systems, and tissue engineering. Water acts as a plasticizer, softening gelatin and reducing its glass transition temperature. Using AFM-based nanoindentation experiments, we examined the mechanical response of a gelatin film to nanoindentations under constant strain (force relaxation) or constant stress (creep compliance) at a wide range of tip approach velocities and relative humidity levels. Scaling analysis using a fractional rheology model reveals that force relaxation and creep compliance exhibit universal power-law behavior. Temporal evolution depends only on the tip indentation time, which defines the externally imposed timescale of the process, and the power-law exponent α, which characterizes the degree of viscoelasticity. At relative humidity > 85%, the α values differ between the force relaxation and creep compliance data. This indicates differences in the underlying molecular processes.

15 min. break

Invited Talk BP 26.7 Thu 11:15 BAR/SCHÖ

Directed evolution of material-producing bacteria — •André Studart — Complex Materials, Department of Materials, ETH Zürich

Engineers often use high temperatures, pressures and polluting chemicals to make synthetic materials. By contrast, biology produces remarkable materials like wood and bone using widely available chemicals in water and at ambient temperature. The ability of organisms to create materials under mild conditions relies on the intricate biological machinery of living cells. Notably, natural selection processes have evolved such machinery for hundreds of millions of years to fulfill the demands of biological environments. Can we harness the machinery and evolutionary processes of biology to create materials more sustainably while still meeting engineering needs ? To explore this question, we utilized a microfluidic platform to evolve material-forming microorganisms towards cell mutants that meet the high productivity needed in industrial processes. Using cellulose-producing bacteria as an example, we show that this directed evolution approach enabled the isolation of a bacterial mutant that produces up to 70% more cellulose than its native counterpart. The overproducing bacterial strain offers an attractive alternative to wood to meet the growing demand for cellulose in the textile, medical and packaging industries. Beyond cellulose, the proposed technology offers a compelling approach to isolate bacteria for the biofabrication of other sustainable materials, such as silk, polyesters and clay-based bricks.

BP 26.8 Thu 11:45 BAR/SCHÖ

Controlling Axonal Outgrowth of Organoids by 3D Nanoprinted Scaffolds — •Tobias Müller[1], Malte Siegmund[1], Emma Wollesen[1], Kim Krieg[2], Ole Pless[2], Jan Hahn[3], Robert Zierold[1], and Robert Blick[1] — [1]Center for Hybrid Nanostructures, University of Hamburg, 22761 Germany — [2]Fraunhofer ITMP, Discovery Research Screening Port, 22525 Germany — [3]Section Facility Mass Spectrometry and Proteomics, University Medical Center Hamburg-Eppendorf, 20246 Germany

Cortical organoids are promising models for neurodegenerative disease research, yet their integration into defined neural networks remains challenging. We use two-photon polymerization (2PP) to fabricate three-dimensional scaffolds that direct axonal outgrowth and support organoid integration into engineered circuits.

Scaling structures from single neurons to millimeter-scale organoids introduces adhesion and imaging challenges. We address this by combining tailored scaffold geometries with a polydimethylsiloxane (PDMS)-based anchoring strategy, critical-point drying and quantitative analysis of electron microscopy images. Walls, stairs and microwires enhance organoid-scaffold interactions, promoting axonal outgrowth along intended paths and reducing extension into non-target regions.

These results demonstrate that 2PP-fabricated microarchitectures can guide axon growth and stabilize organoid-substrate contact, enabling more controlled organoid-based neuronal networks and advancing brain-on-a-chip approaches.

BP 26.9 Thu 12:00 BAR/SCHÖ

Stimulus-induced biomechanical perturbations via smart hydrogel microstructures — •Katja Zieske — Max Planck Institute for the Science of Light, Erlangen, Germany

Cells reside within complex three-dimensional extracellular matrices, where mechanical interactions play essential roles in tissue development, and disease progression. To mimic these interactions, we developed a lab-on-a-chip platform that applies spatially and temporally controlled mechanical perturbations using intelligent hydrogel microstructures.

First, we optimized material composition and photopolymerization parameters and demonstrated reliable, stimulus-dependent expansion and contraction of the hydrogel microstructures within microfluidic chambers. Using these microstructures, we then applied compressive forces to Matrigel and collagen networks. Finally, we applied mechanical perturbations to cellular systems.

By mimicking cellular pushing forces with hydrogel microstructures, this lab-on-a-chip system provides a versatile tool for studying mechanical remodeling of biopolymers and cellular systems.

BP 26.10 Thu 12:15 BAR/SCHÖ

Functionally Connecting High- and Low-Density Neuronal Networks Using 3D-Nanoprinted Structures — •Emma Wollesen, Malte Siegmund, Tobias Müller, Josephine Hoppe, Robert Zierold, and Robert Blick — Center for Hybrid Nanostructures, University of Hamburg, 22761 Hamburg, Germany

Tracing the propagation of interneural communication from high- to low-density networks is essential for exploiting information processing at the single-cell level. Given the multitude of synaptic connections, high-density networks of hiPSC-derived neurons may generate bursts of action potentials, a key communication mode that can be analyzed at the single-cell level in receiving low-density networks. Here, we move toward such a cultivation platform by evaluating 3D nanoprinted (3DN) structures fabricated by two-photon polymerization for their efficiency in facilitating connected high- and low-density networks. We demonstrate the prerequisite formation of hiPSC-derived low-density neuronal networks in tower-shaped 3DN structures. For augmentation with high-density networks, a stomach-shaped structure and connecting elements were fabricated. A minimum structure height of 30 micrometers proved critical for clear network demarcation. For future region-specific chemical stimulation, millimeter-scale structures for media reservoir separation were conceptualized, and fabrication feasibility was confirmed, requiring a 10 micrometer overlap and a suitable shear angle at structure interfaces. These results extend established 3DN platforms for low-density networks and support the integration of neural networks into Brain-on-a-Chip applications.

BP 26.11 Thu 12:30 BAR/SCHÖ

Multiplex sensing of respiratory viruses using surface plasmon resonance spectroscopy — •Ghazaleh Eshaghi[1], David Kaiser[1], Hamid Reza Rasouli[1], Dominik Gary[2], Tobias Fischer[2], Katrin Frankenfeld[2], Abhishek Sharma[3], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena — [2]Forschungszentrum für Medizintechnik und Biotechnologie (fzmb) GmbH, 99947 Bad Langensalza, Germany — [3]BioNavis Ltd., Hermiankatu 6-8H, 33720 Tampere, Finland

We present label-free and real-time biosensing of three major respiratory viruses using the Multi-Parametric Surface Plasmon Resonance (MP-SPR) technique. In this approach, MP-SPR SPR Au sensors are functionalized with ultrathin (~1 nm) azide-terminated carbon nanomembranes (N3-CNMs), enabling covalent attachment of virus-specific antibodies and thereby providing selective immobilization of target antigens on the sensor surface. We demonstrate specific detection of SARS-CoV-2, Influenza A, and Respiratory Syncytial Virus (RSV) antigens with negligible cross-reactivity and high reproducibility in both PBS-P buffer (physiological pH) and clinically relevant nasopharyngeal swab matrices. For SARS-CoV-2, Influenza A, and RSV antigens, we determine dissociation constants (KD) of 7.0 * 0.5 nM, 86 * 4 pM, and 3.0 * 0.2 pM, respectively, with corresponding limits of detection (LOD) of ~65 pM, ~80 pM, and ~2 pM.

BP 27: Cell Mechanics I

Time: Thursday 9:30–12:45 Location: BAR/0205

Invited Talk BP 27.1 Thu 9:30 BAR/0205

Tissue interplay and the coordination of morphogenesis — •Elias Barriga — Physics of Life (PoL), Dresden, Germany

How tissues achieve robust morphogenesis in development and regeneration is the driving question in our research. In my talk I will share our results arising from a combination of mechanical and electrical measurements and perturbations in living tissues; and will discuss how our work support the exciting idea that biophysical properties emerging from tissue interplay coordinate morphogenesis in time and space.

BP 27.2 Thu 10:00 BAR/0205

Mechanical polarity in cell migration — •Steffen Grosser[1], Leone Rossetti[2], Isabela Corina Fortunato[3], Ricard Alert[4,5], and Xavier Trepat[1,5,6,7] — [1]Institute for Bioengineering of Catalonia (IBEC), Barcelona — [2]Faculty of Dentistry, Oral & Craniofacial Sciences, King's College, London — [3]Institut d'Investigació Sanitària Illes Balears (IdISBa), Palma — [4]MPI für Physik komplexer Systeme (MPI-PKS), Dresden — [5]University of Barcelona, Barcelona — [6]ICREA, Barcelona — [7]CIBER-BBN, Barcelona

Cells migrate on substrates in the absence of any net force, which poses a fundamental challenge in cell dynamics. All forces transmitted from the cells to the substrate cancel out. Neither force magnitude nor force dipole are related to neither cell speed nor direction.

We have recently found, however, that a higher moment of the cell traction distribution, the quadrupole, is in fact closely related to cell velocity - to both speed and direction. The quadrupole characterizes the asymmetry of the traction distribution, even when the total net force cancels out. It can be thought of as a mechanical cell polarity readout. Experimentally, the relation between force asymmetry and velocity holds for single cells and for short multicellular trains, and even for cells moving along gradients of adhesion.

To interpret this traction asymmetry, we propose to decompose the force into an active, unbalanced part that drives cell motion, and a frictional component. This leads to a novel, actual force-velocity relation for cell dynamics.

BP 27.3 Thu 10:15 BAR/0205

Mechanics of "apical bulkheads" in the bile canaliculi of the liver — •Matthew J. Bovyn[1,2,3], Maarten P. Bebelman[2], Yannis Kalaidzidis[2], Marino Zerial[2,4], and Pierre A. Haas[1,2,3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden — [3]Center for Systems Biology Dresden — [4]Human Technopole, Milan

In the liver, bile is transported through the network of bile canaliculi. They are bicellular tubes ("lumina"), in which the apical cortices of apposed cells bear bile pressure. When bile canaliculi must hold high pressures, either in development or disease, they generate folds protruding into the tubes, termed "apical bulkheads". These structures are under tension and contribute significantly to the ability of the bile canaliculus as a whole to bear pressure [1]. Here, we use lightsheet microscopy to discover that bulkheads are also dynamic, forming and retracting on a timescale of 20 min. We investigate the mechanical origins of this process by constructing a mechanical model balancing pressure and anisotropic surface tensions and spontaneous curvature of the apical cortices. We discuss the cell biological origins of these mechanical ingredients, the experimental evidence for them, and their role in bulkhead formation.

[1] Bebelman, M. P., Bovyn, M. J., *et al.* Hepatocyte apical bulkheads provide a mechanical means to oppose bile pressure. J. Cell Biol. **222**, e202208002 (2023).

BP 27.4 Thu 10:30 BAR/0205

Blebbing under confinement functions as a pressure-relief mechanism following cortical contraction — •Fatemeh Abbasi[1,2], Timo Betz[2], and Eva Kiermaier[1,3,4] — [1]Life and Medical Sciences (LIMES) Institute, Immune and Tumor Biology, University of Bonn, Bonn, Germany. — [2]Third Institute of Physics-Biophysics, Georg August University Göttingen, Göttingen, Germany. — [3]Department of Medicine, Friedrich-Alexander University Erlangen-Nürnberg (FAU), Erlangen, Germany. — [4]Deutsches Zentrum Immuntherapie (DZI), Universitätsklinikum Erlangen, Erlangen, Germany.

Cells migrating through tissues experience mechanical confinement that reshapes their morphology and internal stress. Using Confinement Force Microscopy (CFM), we dynamically controlled vertical confinement during live imaging and quantified 3D stress responses. A single confinement step triggered a biphasic response: an immediate passive stress spike from nuclear compression followed by a slower, actomyosin-driven buildup linked to bleb formation. Both blebbistatin and Y-27632 reduced traction stresses; notably, Y-27632 fully blocked blebbing, while blebbistatin allowed it only under strong compression, indicating partial decoupling between contractility and morphology. Blebbistatin also lowered cellular stiffness and viscosity, promoting rapid stress relaxation. These results suggest that blebbing functions as a pressure-relief mechanism allowing cells to maintain mechanical balance under confinement.

BP 27.5 Thu 10:45 BAR/0205

Moving without motors: Amoeboid cell migration and shape dynamics driven by actin polymerization — •Winfried Schmidt, Alexander Farutin, and Chaouqi Misbah — Univ. Grenoble Alpes, CNRS, LIPhy, F-38000 Grenoble, France

Mammalian cell migration is essential for many physiological and pathological processes, such as embryonic development, wound healing, and cancer metastasis. Cells have developed the amoeboid migration mode, which is characterized by large, dynamic shape deformations. This strategy allows cells to move rapidly and in the absence of strong adhesion across a variety of different environments, including two-dimensional confinement, three-dimensional matrix, and bulk fluids. Molecular motors, such as myosin, are traditionally considered essential for cell polarization or motility. Here, a model of an amoeboid cell is analyzed both analytically and numerically. It is shown that actin polymerization alone is sufficient to trigger both cell polarity and motility, in line with recent experiments on T-lymphocytes showing that inhibition of molecular motors does not significantly affect motility. Depending on parameter values, the cells exhibit straight, circular, or even chaotic trajectories. A similar variety of motion is observed in experiments across multiple motile cells. These findings open up a new perspective on amoeboid motility, providing a scenario for the onset of polarity, migration, and dynamical cell shape changes without contractile activity.

15 min. break

BP 27.6 Thu 11:15 BAR/0205

Living Cells Respond to the Surface Tension of Soft Solids — •Johannes Rheinlaender, Leah Gumbsch, Hendrik von Eysmondt, and Tilman E. Schäffer — Institute of Applied Physics, University Tübingen, Germany

It is widely known that living cells respond to the stiffness of their environment in terms of spreading area as well as other properties such as the cytoskeletal structure, migration, or gene expression. These effects are usually investigated by seeding cells on elastic substrates with varying bulk stiffness, either hydrogels or soft elastomers. However, cellular behavior differs on hydrogels and elastomers, which has been attributed to various material properties like surface roughness or porosity. Using scanning ion conductance microscopy (SICM), we show that elastomers routinely used in mechanobiology studies exhibit a significant surface tension on the order of several tens of mN/m, independent of their bulk stiffness. We thereby demonstrate that living cells mostly respond to the surface tension rather than the bulk stiffness of the substrate on soft elastomers with Young's moduli below approximately 10 kPa and introduce possible solutions to address this problem. To conclude, the influence of surface tension is an important yet underestimated aspect in cellular mechanobiology.

BP 27.7 Thu 11:30 BAR/0205

Complex Rheology in Single Cells: Compression Stiffening but Shear Softening — •James P. Conboy[1], Luis Alonso[2], Haiqian Yang[2], Nicole van Vliet[1], Pouyan E. Boukany[1], Fred C. MacKintosh[3], and Gijsje H. Koenderink[1] — [1]TU Delft, NL — [2]MIT, USA — [3]Rice University, USA

In multicellular organisms, cells are constantly subjected to physical forces. Cells in the heart, lungs and skin experience primarily compression and stretching, whereas shear forces are dominant in the brain and in blood vessels. The mechanical resilience to compression and shear forces is essential for preventing cell damage or even rupture. Our aim is to understand the response of cells to external mechanical cues. For this purpose, we have developed a novel single cell rheology setup that allows us for the first time to make direct comparisons between a living mammalian cell's response to compression and shear strain. In this work, we have identified the relative contribution of actin and vimentin intermediate filaments in uniaxial compression experiments on single fibroblasts. Our findings reveal that individual fibroblasts undergo stiffening under physiologically relevant compressive strains, but the removal of vimentin reduces this stiffening effect. Furthermore, we present, to our knowledge, the pioneering example of single-cell shear rheology experiments, where we discovered that cells soften when sheared, in stark contrast to their stiffening behaviour under compression. Finally, we propose a minimal model to elucidate these phenomena and compare our results to semiflexible polymer models used to explain the mechanics of reconstituted cytoskeletal systems.

BP 27.8 Thu 11:45 BAR/0205

Intracellular ROS generation under ultra-high dose rate electron irradiation at FLASHlab@PITZ — •Y. Komar[1,2,3], E. Fujan[2], C Richard[1], X. Li[1], N. Aftab[1], A. Aksoy[1], Z. Amirkhanyan[1], A. Chiravuri[1,2], J. Good[1], M. Gross[1], F. Hausmann[3], S. Khammee[1], M. Krasilnikov[1], B. Li[1], Z. Lotfi[1], G. Montoya-Soto[1], F. Müller[1], A. Oppelt[1], F. Riemer[1], K. Suzart[1], E. Tarakci[1,2,3], I. Tinhofer[3], D. Villani[1], S. Worm[1], D. Xu[1], S. Zeeshan[1], M. Frohme[2], F. Stephan[1], S. Aminzadeh[1,2], and A. Grebinyk[1,2] — [1]Deutsches Elektronen-Synchrotron, Zeuthen, Germany — [2]Technical University of Applied Sciences Wildau, Wildau, Germany — [3]Charité University Medicine Berlin, Corporate Member of Freie Universität Berlin and Humboldt-Universität zu Berlin, Berlin, Germany

The new FLASHlab@PITZ beamline commissioning started in August 2025 for radiobiological studies at the Photo-Injector Test Facility at DESY in Zeuthen (PITZ). It enables irradiation with dose rates ranging from conventional (CDR, 0.05Gy/s) up to ultra-high (UHDR, 10^14Gy/s). The in vitro effects of UHDR versus CDR irradiation were examined using human lung cancer A549 and healthy HEL299 cells exposed to CDR (0.05Gy/s) and UHDR (7.8*10^5Gy/s). Reactive oxygen species production assessment showed 84% decrease in HEL299 cells and no difference in A549 at ~7.5Gy under UHDR compared with CDR. That indicates UHDR irradiation having a milder impact on healthy than on cancer cells, highlighting the potential of FLASHlab@PITZ for future in vivo studies.

BP 27.9 Thu 12:00 BAR/0205

Probing the influence of mechano-chemical cues on the size of nuclei — •Pooja Yadav, Florian Rehfeldt, and Matthias Weiss — University of Bayreuth, Experimental Physics I,95447,Bayreuth

The size of nuclei in eukaryotes is frequently observed to scale with the size of the cell that harbours them. Yet, our understanding of how cells can measure and regulate nuclear size is still fragmentary. A recently developed model suggests nuclear size to be determined by a dynamically maintained but limited amount of membrane material that needs to be distributed between organelles and the plasma membrane. Given that membrane homeostasis and cell morphology can be altered biochemically and mechanically, we have used drug treatments and polyacrylamide (PA) hydrogels of varying stiffness as a substrate for cells. As a result, we have found that softening the substrate alters the shape and size of cells and nuclei, but maintains the ratio of their projected areas. Similarly, affecting the actomyosin cortex had little effect on this ratio. However, when enforcing changes in membrane homeostasis by pharmaceuticals, the ratio of cellular and nuclear cross-sectional areas was markedly altered. Altogether, our data suggest that dynamically maintaining and limiting membrane material is a core mechanism of how cells determine the size of their nuclei.

BP 27.10 Thu 12:15 BAR/0205

Nuclear downsizing: Dynamic volume and cell-cycle control in emerging tumour spheroids — •Vaibhav Mahajan[1], Keshav Gajendra Babu[1], Markus Mukenhirn[1], Antje Garside[1], Timon Beck[1,2], Byung Ho Lee[3], Kyoohyun Kim[2], Carsten Werner[4], Alf Honigmann[1], Sebastian Aland[5], Raimund Schlüssler[1], and Anna Taubenberger[1,4] — [1]Dresden University of Technology, Dresden, Germany — [2]Max Planck Institute for the Science of Light, Erlangen — [3]MPI-CBG, Dresden — [4]Leibniz Institute of Polymer Research Dresden — [5]Hochschule für Technik und Wirtschaft Dresden

Tumour development involves biophysical changes across scales, yet how cancer cells regulate properties such as volume and mechanics within dense multicellular environments remains unclear. Using tuneable biohybrid hydrogels, we quantified cell and nuclear volumes as single cancer cells formed multicellular tumour spheroids. We found that transition to multicellularity led to strong reductions in cellular and nuclear volumes, delayed cell-cycle progression, and altered mechanics, with these changes tightly coupled. Nuclear volume dropped by up to 60%, not primarily due to confinement but due to cell-cycle adaptations, namely accumulation of smaller-sized G1 cells-an effect reversed by CDK1 inhibition. Additional nuclear volume decreases within clusters were associated with increased mass density and cell stiffness, both reversible upon cell release. Conversely, cells invading out of spheroids increased nuclear volumes and softened. These findings reveal how cancer cells dynamically adjust volume, cell-cycle state, and mechanics in the multicellular context.

BP 27.11 Thu 12:30 BAR/0205

A protein-DNA surface hydrogel mechanically reinforces the cell nucleus — •Yahor Savich[1,2,3], Ramesh Adakkattil[1], Pranay Mandal[1,2,3], Valentin Ruffine[4], Mareike Jordan[1], Henrik Dahl Pinholt[5], Elisabeth Fischer Friedrich[4], Frank Jülicher[2,3,4], Stephan Grill[1,3,4], and Alexander von Appen[1,4] — [1]MPI-CBG, Dresden — [2]MPI-PKS, Dresden — [3]Center for Systems Biology Dresden — [4]TUD, Dresden — [5]MIT, Cambridge

Cells safeguard their genome while nuclei are deformed. The nuclear envelope is known to protect DNA from such mechanical stress, but how forces are buffered across the scales from individual DNA strands to the nucleus remains unknown. We show that the nuclear envelope protein LEM2 and the DNA-binding protein BAF, together with DNA, form an unconventional stiffening system. When DNA is held at a given force in optical tweezers, the addition of these proteins causes a force increase proportional to the initial force. This behaviour can be captured by an effective spring model that emerges from multivalent protein-protein and protein-DNA interactions. At the nuclear surface, the same components form an elastic surface hydrogel in which the multivalent interactions contract the surface hydrogel relative to its relaxed state, introducing a pre-stress. Using parameters obtained at the molecular scale, a continuum model of this surface hydrogel yields free-energy-minimizing nuclear shapes and an area stiffness that are in agreement with measurements in control and LEM2 knockdown cells. These results identify a load-bearing, mesoscale protein-DNA surface hydrogel that mechanically reinforces the nucleus.

BP 28: Active Matter V (joint session DY/BP)

Time: Thursday 9:30–12:45 Location: ZEU/0160

See DY 49 for details of this session.

BP 29: Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates I (joint session CPP/BP)

Biomolecular condensates play a central role in many cellular processes and provide a fascinating example of self-organized, highly dynamic systems. Physical methods, particularly from statistical physics and soft matter, have emerged as valuable tools for understanding and predicting their fundamental properties. Conversely, the complexity and diversity of biological systems open new perspectives and challenges for physical modeling. This focus session will highlight current research at the interface of physics and biology, with an emphasis on theoretical modeling and simulation of the physics of biomolecular condensates.

Organized by Arash Nikoubashman, Tyler Harmon and Lukas Stelzl.

Time: Thursday 9:30–11:15 Location: ZEU/0260

Topical Talk BP 29.1 Thu 9:30 ZEU/0260

Wetting transitions in biomolecular coacervates — •Susanne Liese[1], Tiemei Lu[2], Evan Spruijt[3], and Christoph Weber[1] — [1]University of Augsburg — [2]University of Oxford — [3]Radboud University

Biomolecular coacervates are liquid-like droplets that can interact with membranes and self-organize into complex structures. Understanding the principles governing their shapes and higher-order assemblies is crucial for controlling compartmentalization in biological and synthetic systems.

We present a theoretical framework describing the shape and organization of biomolecular coacervates interacting with membranes and each other. Large coacervate droplets adopt morphologies determined by the balance of surface tensions, from partial adhesion to full engulfment. Scaled membrane tension and droplet-membrane interactions predict transitions between spherical, lens-shaped, partially wrapped, and endocytosed droplets, with composition-dependent contact angles linking molecular properties to macroscopic shapes.

For multiphase coacervates, we model the impact of interfacial species on droplet organization. Enrichment of an interfacial component at phase boundaries drives partial wetting between droplets, promoting the formation of dimers and extended chains. Numerical simulations show that surface tension minimizes the contact area, straightening droplet arrangements and generating polymer-like behavior with bending stiffness and segment-length constraints.

BP 29.2 Thu 10:00 ZEU/0260

Elastic regulation of biomolecular condensates — •Oliver Paulin and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany

In recent years, biomolecular condensates have emerged as a vital component of sub-cellular organisation. Here, we discuss the role that elastic interactions can play in regulating condensate size, count, and mechanical properties. First, we focus on the impact of 'external' elasticity that arises from a confining mesh such as the cytoskeleton. We find that the additional energetic cost of network deformations induced by condensate growth limits condensate size, and can even suppress condensate formation entirely. Additionally, when condensate size is comparable to characteristic heterogeneities of the network, non-local interactions may arrest thermodynamic coarsening and drive the formation of stable patterned states with an energetically selected length scale. Second, we study how 'internal' elasticity, resulting from the intrinsic viscoelasticity of condensate material, can inhibit condensate growth, but also impart condensates with mechanical strength. For the case in which condensate growth is driven by active incorporation of new material, we demonstrate how a delicate balance of material properties provides condensates with solid-like mechanical strength, without compromising their liquid-like ability to form and grow rapidly. For both examples, we construct dynamic continuum models that couple phase separation with elastic deformation, analysing the key parameters that control condensate form, and identifying how cells can use elasticity to fine-tune condensate behaviour to fulfil a specific function.

BP 29.3 Thu 10:15 ZEU/0260

Phase Separation of a Nucleator in a Self Straining Active Filament Network — •Jakob Schindelwig[1], Quentin Bodini-Lefranc[1,2], and Sebastian Fürthauer[1] — [1]Institute of Applied Physics, TU Wien, Lehargasse 6, 1060 Vienna, Austria — [2]Ecole polytechnique, Institut Polytechnique de Paris, Route de Saclay, 91120 Palaiseau, France

Many membraneless compartments of cells, such as stress-granules, form via liquid-liquid phase separation. In cells many compartments of the same type and similar sizes can coexist. Since this is inconsistent with equilibrium phase separation physics, we ask if active mechanics could explain this observation. We develop a model coupling dynamics of the droplet material to an active self-straining filament network. This model shows (i) arrested coarsening , (ii) oscillations, (iii) scale selection. We establish that our model is physiologically plausible by comparing to recent work on a phase separating nucleator of actin.

BP 29.4 Thu 10:30 ZEU/0260

Active Transport as a Mechanism of Microphase Selection in Biomolecular Condensates — •Le Qiao, Peter Gispert, and Friederike Schmid — Institut für Physik, Johannes Gutenberg-Universität Mainz, D55099 Mainz, Germany

Cells control the size and organization of biomolecular condensates formed by liquid-liquid phase separation (LLPS), yet the underlying physical principles remain incompletely understood. We propose a transport-driven mechanism in which undirected motor-mediated motion along cytoskeletal filaments redistributes phase-separating components, generating an effective non-equilibrium long-range repulsion that arrests coarsening. This is explored using a minimal reaction-diffusion-transport model that captures the interplay between binding-release kinetics, diffusion, and active transport. A linear stability analysis and three-dimensional simulations reveal a transition from macroscopic to microphase separation at remarkably low binding/release fractions, corresponding to minute fractions of motor-bound proteins. Tuning motor binding rates b or transport velocities enables sublinear control of condensate dimensions ($L \sim b^{1/4}$) from nanometers to micrometers. This mechanism provides a simple physical route for spatially programmable condensate organization in living cells and active materials.

BP 29.5 Thu 10:45 ZEU/0260

Positive feedback in chemically active droplets — •Xi Chen[1], Jens-Uwe Sommer[1,2], and Tyler Harmon[1] — [1]Leibniz Institute of Polymer Research, Dresden, Germany — [2]Dresden University of Technology

Biomolecular condensates are dynamic compartments that can be maintained far from equilibrium by active chemical reactions. Active condensates can be driven by phase-dependent reaction fluxes, for example via localized enzymatic activity, and thereby exhibit emergent behaviors that cannot be realized in equilibrium condensates. We analyzed condensates with positive feedback between phase separation and reactions: droplets enhance reactions, and the resulting products stabilize the droplets. We show that this feedback produces pronounced hysteresis, making droplets resilient to cellular fluctuations. We show the hysteresis persists across a broad range of reaction schemes and parameter choices, indicating that it is a robust feature of droplets with positive feedback. Condensates that form to satisfy transient cellular needs may benefit from such hysteresis, because it ensures that they persist long enough to carry out their functions despite fluctuating conditions.

BP 29.6 Thu 11:00 ZEU/0260

Chemically driven simulations of enzymatic phosphorylation in protein condensates — •Emanuele Zippo[1], Dorothee Dormann[1,2], Thomas Speck[3], and Lukas Stelzl[1,2] — [1]Johannes Gutenberg University Mainz, Mainz, Germany — [2]Institute of Molecular Biology (IMB), Mainz, Germany — [3]University of Stuttgart, Stuttgart, Germany

The condensation and aggregation of intrinsically disordered proteins (IDPs) in cells are governed by enzyme-driven, non-equilibrium processes. Kinases such as Casein kinase 1 delta (CK1d) phosphorylate proteins using ATP as chemical fuel, tuning intermolecular interactions and modulating condensate assembly. The neurodegeneration-linked protein TDP-43 undergoes CK1d-mediated hyperphosphorylation, proposed as a cytoprotective mechanism through condensate dissolution, yet the mechanisms underlying kinase-condensate interactions remain unclear. Using coarse-grained molecular dynamics simulations, we investigate how CK1d phosphorylates TDP-43 and how this reaction drives the structural reorganization and dissolution of its condensates. To ensure thermodynamic consistency in such fuel-driven simulations, we employ an automatic, generally applicable Markov state modeling framework. Post-translational modifications (PTMs), such as phosphorylation, can actively regulate condensate stability and suppress Ostwald ripening, offering a mechanism to control mesoscale structure in soft materials. Understanding such reaction-structure coupling in non-equilibrium environments is key to explaining cellular self-organization and designing biomimetic systems.

BP 30: Focus Session: Controlling Microparticles and Biological Cells by Ultrasound (joint session BP/CPP/DY)

Recently ultrasound has emerged as a very promising physical modality to control the behavior of microparticles and even of biological cells, which can be moved and stimulated by sound waves. For biological cells, one can further control the effect of sound through gene expression (sonogenetics), similar to the control by light (optogenetics). However, because the wavelength of sound is much larger than the one of light, one of the challenges is to localize the effect of sound waves, e.g. by using gas bubbles. Here, we bring together experimental and theoretical researchers who currently explore the potential of ultrasound to control active and passive microsystems and to develop new applications ranging from biomedicine to soft robotics.

Organized by Peer Fischer and Ulrich S. Schwarz (Heidelberg)

Time: Thursday 10:15–12:45 Location: BAR/0106

Invited Talk BP 30.1 Thu 10:15 BAR/0106

Mechanogenetics for Cell ImmunoTherapy — •Yingxiao Wang — 1002 childs way, Los Angeles, CA 90089

Cell-based cancer immunotherapy is a promising therapeutic intervention for cancer treatment. However, non-specific toxicity against healthy tissues (e.g. off-tumor toxicity) is a major hurdle for solid tumor treatment. We have developed controllable on-switch gene cassettes in which a specific antigen production on the target cancer cell can be remotely and mechanically induced by an external focused ultrasound (FUS). FUS was applied to stimulate the production of the synthetic and clinically validated antigen on tumor cell surface orthogonal to the endogenous proteins. SynNotch was further engineered into primary human T cells (SynNotch-CAR T) to recognize the synthetic antigen expressed on the ultrasound-induced tumor cells and activate the production of CAR, which can lead to the recognition of a native tumor specific antigen (TSA) universally expressed on the whole population of tumor cells for immunotherapy. We applied this system to treat prostate cancer cells whose locally metastasized tumors are confined in space but intermingled with vessels and nerves. Our results showed that FUS can mechanically induce the synthetic antigen production in prostate cancer cells, which results in the engagement and activation of SynNotch CAR T cells for the tumor eradication. This local activation of engineered tumor cells by FUS should allow a high precision and safety in eradicating tumors. Hence, this approach for immunotherapy should open new opportunities to integrate engineering mechanics with genetic medicine for successful translation.

BP 30.2 Thu 10:45 BAR/0106

Shaping sound to tickle cells — •Dimitris Missirlis[1,2], Athanasios Athanassiadis[1,2], Rom Lerner[1,2], and Peer Fischer[1,2] — [1]Institute for Molecular Systems Engineering and Advanced Materials, Im Neuenheimer Feld 225, 69120 Heidelberg, Germany — [2]Max Planck Institute for Medical Research, Jahnstr. 29, 69120, Heidelberg, Germany

The ability to shape ultrasonic waves precisely is finding growing relevance in biomedical applications, where ultrasound is increasingly used to noninvasively stimulate biological tissues for therapeutic purposes. However, it remains an unsolved question how high-frequency ultrasound can interact with cells to excite biological responses. Our recent work on shaping and controlling ultrasound waves has provided us with a new tool to address the fundamental question how ultrasound interacts with and influences cells. To this end we have developed adaptable setups where we can control relevant ultrasound parameters in vitro as well as in vivo. By systematically examining the critical parameters, we discuss the role of different ultrasonic effects, including thermal effects, radiation forces, and sound-induced shear flows. Further, we discuss both physical and sonogenetic methods that can be used to enhance the coupling of ultrasound to cells.

BP 30.3 Thu 11:00 BAR/0106

A Theoretical Model for Ultrasound-Induced Intracellular Streaming — •Niels Gieseler[1,2,3], Falko Ziebert[1,2], and Ulrich S. Schwarz[1,2] — [1]Institute for Theoretical Physics, Heidelberg University, Philosophenweg 19, Heidelberg 69120 Germany — [2]BioQuant, Heidelberg University, im Neuenheimer Feld 267, Heidelberg 69120 Germany — [3]Max Planck Institute for Medical Research, Jahnstrasse 29, Heidelberg 69120, Germany

Ultrasound is not only the basis of an essential imaging method for biomedicine, recently it has also become a promising avenue to control biological systems, for

example, in sonogenetics or ultrasound neuromodulation. However, the underlying physical effects are not well understood, and a complete theoretical description is missing. In fact, many different physical effects compete, including radiation forces, streaming, cavitation, and local heating. Here, we focus on intracellular streaming, which might induce organelle movement or alter gene expression, as the steady second-order rotational flow generated by an acoustic source. As a model for the viscoelastic nature of cells and their surroundings, we use Oldroyd-B fluids. Building on existing work, we calculate the streaming flows inside and outside of a sphere sonicated with a plane wave. The streaming is treated as a second-order perturbation expansion of the Navier-Stokes equations, which is solved separately for both media and combined using suitable boundary conditions. Our work shows under which conditions intracellular streaming can be induced in biological cells.

15 min. break

Invited Talk BP 30.4 Thu 11:30 BAR/0106

Recent theoretical progress on sound-propelled microsystems — •Raphael Wittkowski — Department of Physics, RWTH Aachen University, 52074 Aachen, Germany — DWI – Leibniz Institute for Interactive Materials, 52074 Aachen, Germany

The research area of sound-propelled microsystems is growing fast and has a great potential for various future applications in engineering, medicine, and other fields. The progress in this area is accelerated by theoretical methods, as analytical modeling and computer simulations can provide new insights that cannot be obtained by experiments.

In this talk, I will address the theoretical investigation of sound-propelled microsystems and present examples from the recent research progress in this area. The talk will cover different types of sound-propelled microsystems including microrobots, micromachines, artificial muscles, and soft robots.

Funded by the Deutsche Forschungsgemeinschaft (DFG) – 535275785.

BP 30.5 Thu 12:00 BAR/0106

Rarefaction wave amplification from non-resonant deforming bubbles — Yuzhe Fan, Saber Izak Ghasemian, and •Claus-Dieter Ohl — Otto-von-Guericke University, Magdeburg, Germany

Gas bubbles in liquids or soft matter exposed to acoustic waves behave as oscillators, with maximum response at their resonance frequency. When driven below resonance at sufficient pressure amplitudes, bubbles can collapse with strong energy focusing and even emit light; when driven near resonance, surface instabilities and fast jet flow develop during oscillation. Like other oscillators, bubbles cease to respond when driven far above resonance. Although their oscillations are minimal, bubbles in this regime act as pressure-release interfaces, can reflect high peak pressure shock into rarefaction wave, and may therefore seed cavitation when interacting with high-power therapeutic ultrasound. Yet, here we show that even diagnostic ultrasound with peak positive pressures as low as ~10 MPa can nucleate cavitation in microseconds. This is caused through the non-resonant deformation of the bubble into a concave shape that refocuses scattered waves, amplifying the tension leading to microcavitation. Our findings reveal that cavitation can be triggered by high-frequency positive pressure over a much wider amplitude range than previously recognized, offering a new perspective for current safety guidelines for ultrasound bioeffects and applications in medical ultrasound.

BP 30.6 Thu 12:15 BAR/0106

Optimizing acoustically propelled microrobots using genetic algorithms — •Lennart Gevers[1,2,3] and Raphael Wittkowski[1,2,3] — [1]Department of Physics, RWTH Aachen University, Aachen, Germany — [2]DWI – Leibniz Institute for Interactive Materials, Aachen, Germany — [3]Institute of Theoretical Physics, Center for Soft Nanoscience, University of Münster, Münster, Germany

The promising potential applications of acoustically propelled microparticles demand methods to create particle designs that allow for targeted autonomous motion. Current methods remain largely based on experiments due to the intricate nature of the underlying dynamics. Large-scale computational studies, specifically when combined with optimization algorithms, are impeded by the cost of traditional acoustofluidic simulations.

In this talk, we present the implementation of an analytical framework describing non-Brownian motion of colloidal molecules driven by acoustic streaming. The analytical framework is combined with vectorized, GPU-accelerated, and distributed computation. This enables fast, large-scale simulations, where 10^5 trajectories over 10 s real time can be simulated on a normal personal computer within one minute. Coupling this approach with genetic algorithms reveals particle geometries, control parameters, and underlying principles for acoustically propelled particles that exhibit controllable and stable behavior over long times.

Funded by the Deutsche Forschungsgemeinschaft (DFG) – 535275785.

BP 30.7 Thu 12:30 BAR/0106

Equations of motion for arbitrarily shaped acoustically propelled rigid microparticles — •Justus Schnermann[1,2,3] and Raphael Wittkowski[1,2,3] — [1]Department of Physics, RWTH Aachen University, Aachen, Germany — [2]DWI – Leibniz Institute for Interactive Materials, Aachen, Germany — [3]Institute of Theoretical Physics, Center for Soft Nanoscience, University of Münster, Münster, Germany

Much experimental research concerns the acoustic propulsion of microparticles, but theoretically, only axisymmetric particles with a stable orientation have been studied thus far. In this talk, we present an analytical derivation of the ordinary differential equation of motion for an arbitrarily shaped acoustically propelled rigid microparticle. This equation governs the time evolution of the orientation and position of the particle. Its parameters depend only on the particle's leading-order oscillation velocity field. Based on this equation, we classify qualitatively the possible long-term trajectories of arbitrary particles in unidirectional ultrasound.

Funded by the Deutsche Forschungsgemeinschaft (DFG) – 535275785.

BP 31: Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates II (joint session CPP/BP)

Time: Thursday 11:30–12:45 Location: ZEU/0260

BP 31.1 Thu 11:30 ZEU/0260

Exponential Size Control in Biomolecular Condensates via Universal Scaling of Power-Law Distributions — •Yifan Huang[1], Chuan Tang[1], Haoyu Song[2], Bing Miao[3], and Qiyun Tang[1,4] — [1]Key Laboratory of Quantum Materials and Devices of Ministry of Education, School of Physics, Southeast University, Nanjng 211189, China — [2]School of Physics, Zhejiang University, Hangzhou 310058, China — [3]Center of Materials Science and Optoelectronics Engineering, College of Materials Science and Opto-Electronic Technology, University of Chinese Academy of Sciences, Beijing 100049, China — [4]Jiangsu Physical Science Research Center, Nanjing 210093, China

Power-law distributions are ubiquitous phenomena in diverse systems, whereas concomitant scale invariance hinders the exploration of precise size control for biocondensates in recent experiments. Using massive computer simulations and the kinetic theory of coalescence, we demonstrate that the cutoff volume can collapse all power-law distributions of biocondensates in different parameters onto one master curve. Remarkably, the cutoff size can increase exponentially by increasing monomer concentrations $R \sim e^{\phi}$, of which nanometer condensates in simulations can be extrapolated to micrometer droplets in experiments. The findings provide a new mechanism to rapidly tailor the biocondensates to appropriate sizes through power-law distributions, which can stimulate explorations in biological and other nonequilibrium systems

BP 31.2 Thu 11:45 ZEU/0260

Droplet-assisted folding of long regulatory RNAs — Simon Doll[1], Lukas Pekarek[1], Fathima Ferosh[1], Jovana Vasiljević[1], Marcus Jahnel[1], and •Tyler Harmon[2] — [1]BIOTEC, Dresden, Germany — [2]IPF, Dresden Germany

Long regulatory RNA regions orchestrate complex cellular processes, including gene expression and epigenetic modifications. How these RNAs dynamically fold and refold in response to cellular signals remains poorly understood. Given that RNAs interact with ubiquitous RNA-binding proteins (RBPs) prone to form biomolecular condensates, we explore how protein droplets interacting along an RNA impact its folding process. Attached droplets prevent premature folding by competing with RNA:RNA interactions. When droplets dissolve due to cellular signals, capillary effects cause the RNA to collapse while refolding. We test this process of condensate-guided RNA folding by adapting established RNA secondary structure predictors to mimic various folding pathways and supplement this with coarse-grained simulations. We find that interactions with transient droplets robustly leads to the formation of long-range RNA contacts, which are otherwise hard to achieve. Our results compare favorably with available experimental data. We propose that this strategy, which we call droplet-assisted RNA folding, represents a previously unexplored mechanism for shaping RNA structures. Given the widespread propensity of RBPs to form condensates, this process could play a fundamental role in the structural organization, conditional reshaping, and functional regulation of long regulatory RNAs.

BP 31.3 Thu 12:00 ZEU/0260

Simulation Insights into the Assembly of Polyplexes for RNA Delivery — •Jonas Hans Lehnen[1], Jorge Moreno Herrero[3], Heinrich Haas[3], Friederike Schmid[1], and Giovanni Settanni[1,2] — [1]Department of Physics, Johannes-Gutenberg University Mainz — [2]Faculty of Physics and Astronomy, Ruhr University Bochum — [3]BioNTech SE, Mainz

RNA-based pharmaceuticals proved successful with the COVID-19 vaccines and are now undergoing clinical trials for a broad range of therapeutic indications. Lipid-based nanoparticles (LNPs) have been used so far as delivery systems, although alternatives are still needed to meet efficacy and safety requirements across a broader range of applications. Polyplexes, formed by the self-assembly of cationic polymers with the anionic nucleic acids, constitute a valuable substitute, especially if precise control of the number and shape of the encapsulated RNA chains is possible. Here[1], we use molecular dynamics simulations of a coarse-grained polyplex model to show that the most important factors controlling it are the charge ratio between polyelectrolytes and RNA and their concentration during assembly. Close to the isoelectric point, the polyplexes are large, whereas in large excess of cationic polymer, their size decreases, allowing one RNA copy per nanoparticle. Our results are consistent with recent experimental work on polyethylenimine polyplexes.

[1] Simulation Insights into the Assembly of Polyplexes for RNA Delivery, Lehnen et al., Biomacromolecules (2025), DOI: 10.1021/acs.biomac.5c01219

BP 31.4 Thu 12:15 ZEU/0260

Polymer-assisted condensation as key to chromatin localization — •Arghya Majee[1] and Jens-Uwe Sommer[1,2,3] — [1]Leibniz Institute of Polymer Research Dresden, Germany — [2]Institute for Theoretical Physics, TU Dresden, Germany — [3]Cluster of Excellence Physics of Life, TU Dresden, Germany

We put forward a novel mechanism [1] to account for the experimentally observed [2] positional shifts of chromosomes within the cell nucleus, which appear to be driven by compositional alterations in the nuclear lamina. By considering chromatin as a biomolecular condensate we demonstrate that the adsorption of the chromatin-binding proteins at the lamina leads to a wetting of the condensate while spreading of the chromatin on the lamina is avoided. This leads to the non-monotonous density profile of the polymer with respect to the surface which can be explained by the competition between the tendency of the protein component to wet the surface and the conformational restrictions of the polymer near the impenetrable surface. A change in the composition of the the lamina can lead to repositioning of chromatin towards the center of the nucleus. Our theory not only offers an explanation for specific chromatin conformation experiments, but also contributes to the broader understanding of wetting onto responsive surfaces in multi-component systems.

[1] A. Majee and J.-U. Sommer, bioRxiv 2025.06.11.658974 (submitted).
[2] Amiad-Pavlov *et al.*, Sci. Adv. **7**, eabf6251 (2021).

BP 31.5 Thu 12:30 ZEU/0260

Bridging Scales to Understand the Role of Ubiquitylation and Sumoylation in Protein Phase Separation — •Supriyo Naskar, Kurt Kremer, and Oleksandra Kukharenko — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

The post-translational modifiers, such as mono- and poly-ubiquitins and SUMOs, are known for their ability to modulate protein-protein interactions by becoming covalently attached to other target proteins. Despite the high similarity in the tertiary structure and sequence, they differentially influence the target protein properties. In this work, we employed a multiscale simulation approach that encompasses atomistic to different levels of coarse-grained modeling techniques, combined with data-driven methods, to explore the structural differences and multidimensional energy landscapes of ubiquitin, SUMO, and their conjugates. We finally investigate the influence of distinct features of the targets and modifiers on protein phase separation and aggregation, providing molecular-level insight into the corresponding in vitro measurements and informing further experiments through the adjustment of relevant parameters.

BP 32: Statistical Physics of Biological Systems III (joint session BP/DY)

Time: Thursday 15:00–18:15 Location: BAR/SCHÖ

BP 32.1 Thu 15:00 BAR/SCHÖ

Efficiency of Droplet Formation and Dissolution by Chemical Reactions — •Gerrit Wellecke[1,2], Riccardo Rossetto[1,2], Jan Kirschbaum[1], and David Zwicker[1] — [1]Theory of Biological Fluids, Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany — [2]University of Göttingen, Institute for the Dynamics of Complex Systems, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Droplets formed by phase separation are vital for intracellular organization, and cells often control the formation and dissolution of these droplets through chemical reactions. To understand how cells can influence droplets in space and time, we consider a ternary system that exhibits a bistability between homogeneous and phase-separated states. We use a thermodynamically consistent approach to describe the diffusive and reactive dynamics, which allows us to quantify the energy dissipation and entropy production during transitions between these states. We find that reaction-controlled droplet formation and dissolution in the bistable regime are fundamentally different processes. While droplet formation is generally aided by relaxation to equilibrium, we find that a droplet's size determines whether it is best dissolved internally or externally. Further, our model identifies plausible mechanisms by which cells may regulate their intracellular droplets, providing insights that could guide the development of synthetic soft matter systems with tunable droplet behaviour.

BP 32.2 Thu 15:15 BAR/SCHÖ

Size control and fluctuations of chemically active droplets — •Guido Kusters and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Biological cells use liquid-liquid phase separation to dynamically compartmentalize their environment for various applications, many of which require size control. This process is challenging because (i) large droplets tend to grow at the expense of smaller ones, and (ii) thermal fluctuations can disturb droplets since cells are typically small and soft. Chemical reactions can, in principle, control droplet sizes, but there are no clear guidelines on how to robustly achieve size control. To provide guidelines, we consider a binary fluid model driven out of equilibrium by chemical reactions. We reveal two different classes of size-controlled droplets, depending on the ratio of droplet radius to the reaction-diffusion length. Moreover, we determine parameter regimes in which droplets become small. To study fluctuations in this case, we use fluctuation-dissipation arguments to predict the size fluctuations of size-controlled droplets, consistent with our numerical simulations. Taken together, our theory allows us to predict the chemical reactions necessary for maintaining small droplets, e.g., in biological cells or synthetic applications.

BP 32.3 Thu 15:30 BAR/SCHÖ

Anomalous diffusion and directed coalescence of condensates out of equilibrium — •Andriy Goychuk — Helmholtz Centre for Infection Research, Braunschweig, Germany — Lower Saxony Center for Artificial Intelligence and Causal Methods in Medicine, Hannover, Germany

Phase separation is ubiquitous in engineered and in biological systems. For example, biomolecular condensates contribute to the organization of the cytoplasm and nucleoplasm in cells. Here, I will first extend our understanding of textbook phase separation models by showing how condensates consisting of nonpolar molecules can effectively polarize and undergo coarsening by directed coalescence when subjected to a global drift, for example due to electrostatic potential gradients, chemical concentration gradients, or gravitation. Next, to better model the intracellular solution, I will incorporate viscoelastic stress propagation and nonequilibrium fluctuations. In this context, the Brownian motion of condensates has been barely explored despite being a cornerstone of statistical and colloidal Physics. If the active stresses, for example generated by molecular motors, have a different correlation time than the viscoelastic relaxation time of the solution, then the fluctuation-dissipation theorem is broken and the mixture is driven out of equilibrium. In this case, the size-dependence of the center-of-mass diffusion coefficient of the condensates can be either suppressed or enhanced, and the droplet can show superdiffusive motion. Together, these findings improve our understanding of the dynamics of domains in viscoelastic media and conserved order parameters in general.

BP 32.4 Thu 15:45 BAR/SCHÖ

A Minimal Theoretical Framework Linking Translation Activity to Stress-Induced Condensates — •Pascal S. Rogalla[1], Alessandro Barducci[1], and Luca Ciandrini[1,2] — [1]Centre de Biologie Structurale, Université de Montpellier, CNRS, INSERM, Montpellier, France. — [2]Institut Universitaire de France

The formation of intracellular membraneless organelles, such as stress-granule-like condensates formed via liquid-liquid phase separation (LLPS), is a common response to cellular stress. RNA, including mRNA, promotes the assembly of many of these condensates, while the resulting aggregation of mRNAs reduces their availability for translation and thereby modulates ribosome loading. This establishes a feedback loop between condensate formation and translational activity. Here we develop a minimal physical model that makes this coupling explicit by combining Flory-Huggins theory for LLPS with the Totally Asymmetric Simple Exclusion Process (TASEP) for ribosomal traffic on mRNAs. This hybrid framework provides a proof-of-principle description of how LLPS and translation dynamically influence one another. Our analysis reveals that the phase behaviour of both subsystems becomes mutually dependent: a

low-occupancy ribosomal phase promotes mRNA aggregation, whereas a high-occupancy phase suppresses condensate formation. These results suggest that cells may regulate condensate formation through translation modulation and, conversely, that LLPS can reshape the translatome. This provides a first proof-of-principle framework for quantifying stress-induced reorganisation of the translational landscape.

BP 32.5 Thu 16:00 BAR/SCHÖ

Optimal sensing through phase separation — •Henry Alston[1], Mason Rouches[2], Arvind Murugan[2], Aleksandra Walczak[1], and Thierry Mora[1] — [1]Laboratoire de Physique, Ecole Normale Superieure — [2]The James Franck Institute & Department of Physics, The University of Chicago

Cells are constantly tasked with making accurate measurements of their surroundings. A paradigmatic example is the sensing of signalling molecule concentrations: the work of Berg and Purcell derived limits for the precision and speed of this sensing through ligand-receptor binding. However, recent experimental work has identified the formation of condensates (liquid droplets coexisting with the cell cytoplasm through phase separation) as a potential mechanism for selectively initiating downstream processes by effectively amplifying small concentration differences between competing signalling molecules. Using a minimal model for droplet nucleation and growth in a fluid mixture, we observe that phase separation can distinguish concentration differences of 1% in minutes, a significant improvement upon well-established pathways for precise concentration sensing.

BP 32.6 Thu 16:15 BAR/SCHÖ

Thermodynamics of DNA sequence recognition by a transcription factor — •Jonas Neipel[1,2,3], Anne Schwager[1], Yahor Savich[1,2,3], Douglas Diehl[1], Anthony A. Hyman[1], Frank Jülicher[2,3], and Stephan W. Grill[1,3] — [1]Max Planck Institute for Molecular Cell Biology and Genetics, Dresden Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden Germany — [3]Center for Systems Biology Dresden, Dresden, Germany

Transcription factors (TFs) are proteins that regulate the transcription of genes by binding to specific genomic positions defined by the DNA sequence. The sequence of preference of a TF is typically characterized by a single sequence motif that maximizes binding affinity. However, eukaryotic TFs bind to a spectrum of low affinity binding sites that vastly outnumber canonical motif sequences in the genome. Here, we develop an Ising model of DNA sequence recognition that yields quantitative prediction of TF binding energies across sequence space for the human TF KLF-4. The model is parametrized by in vitro experiments, where we quantify relative binding energies for various sequences in a competitive assay using fluorescence anisotropy. Strikingly, we find that the thus fully parametrized thermodynamic model quantitatively predicts KLF-4 occupancy across the human genome. Finally, we discuss how this genomic energy landscape guides the formation of TF condensates.

15 min. break

BP 32.7 Thu 16:45 BAR/SCHÖ

Kinetic inference of entropy production — •Ivan Di Trelizzi — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Nonequilibrium steady states, from planetary dynamics to biological processes, constantly dissipate energy to their environment, producing entropy at a constant rate. Quantifying this dissipation is key to understanding how far systems operate from equilibrium but remains experimentally challenging. I will present a new approach to infer entropy production directly from trajectory data, using measurable kinetic quantities known as traffic and inflow rate, without requiring knowledge of microscopic forces or fluxes. The method remains effective even under partial observation, providing a practical framework to quantify nonequilibrium behaviour in complex physical and biological systems.

BP 32.8 Thu 17:00 BAR/SCHÖ

Frequency-space trajectory Fisher Information to quantify sensitivity in complex living systems — •Zhiheng Wu[1] and Isabella Graf[1,2] — [1]European Molecular Biology Laboratory, Heidelberg, Germany — [2]Department of Physics and Astronomy, Heidelberg University, Heidelberg, Germany

Living systems sense their environment by stochastically mapping external signals onto internal states. For example, several animals including fruit flies and pit vipers encode small changes in the ambient temperature in terms of changes in the interspike time of neurons. The sensitivity of these measurements can be evaluated by the so-called Fisher information (rate). While living systems constantly adapt to changing environments, calculations of Fisher information have so far mostly focused on static signals and internal states. To evaluate measurement sensitivity in the non-static case, we evaluate the trajectory Fisher information and show that, under common assumptions, it can be expressed as an integral over frequency space involving the power spectral density. This expression provides a tractable way to quantify information in adaptive and complex biological systems and we discuss some interesting applications.

BP 32.9 Thu 17:15 BAR/SCHÖ

Ergodicity shapes inference in biological reactions driven by a latent trajectory — •Ricardo Martinez-Garcia[1], Benjamin Garcia de Figueiredo[2], Justin Calabrese[1], and William Fagan[3] — [1]CASUS-HZDR, Görlitz, Germany. — [2]Princeton University, Princeton NJ, USA. — [3]University of Maryland, College Park MD, USA.

Many natural phenomena, from intracellular reactions to predator-prey encounters, can be described as counts of events triggered at random intervals when an underlying dynamical system enters reactive regions of its phase space. These reactions control biological functions across scales, from cellular processes to ecosystem services and stability. We compute the exact distribution of inter-count times under the only assumption that the latent dynamical system is Markovian and ergodic, recovering widely used Poisson statistics as a limiting case. These results limit what information about the latent process can be inferred from a local detector, which we explore in two biophysical scenarios. First, in estimating an animal's activity from detector crossings, we show that mean counts may fail to capture movement parameters, encoded in higher-order moments. Second, we show that the variance of inter-reaction times imposes a fundamental limit on how precisely detector measurements can infer the size of an ensemble of trajectories, generalizing the Berg-Purcell limit for chemosensation. Overall, we develop a flexible framework for quantifying inter-event time distributions in reaction-diffusion systems that shows which properties of latent processes are inferable from observed reactions.

BP 32.10 Thu 17:30 BAR/SCHÖ

Information Bottleneck in Gene Regulation — •Marianne Bauer — TU Delft

Biological systems need to process information in order to perform specific functions. In the context of gene regulation, regulatory regions process transcription factor signals in order for cells to differentiate towards correct fates. Previously, we have shown that the information bottleneck (IB) framework provides a useful framework for understanding regulatory binding site regions. Here, I will discuss two recent collaborative advances to provide an improved biological understanding from IB based predictions. First, using two complementary models for clustering transcription factors at binding site sensors, we can study information transfer during early fly embryo development with local transcription factor clustering. We find that weak cooperativity or clustering can allow for maximal information transfer, especially about the relevant variable, and that weak clustering also allows the binding site sensors to achieve optimality consistent with the IB bound. Second, we investigate how optimal activation changes when multiple binding site elements can process information, and find that activation profiles consistent with IB optimality resemble gene expression profiles in the early fly embryo.

BP 32.11 Thu 17:45 BAR/SCHÖ

Binary karyotypes are universally selected for across cancers — •Lucija Tomašić[1], Shane A. Fiorenza[1], Hajime Okada[2], Thomas W. van Ravesteyn[3], Uri Ben-David[2], Geert J.P.L. Kops[3], and Nenad Pavin[1] — [1]Univ. of Zagreb, Zagreb, Croatia — [2]Tel Aviv University, Tel Aviv, Israel — [3]Hubrecht Institute, Utrecht, the Netherlands

Aneuploidy, an abnormal chromosome number, is a defining feature of most cancers, yet its vast diversity has made it difficult to identify universal evolutionary rules. By analyzing over 90,000 patient-derived cancer karyotypes using a new visualization approach and mathematical modeling, we uncover a simple organizing principle. Across cancer types, and even in yeast, aneuploid genomes overwhelmingly assemble into "binary karyotypes" composed of only two chromosome copy numbers. Despite the enormous space of theoretically possible chromosome configurations, these states dominate patient data, comprising more than three-quarters of observed karyotypes. Our model shows that this pattern arises from a modest but consistent fitness advantage of binary karyotypes over more complex configurations. This principle also provides insight into how aneuploid cells withstand stress responses, as binary karyotypes exhibit lower rates of tumor suppressor gene inactivation. Together, our results identify binary karyotypes as a conserved evolutionary class of aneuploidy, governed by global organizational rules that may reveal shared vulnerabilities across cancers.

BP 32.12 Thu 18:00 BAR/SCHÖ

Inertial instability of blood in cross microchannels — •Joséphine Van Hulle and Christian Wagner — Experimental Physics, Saarland University, Germany

A localized reduction of vessel diameter (stenosis) increases the local blood flow speed and can trigger downstream recirculation which promotes conditions for the vessel blockage (thrombosis). The role of fluid elasticity in these flows remains underexplored. We isolate the extensional effects using cross-slot microfluidics, which creates an elongation plane with a well-defined inertial instability. By varying the hematocrit and plasma composition, we show that red blood cell deformability and plasma viscoelasticity lower the critical Reynolds number for the onset of vortex formation. These results highlight that even weak elastic stresses of blood can favor recirculation, a characteristic rarely modeled but necessary for physiologically realistic arterial simulations.

BP 33: Bioimaging

Time: Thursday 15:00–18:30 Location: BAR/0205

Invited Talk BP 33.1 Thu 15:00 BAR/0205

Expanding the Bag of Optical Tricks for (Neuro)Biology — •Fabian F. Voigt — Department for Molecular and Cellular Biology, Harvard University, Cambridge, USA — Max Planck Institute for the Science of Light, Erlangen, Germany — Max Planck Center for Physics and Medicine, Erlangen, Germany

Seeing is believing and thus, optical imaging techniques are extremely useful to study brain structure and function. I will present several projects aimed at providing the neuroscience community with bet- ter instrumentation: These range from open-source light-sheet micro- scopes for imaging cleared tissue (https://mesospim.org/) to novel multi-immersion microscope objectives that take inspiration from scallops and astronomical telescopes as well as utilizing metasurfaces for improving light collection efficiency in light-sheet microscopy.

BP 33.2 Thu 15:30 BAR/0205

Using Rotating Coherent Scattering (ROCS) Microscopy for Binding and Uptake Analysis of Virus-Mimicking Particles — •Dominik Huber and Alexander Rohrbach — Lab for Bio- and Nano-Photonics, University of Freiburg, Germany

The investigation of viruses with their host cell is an important topic in medical research, yet direct observation of these nanoscale dynamics remains challenging, since conventional fluorescence microscopy is limited by photobleaching and labelling constraints. To address these limitations, we employ label-free Rotating Coherent Scattering (ROCS) microscopy, an imaging approach that enables high-speed, high-resolution visualization of virus-mimicking particle behaviour at the cell.

ROCS microscopy uses backscattering of oblique illumination of a rotating laser beam to achieve around 160 nm spatial resolution at imaging rates up to around 200 Hz. By combining several illumination wavelengths and illumination angles, ROCS microscopy can be used in brightfield and darkfield as well as in total internal reflection mode. Leveraging this flexibility in imaging, allows us to capture the binding dynamics of particles to cells and to investigate them from their first attachment up to the investigation of single particle uptake events.

The analysis of particle fluctuation widths and mean square displacements enabled us to detect differences in binding characteristics of two different types of virus-mimicking particles, thus demonstrating that ROCS microscopy provides a powerful tool for investigation of particle-cell interactions at the single-particle level.

BP 33.3 Thu 15:45 BAR/0205

Pharmacological modulation of intrinsic tissue transparency for enhanced microscopy — •Adrián Puerta, Susan Wagner, and Moritz Kreysing — Institute of Biological and Chemical Systems, Karlsruhe Institute of Technology, 76344 Eggenstein Leopoldshafen, Germany

Light microscopy remains as one of the primary methods for data acquisition in biological research, yet its performance is frequently limited by the strong scattering properties of experimental tissues. Hence, the use of clearing agents that are incompatible with living samples is often required (1). To overcome these limitations, we aim to modulate the intrinsic transparency of biological samples, enabling more effective live-cell imaging.

Conventional clearing strategies rely on chemicals that modify the refractive index of aqueous or lipid-rich tissue components (2). In contrast, our approach involves screening small molecules with pharmacological properties that may enhance transparency in mammalian cells. To investigate this, we have developed a high-throughput screening system based on flow cytometry that will allow us to identify potential changes at a single-cell scale.

(1) Yu, T. et al. Physical and chemical mechanisms of tissue optical clearing. iScience 24, 102178 (2021).

(2) Ou, Z. et al. Achieving optical transparency in live animals with absorbing molecules. Science 385, eadm6869 (2024).

BP 33.4 Thu 16:00 BAR/0205

Imaging viral infection in live cells with confocal interferometric scattering microscopy (iSCAT) — •Anirudh Khemani[1], David Albrecht[1], Jan Renger[1], Marco Heisig[1], Kiarash Kasaian[1], and Vahid Sandoghdar[1,2] — [1]Max Planck Institute for the Science of Light, 91058 Erlangen, Germany — [2]Max-Planck-Zentrum für Physik und Medizin, 91054 Erlangen, Germany.

Fluorescence-based microscopy can suffer from observational bias, functional perturbation, phototoxicity, or insufficient signal. Confocal interferometric scattering microscopy [1] provides quantitative, label-free imaging of nanoscale dynamics in live-cell processes. iSCAT is a shot-noise-limited homodyne interferometric technique. By rejecting out-of-focus light, confocal iSCAT yields high structural contrast of nano-bioparticles, like vesicles and viruses, and we validate structural assignments with fluorescence. We apply this platform to study rare, dynamic events in the vaccinia virus life cycle. To improve experimental control and statistics, we developed a microfluidic system to deliver individual virions with defined timing and position. Furthermore, we combine confocal SCAT with concomitant wide-field iSCAT [2] to span a large range of spatial and temporal resolutions. We report on complex processes such as virus-induced nucleation of actin tails and high-speed tracking of single virions at cell-cell junctions and on membranes.

[1] Küppers, M., Albrecht, D., *et al. Nat. Commun.* **14**, 1962 (2023).

[2] Mazaheri, M., Kasaian, K., *et al. Optica* **11**, 1030 (2024).

BP 33.5 Thu 16:15 BAR/0205

Image segmentation of treated and untreated tumor spheroids by fully convolutional networks — Matthias Streller[1], Soňa Michlíková[2], Katharina Lönnecke[1], Leoni A. Kunz-Schughart[2], Anja Voss-Böhme[1], and •Steffen Lange[1,2] — [1]HTW Dresden — [2]OncoRay, TU Dresden, HZDR, Germany

Multicellular 3D tumor spheroids (MCTS) are advanced preclinical cell culture systems for assessing the impact of combinatorial radio(chemo)therapy as they exhibit therapeutically relevant in vivo-like characteristics. State-of-the-art assays quantify long-term curative endpoints based on collected brightfield image time series from large treated spheroid populations, which requires laborious spheroid segmentation of up to 100,000 images per treatment arm. While several image analysis algorithms are available for spheroid segmentation, they all focus on compact MCTS with a clearly distinguishable outer rim throughout growth and often fail for the common case of treated MCTS, which may partly be detached and destroyed and are usually obscured by dead cell debris. To address these issues, we successfully train 2 fully convolutional networks, UNet and HRNet, and optimize their hyperparameters to develop an automatic segmentation for both untreated and treated MCTS[1]. We extensively test the automatic segmentation on larger, independent datasets and observe high accuracy for most images with Jaccard indices around 90%, with deviations consistent to inter-observer variability. We also successfully test against previously published datasets and spheroid segmentations.

[1] Streller et.al, GigaScience 2025, doi.org/10.1093/gigascience/giaf027

BP 33.6 Thu 16:30 BAR/0205

Predicting treatment response of tumor spheroids from radiomics analysis of post-treatment dynamics — Pejman Shojaee[1,2], Tom Bischopink[1], Daria Bolotova[1], Sona Michlikova[2], Leoni A. Kunz-Schughart[2], Steffen Lange[1,2], and •Anja Voss-Böhme[1] — [1]DataMedAssist Group, Faculty of Informatics/Mathematics, HTW Dresden — [2]OncoRay - National Center for Radiation Research in Oncology Dresden

Radiomics has significantly advanced radiation oncology by providing quantitative, objective metrics to predict therapeutic efficacy. However, these methods have not been applied to three-dimensional, multicellular tumor spheroids yet, which are the preferred in vitro model for pre-animal, pre-clinical selection of novel, future-oriented treatment modalities. We present an AI-driven predictive modeling workflow to predict long-term tumor spheroid relapse using radiomics data from early post-treatment imaging of spheroids of two human cancer cell lines subjected to radiation therapy and hyperthermia. Our approach integrates multiple feature selection methods and machine learning algorithms for optimal classification performance. A detailed evaluation of the model performance reveals a time gain by early prediction of 2-14 days, while cases of late relapse remain challenging. The presented radiomics-based approach reduces the resource-intensive demands associated with prolonged experimental monitoring and allows accurate prediction for up to three days beyond the observation horizon.

15 min. break

BP 33.7 Thu 17:00 BAR/0205

Photothermal chemical imaging of nano-structured cells and cell organelles with less than 5 nm resolution — Maryam Ali[1,2], Christin David[1,3], and •Daniela Täuber[1,2] — [1]Friedrich Schiller University Jena — [2]Leibniz Institute of Photonic Technology, Jena — [3]University of Applied Sciences Landshut, Germany

Mid-infrared photoinduced force microscopy (PiF-IR) is a new imaging technique that enables the chemical characterization of surfaces with an unprecedented spatial and high spectral resolution. PiF-IR bridges the gap between high-resolution structure elucidation using electron microscopy, fluorescence microscopy and conventional infrared spectroscopy. It is complementary to tip-enhanced Raman spectroscopy (TERS). PiF-IR was successfully applied to map the local chemistry and structure of the antibiotic interaction on the surface of individual bacterial cells with a resolution of a few nanometers using the model system Bacillus subtilis and vancomycin [Ali et al., Anal. Chem., 2025, 97, 23914] and to map the surface of retina pigment organelles. Frequently observed anisotropic signal distributions on soft nanostructures in tip-enhanced

photothermal imaging methods could be attributed to hybrid field coupling in a study combining modeling and experiment [Anindo et al., J. Phys. Chem. C, 2025, 129, 4517].

BP 33.8 Thu 17:15 BAR/0205

Phase Analysis of Photothermal Signal Enables Sub-Cellular Chemical Mapping of Complex Biological Systems — •Felix Hermann Patzschke and Frank Cichos — Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, Leipzig University, Linnéstraße 5, 04103 Leipzig

Optically probed Photothermal Infrared (O-PTIR) microscopy is a powerful technique for label-free chemical imaging at sub-micron resolution, promising for cell and tissue analysis. However, the mechanism of signal generation is complex, suffering from the dynamic crosstalk between background and target heating. This lack of a rigorous, quantitative understanding of these dynamics currently forces users to sacrifice either chemical specificity or spatial resolution.

We conducted systematic experiments on defined nanoscale structures to motivate and validate a quantitative theoretical model based on the transient heat equation. This model reveals that the phase of the photothermal signal, a dynamic quantity often neglected, contains essential, localized information.

This phase directly encodes the time delay associated with thermal wave propagation, allowing for precise quantification of sub-cellular structural detail through effective thermal distance, even when the amplitude signal is insufficient to resolve closely-spaced features. By leveraging the full phase and amplitude response, we overcome existing spatial resolution limits, achieving enhanced, label-free chemical mapping for next-generation bioimaging, using existing hardware.

BP 33.9 Thu 17:30 BAR/0205

Effects of Optical Stimulation on the Adhesion of Human Osteoblasts — •Franziska Dorn[1], Wiebke Wollenberg[2], Meike Bielfeldt[3], Regina Lange[1], Susanne Stählke[3], Ingo Barke[1], Henrike Rebl[3], Berit Zeller-Pulmhoff[2], and Sylvia Speller[1] — [1]Physics of Surfaces and Interfaces, University Rostock — [2]Data-Driven Analysis and Design of Materials, University of Rostock — [3]Institute of Cell Biology, University Medical Center Rostock

Accelerated growth of autologous bone tissue is a promising strategy in regenerative medicine. In this study, we investigated how optical stimulation influences cell adhesion. We cultured the osteoblast-like (MG-63) cells in fetal bovine serum-free physiologic medium. As substrates, we used plain glass and glass surfaces with structured gold nanotriangular islands fabricated by nanosphere lithography. After cell seeding, the samples were illuminated with green light, inducing a spatially varying light intensity due to reflection and plasmons. Afterwards, we examined the cells using scanning electron microscopy and applied machine-learning-based/random-forest-based segmentation to extract morphological features. We found that opto-stimulated cells form more concave borders than unstimulated controls, suggesting that the cytoskeleton and the focal adhesions develop at non-uniform speed. Additionally, the adhesion area of illuminated cells is substantially larger than that of control cells on glass surfaces. However, when cells are seeded on surfaces with gold nanotriangular islands, this effect is absent. In a next step the peripheral region of the cells, in terms of lamellipodia and filopodia is addressed. (SFB 1270-299150580)

BP 33.10 Thu 17:45 BAR/0205

Imaging biomolecules for improving single-molecule diffraction — •Stefanie Lenzen[1,2], Lukas V. Haas[1,2], Kevin Janson[1], Amit K. Samanta[1,2], and Jochen Küpper[1,2] — [1]Center for Free-Electron Laser Science (CFEL), Deutsches Elektronen-Synchrotron DESY, Hamburg — [2]Department of Physics & Department of Chemistry & Center for Ultrafast Imaging, Universität Hamburg

Determining the structure and dynamics of single native biomolecules is still a challenge. In protein-crystallography and cryo-EM the molecule needs to be fixed, which might lead to structural disentegration, and the temporal resolution of these methods are limited. X-ray free-electron lasers (XFELs) provide ultrashort pulses, enabling diffraction before destruction, and a large number of photons, promising the observation of diffraction patterns *off* single nanoparticles [1]. Aerodynamic-lens stacks were used to deliver focused dense particle beams for such experiments on large nanoparticles [2]. Localization microscopy (LM), based on Mie-scattering is used to study and optimize these beams, an important step in improving single particle imaging. Due to the limitation in particle size [3], small biomolecules do not provide sufficient intensity for being detected with LM. We optimized the optical and analysis system and developed a promising method for the detection of smaller biomolecules, based on fluorescence.

[1] Poudyal, Schmidt, Schwander, *Struct. Dyn.* **7**, 024102 (2020);
[2] Ayyer, et int (39 authors), Chapman, *Optica* **8**, 15-23 (2021);
[3] Worbs, et int (2 authors), Maia, *Commun Phys* **8**, 155 (2025)

BP 33.11 Thu 18:00 BAR/0205

Optically addressable spins in proteins — •Dominik Bucher — Technical University of Munich, TUM School of Natural Sciences, Chemistry Department

Optically addressable spins have attracted significant interest for their potential in quantum sensing technologies. The current workhorses rely on spin defects in solids (such as the nitrogen-vacancy center in diamond), which lack the possibility for precise synthetic control over their properties. In my talk I will highlight our latest research on optically addressable spins in proteins, specifically flavin-based proteins. Upon excitation, these proteins generate radical pairs that can be detected optically via their flourescence and manipulated through radio wave-controlled spin chemistry. We further show that this optical spin interface is tunable by the protein structure. I will explain how these systems differ from the well-established NV center and discuss their potential as genetically encoded quantum sensors for future applications.

K. Meng et al. Optically detected and radio wave-controlled spin chemistry in cryptochrome, BioRxiv https://doi.org/10.1101/2025.04.16.649006 (2025)

BP 33.12 Thu 18:15 BAR/0205

Beyond Molecular Sensitizers: Illuminating the Role of Nanomaterials in Singlet Oxygen Photochemistry — •Zahid Ullah Khan[1], Latif Ullah Khan[2], Hermi Felinto Brito[1], and Paolo Mascio[1] — [1]Institute of Chemistry, University of São Paulo (USP), 05508-000, São Paulo-SP, Brazil — [2]Synchrotron-light for Experimental Science and Applications in the Middle East (SESAME) P.O. Box 7, Allan 19252, Jordan

Singlet molecular oxygen (1O2) plays a crucial role in various fields, including optoelectronics, photooxygenation reactions, and biomedical therapies, particularly as a major contributor to the success of photodynamic therapy (PDT). Since direct excitation of oxygen from the triplet ground state (3O2) to the singlet-excited state is spin-forbidden, thus, making the design of heterogeneous sensitizers crucial for efficient 1O2 production. For this purpose, nanomaterials, such as quantum dots (QDs) and rare earth fluoride nanoparticles (NPs), have emerged as versatile sensitizers for 1O2 generation, either individually or in combination with other inorganic or organic materials. Hence, conjoining the photophysical properties of QDs and rare earth NPs with other materials, e.g., coupling/combining with other inorganic materials, doping with the transition metal ions or lanthanide ions, and conjugation with a molecular sensitizer provide the opportunity to achieve high-efficiency quantum yields of 1O2 which is not possible with either component separately. Hence, the current work focuses the development of semiconductor QDs and rare earth-based nanosensitizer for efficient production of 1O2.

BP 34: Focus Session: Emergent Transport in Active Systems (joint session DY/BP)

Collective motion and directed transport are hallmark phenomena of active matter, arising from the interplay of self-propulsion, interactions, and nonequilibrium fluctuations. Even in the absence of global biases, assemblies of active particles can exhibit spontaneous currents, self-organized chemotaxis, and rectified transport due to broken symmetries or nonlinear feedbacks. Directed transport often emerges in inhomogeneous environments, where variations in particle activity or interaction strength can bias motion and organization. Activity gradients represent a particularly relevant example, providing a tunable mechanism to steer collective motion and pattern formation. These processes link microscopic activity to macroscopic material behavior and transport. This focus session aims to bring together theorists and experimentalists working on the fundamental mechanisms and control of emergent transport in active systems.

Organized by Abhinav Sharma (Augsburg) and Jens-Uwe Sommer (Dresden)

Time: Thursday 15:00–18:00 Location: ZEU/0160

See DY 55 for details of this session.

BP 35: Focus Session: 75 Years Division Polymer Physics: From Curiosity to Smart Materials (joint session CPP/BP)

Polymer materials are ubiquitous in modern society. In recent years, the focus has been on the development of functional, tunable or responsive materials, oftentimes inspired by biological materials. At this, a number of fundamental problems arise, e.g. regarding the interaction of polymers with water, biomolecules or inorganic nanoparticles and the resulting self-assembled morphologies as well as the underlying dynamics and the kinetics of morphological changes upon a stimulus. These problems are nowadays addressed in an interdisciplinary way by experimental methods, computer simulations and theory, often in close collaboration with polymer chemists. In five talks by renowned speakers, the focus session aims at highlighting few of these aspects that are currently under investigation worldwide. The fact that the Polymer Physics Division of the German Physical Society was founded in 1951 and hence, 2026 is the 75th anniversary, seems to be a good occasion to bring modern polymer physics into the focus.

Organized by Christine M. Papadakis, Christian Holm, Tayebeh Ameri and Kristian Franze.

Time: Thursday 15:15–17:45 Location: ZEU/LICH

Topical Talk BP 35.1 Thu 15:15 ZEU/LICH

The Loops of Life — Brian Chan and •Michael Rubinstein — Duke University, Durham, NC, USA

In mammalian cells, the cohesin protein complex is believed to regulate chromatin during interphase through active loop extrusion, in which dynamic loops are formed by cohesin translocating along chromatin. We developed a theoretical model that quantifies how key parameters, including cohesin residence time on chromatin, extrusion velocity, and the number density of chromatin-bound cohesins, regulate genomic contacts. The model describes chromatin contact probabilities and predicts that loop formation probability is a nonmonotonic function of loop length. Our theory demonstrates that active loop extrusion causes the apparent fractal dimension of chromatin to cross over between two and four at contour lengths on the order of 30 kilobase pairs. This work provides a theoretical basis for the compact organization of interphase chromatin, explaining the physical reason for the segregation of topologically associated domains and suppression of chromatin entanglements by up to a factor of 50, which contributes to efficient gene regulation by distal elements such as enhancers or silencers.

Topical Talk BP 35.2 Thu 15:45 ZEU/LICH

Polyelectrolytes and Biological Systems: A Charged Relationship — •Matthias Ballauff — Chemie und Biochemie, Freie Universitaet Berlin

If charges are appended to linear or crosslinked polymers, a polyelectrolyte results. Polyelectrolytes are ubiquitous and play a major role in biophysics. Important natural polyelectrolytes as e.g. DNA or Heparin are central in biology, and a thorough understanding of these systems and of charge-charge interaction is one of the main tasks of biophysics. In my lecture, I will discuss our recent research done on -Interaction of linear polyelectrolytes with proteins. This problem is also relevant for the formation of biocondensates by the interaction of cationic and anionic proteins; -Charged polymer networks and their interaction with proteins; -Role of polyelectrolytes in virus infections. In all cases, a quantitative understanding of the systems in terms of analytical models can be achieved, which may pave the way for future pharmaceutical applications.

Topical Talk BP 35.3 Thu 16:15 ZEU/LICH

From block copolymer morphologies to functional polymer membranes — •Volker Abetz — Helmholtz-Zentrum Hereon, Institute of Membrane Research, Max-Planck-Str. 1, 21502 Geesthacht, Germany — University of Hamburg, Institute of Physical Chemistry, Martin-Luther-King-Platz 6, 20146 Hamburg, Germany

Depending on solvent selectivity and the time of evaporation different structures can be obtained in cast block copolymers, showing that there is an interplay between kinetics and thermodynamic driving forces during the self-assembly before the sample is dry. When preparing membranes from block copolymer solutions, besides molecular weight, composition of the block copolymer and its concentration, also the choice of solvent, and the casting conditions play an important influence on the obtained morphology of the finally obtained membrane. This is especially important when membranes are prepared via the so-called non-solvent induced phase separation process after initial self-assembly by partial evaporation of solvent. The obtained membranes, when prepared successfully, display a rather isoporous top layer and can be subsequently post functionalized, in order to tune pore size and pore surface property. Different examples of the separation properties will be shown and also the potential use as a membrane reactor will be discussed.

Topical Talk BP 35.4 Thu 16:45 ZEU/LICH

Molecular electronic materials and devices for solar energy conversion — •Jenny Nelson — Imperial College London

To maximize the potential of solar power, new materials will be needed to harvest and convert solar energy alongside existing photovoltaic technologies. Molecular electronic materials, such as conjugated polymers and molecules, can achieve photovoltaic conversion through a process of photon absorption, charge separation at a heterojunction, and charge collection. Through a remarkable series of advances in materials design, the efficiency of photovoltaic energy conversion in molecular materials has risen from 1% to over 20% within two decades. We will discuss the factors that control the function of molecular solar cells including the nature of the charge separating heterojunction, and the impact of chemical and physical structure on phase behaviour, energy and charge transport, light harvesting, and loss pathways, comparing experimental measurements with a computational model of the generation and evolution of excited states and charges in such systems. We identify key molecular parameters that are likely to assist charge generation and consider the extent to which these parameters are optimised in the best performing materials. Finally, we will address the limits to conversion efficiency in such systems.

Topical Talk BP 35.5 Thu 17:15 ZEU/LICH

Control of cell and tissue stiffness by biopolymer networks and particle inclusions — •Paul Janmey — University of Pennsylvania, Philadelphia, PA, USA

Filamentous networks of semiflexible polymers are ubiquitous in biology. Collagen fibers form much of the extracellular matrix, the cytoskeleton controls cell mechanics, and chromatin fibers span the volume of the nucleus. The mechanical properties of the biopolymer fibers, the way in which the fibers link into networks, and the types of cells within the network all affect the way in which tissues respond to mechanical stress.

BP 36: Statistical Physics of Biological Systems IV (joint session BP/DY)

Time: Friday 9:30–12:45 Location: BAR/SCHÖ

Invited Talk BP 36.1 Fri 9:30 BAR/SCHÖ

Swimming in complex environments — •Christina Kurzthaler — Max Planck Institute for the Physics of Complex Systems

Microorganisms are omnipresent in the ocean, the human body, and our soils and therefore play an important role for various geological, biological, and medical processes. To optimize their survival and perform biological functions many microorganisms convert chemical energy into directed motion. In this talk, I will illustrate the underlying physical concepts and show concrete examples of our research, focusing on the interactions of microorganisms with their complex habitats. I will first discuss the motion of sperm in complex fluids and address their emergent dynamics in the presence of a hyperactivation agonist, modifying the sperm beating pattern. Second, I will focus on the first-passage-time statistics of active agents moving towards a target boundary. Our results highlight how swim gait impacts spreading and search efficiency in active systems with potential consequences for sperm motion in the reproductive tract and the accumulation of microbial communities.

BP 36.2 Fri 10:00 BAR/SCHÖ

Motor shot noise explains active fluctuations in a single cilium — •Maximilian Kotz[1], Veikko F. Geyer[2], and Benjamin M. Friedrich[1] — [1]Cluster of Excellence Physics of Life, TU Dresden, Dresden, Germany — [2]B CUBE, TU Dresden, Dresden, Germany

Molecular motors drive seemingly regular motion, making living matter move - yet also cause non-equilibrium fluctuations that can serve as a probe of internal motor dynamics. Here, we use motile cilia as a model system to investigate how small-number fluctuations shape collective dynamics. Motile cilia exhibit regular bending waves; this motion is driven by the self-coordinated activity of thousands of molecular motors inside the cilia's cytoskeletal core. By developing, to the best of our knowledge, the first stochastic model of cilia beating, we show that the finite number of motors leads to active fluctuations on the mesoscale, sufficient to explain frequency jitter in beating cilia observed in experimental data. We rigorously compare observables of this model, including the quality factor of the oscillation, to experimental data in which motors have been partially extracted from cilia. This is a strong test of this stochastic model. The model also reproduces other phenomena of experimental data, like correlation lengths of intra-cilium synchronization and noise-induced phase slips. We propose that active fluctuations are important new observables, which can guide theoretical models of motor dynamics in beating cilia and other motor systems.

BP 36.3 Fri 10:15 BAR/SCHÖ

Theory of Forces Between Crosslinked Filaments — •Cedrik Barutel and Sebastian Fürthauer — Institute of Applied Physics TU Wien Austria

The cytoskeleton drives essential cellular processes like cell division and chromosome segregation. It consists of filaments that are crosslinked by proteins, many of which are molecular scale motors that consume ATP to do work. The forces that crosslinking proteins generate between cytoskeletal filaments are the key drivers of active cellular mechanics. We derive a generic theory to describe such crosslinking forces.

We construct a theory to describe and predict the forces generated collectively by crosslinking proteins between biofilaments using symmetries, conservation laws, and out-of equilibrium thermodynamic principles. Our approach identifies the full set of phenomenological coefficients governing entropic, active, and frictional crosslinking forces, which allows a quantitative comparison between the effects of different crosslinker mixtures between two filaments. We demonstrate the power and validity of this framework by quantitatively explaining a set of different experimental setups, which combine the effects of passive and active crosslinks

BP 36.4 Fri 10:30 BAR/SCHÖ

Modeling Cooperative Remodeling and Energy Landscapes in the Bacterial Flagellar Motor — •Nils-Ole Walliser — Laboratoire Charles Coulomb, University of Montpellier, Montpellier, France

Bacteria use the flagellar motor to adapt their motility to changing mechanical conditions. This rotary motor tunes its torque by recruiting and releasing torque-generating stator units. I will present statistical-physics-based models that use single-motor measurements to infer interaction potentials and energy landscapes in the bacterial flagellar motor. First, using single-motor bead assays that resolve stepwise changes in rotation speed and thus stator occupancy, we model stator recruitment as a finite-size lattice gas and infer stator-stator cooperativity from occupancy fluctuations. This reveals moderate attractive interactions and shows that the motor operates in a regime that balances responsiveness to load changes with noise in stator number. Second, I will discuss experiments where the motor load is actively perturbed, uncovering a strong asymmetry in the relaxation to the steady state when starting from higher versus lower stator occupancy. A two-state catch-bond model quantitatively explains this stoichiometry-dependent asymmetry and captures the mechanosensitive nature of stator anchoring to the cell wall. Finally, I will show how high-temporal-resolution rotation traces can be used to reconstruct, in a model-independent way, the tilted periodic energy landscape of the rotor/LP ring within a Smoluchowski framework, yielding barrier heights, torque and internal friction.

BP 36.5 Fri 10:45 BAR/SCHÖ

Anisotropic (sub)diffusion of organelles in living cells — •Aranyak Sarkar, Pooja Yadav, and Matthias Weiss — Experimental Physics I, University of Bayreuth, Universitätsstraße 30, 95447 Bayreuth

Eukaryotic cells are neatly organized into distinct, membrane-enclosed compartments ('organelles') with specific duties. A prominent example are peroxisomes, which feature vesicle-like shapes with radii 0.1 – 1 μm that are dispersed across the cytoplasm. Using time-lapse fluorescence microscopy, we have tracked the motion of individual peroxisomes over extended periods. Analysis of the experimental data revealed two distinct modes of motion: a prevailing (sub)diffusive motion and a quite rare super-diffusive characteristics that is associated with motor-driven transport along microtubules. Focussing on the seemingly unremarkable subset of (sub)diffusive trajectories, we have found a significant anisotropy in the motion that persisted even when microtubules were disrupted. In particular, diffusive steps along the cells' long axis were seen to be favored over steps in the perpendicular direction, indicating an anisotropic materials characteristic of the cytoplasm. Using a simple model, we were able to capture and explain the observed features of the anisotropic diffusion of organelles.

15 min. break

BP 36.6 Fri 11:15 BAR/SCHÖ

Understanding Influenza A Virus particles detaching from reconstructed cell surfaces — •Thomas Kolbe[1,2], Pierre Gaspard[1], and Bortolo Matteo Mognetti[1,2] — [1]CENOLI, Université Libre de Bruxelles (ULB) — [2]IB2 - Interuniversity Institute of Bioinformatics in Brussels

Influenza infection is a multistage process that involves the trafficking of viral particles across the cell membrane. Before endocytosis, virions target the membrane by binding hemagglutinin ligands to sialic acid residues on cell receptors. After budding, neuraminidase cleaves these residues, enabling virions to detach from the infected cell surface.

We examine detachment dynamics through simulations and theoretical analysis. We explain experimental findings showing that the time required for virions to detach can decrease as the single-trajectory average number of bonds increases - a counterintuitive result specific to neuraminidase activity. Furthermore, we demonstrate that the detachment time is not governed by a Poisson distribution but depends on multiple factors, including ligand-receptor reaction rates, virion size, and receptor diffusion constant. These results clarify how biochemical parameters regulate the residence time of virions at the cell surface.

BP 36.7 Fri 11:30 BAR/SCHÖ

Band pattern formation of erythrocytes in density gradients is due to competing aggregation and net buoyancy — •Felix Maurer[1], Camila Romero[1], Nikolas Lerch[1], Thomas John[1], Lars Kaestner[1,2], Christian Wagner[1,3], and Alexis Darras[1,4] — [1]Experimental Physics, Saarland University, Saarbruecken, Germany — [2]Department of Theoretical Medicine and Biosciences, Saarland University, Homburg, Germany — [3]Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg — [4]School of Physics, University of Bristol, Bristol, United Kingdom

Centrifugation of biological matter in density gradient solutions is a standard method for separating cell types or components. It is also used to separate RBCs by age, as they lose water and become denser over their lifespan. When the density gradient is prepared with Percoll, discrete bands of RBCs are systematically observed, despite the continuous density distribution of RBCs. We developed a continuity equation incorporating cell aggregation to describe the macroscopic evolution of RBC volume fraction in a density gradient, considering a continuous RBC density distribution. Numerical solutions demonstrate that the competition between net buoyancy and aggregation is sufficient to create band patterns. Our model reproduces the temporal evolution observed in experiments, but also predicts several types of bifurcation-like behaviors for the steady-state patterns in constant gradients, depending on RBC volume fraction and aggregation energy.

BP 36.8 Fri 11:45 BAR/SCHÖ

Adaptive self-organization in excitable biological collectives — •Bianca Ariani[1,3], Yunus Sevinchan[2,3], and Pawel Romanczuk[2,3] — [1]Bernstein Center for Computational Neuroscience, Berlin — [2]Science of Intelligence, TU Berlin — [3]Institute for Theoretical Biology, HU Berlin

Biological collectives often display complex, context-dependent behavior, such as coordinated responses to predators, despite individuals following simple local rules. This class of phenomena is broadly understood as self-organization.

We examine a system showing rich spatio-temporal dynamics: Sulphur Mollies, Mexican freshwater fish whose group behavior resembles a stochastic excitable medium. To probe the mechanisms behind their collective activity, we study a bio-inspired agent-based model in which individuals estimate the shoal's mesoscale activity from the cues they perceive as they move. Each agent adjusts its sensitivity to cues through a simple homeostatic plasticity rule, allowing the group to regulate its collective state. This formulation links individual adaptation to population-level patterns.

Our results show that local adaptive regulation reproduces key qualitative features of the biological system. More generally, they illustrate how distributed plasticity mechanisms can support robust self-organization in complex biological collectives.

BP 36.9 Fri 12:00 BAR/SCHÖ

Visual-based Collective Shepherding in Swarm Robotic System — •Yating Zheng[1,2] and Pawel Romanczuk[1,2] — [1]Department of Biology, Humboldt Universität zu Berlin, Berlin, Germany — [2]Research Cluster of Excellence 'Science of Intelligence', Berlin, Germany

Collective shepherding presents a rich example of two interacting multi-agent systems coupled through non-reciprocal interactions. While most existing models assume that shepherd agents have global knowledge of the flock-an unrealistic premise for physical or biological systems-we introduce a vision-based, locally interacting model that captures the essential physics of shepherd-flock coordi-

nation. The model produces robust, self-organized behavior among shepherds without explicit communication, and we analyze how key control parameters, such as flock size and the number of shepherds, shape the resulting dynamics.

The framework also performs effectively in more challenging regimes, including the manipulation of non-cohesive agents and passive (non-self-propelled) agents, demonstrating its broad dynamical applicability. We further validate the model on a mixed-reality swarm-robotic platform, where physical robots successfully shepherd a virtual flock.

Overall, these results provide a minimal yet powerful physics-based description of multi-agent herding using only local visual information, offering insight into non-reciprocal collective behavior and enabling scalable real-world implementations in swarm robotics.

BP 36.10 Fri 12:15 BAR/SCHÖ

Polymer theory shows DNA motors extrude loops in the monomeric mode — Kirill Polovnikov[1,2] and •Dmitry Starkov[2] — [1]Institute for Physics and Astronomy, University of Potsdam, Potsdam-Golm, Germany — [2]Moscow, Russia

Cohesin-dependent loop extrusion is a key active mechanism of DNA organization, yet it remains unclear whether chromatin loops in living cells are generated primarily by individual cohesin motors or by higher-order structures. To fill this major gap, we build an analytical polymer-physics model that extracts a missing parameter - *the linear density of loops* - directly from Hi-C data. We focus on short genomic distances, where contact statistics simplify, resulting in a perturbative expression for the contact probability of a looped chain under a finite contact-detection radius. Our theory recapitulates a characteristic dip in the *logarithmic derivative* of the contact-probability that is *broadly observed in experiments*. By fitting this minimal model to a diverse range of mammalian Hi-C datasets, we infer approximately six loops per megabase. Independent imaging and mass spectrometry measurements of cohesin density are consistent with our inferred loop density, supporting the monomeric mode of DNA motors extrusion.

BP 36.11 Fri 12:30 BAR/SCHÖ

Universal loop statistics from active extrusion — •Anastasia Chervinskaya[1] and Kirill Polovnikov[1,2] — [1]Moscow, Russia — [2]Institute for Physics and Astronomy, University of Potsdam, Potsdam-Golm, Germany

Cohesin-dependent loop extrusion is a key active mechanism of genome organization, yet quantitative links between extrusion kinetics and measurable loop statistics remain incomplete. We develop an analytical model that predicts the mean loop scale, full loop-length distributions, state composition, and arm-arm correlations for one-sided versus two-sided extrusion. The theory maps the master equations onto diffusion on a state graph yielding state-resolved loop-length PDFs.

We show that one-sided extrusion yields a universal exponential loop-length distribution, whereas two-sided extrusion generates a sum of exponentials that approaches a gamma-like form at high barrier density. The model also predicts a strictly positive lower bound of 1/4 on arm-arm correlations.

Parameterized with independent measurements for HeLa G1 (cohesin residence and spacing; barrier densities and lifetimes), our model quantitatively accounts for the observed loop size. Also, it reproduces the experimentally measured distribution of CTCF-CTCF loop lengths under the assumption of two-sided extrusion, providing additional evidence that cohesin extrusion in living cells is predominantly bidirectional. Our results provide a compact route to infer biophysical parameters of active extrusion from experimental data.

BP 37: Tissue Mechanics II

Time: Friday 9:30–12:45 Location: BAR/0106

BP 37.1 Fri 9:30 BAR/0106

Active rheology and feedback-controlled stress in a multi-purpose platform for tissue mechanics — •Anna Mukhina[1,2], Till Muenker[1], Mattias Luber[1], Polina Malova[1,2], and Timo Betz[1,2] — [1]Third Institute of Physics - Biophysics, University of Goettingen — [2]Max Planck School Matter to Life

3D tissue engineering offers unique opportunities to study simplified, but accurate models of complex biological systems, where especially force generation, mechanical properties, and active regulation can be addressed. However, most current methods to raise engineered tissues do not allow quantitative characterization of their mechanics without a strong perturbation of these delicate systems.

Here, we present a novel experimental platform to apply well-defined strain to tissues and measure the resulting forces with an optical readout. Tissues are grown between flexible posts, where one post can be actuated by a piezo bending element, and direct optical detection of both posts movement allows for precise force and strain measurement. With this setup, we avoid complex microscopy measurements, can position the system in an incubator, and the rapid readout enables a large variety of experimental protocols. The system can conduct oscillatory rheology, simulate isometric/eccentric contractions, reproduce changes in environmental stiffness during physiological and pathological processes, and adapt stress or strain to mechanical changes of the system. We demonstrate the potential of the developed setup by carrying out oscillatory rheology of engineered skeletal muscles over the course of their maturation, covering three orders of frequency magnitude.

BP 37.2 Fri 9:45 BAR/0106

demonstrating normal tissue sparing with pitz PITZ electron beams in zebrafish embryos — •E Tarakci[1,2,3], C Schulze[2], C Richard[1], M Gross[1], N Aftab[1], A Aksoy[1], Z Amirkhanyan[1], A Chiravuri[1,2], J Good[1], F Hausmann[3], S Khammee[1], Y Komar[1,2,3], M Krasilnikov[1], B Li[1], X Li[1], Z Lotfi[1], G Montoya-Soto[1], F Mueller[1], A Oppelt[1], F Riemer[1], K Suzart[1], I Tinhofer[3], D Villani[1], S Worm[1], D Xu[1], S Zeeshan[1], M Frohme[2], F Stephan[1], S Aminzadeh Gohari[1], and A Grebinyk[1] — [1]Deutsches Elektronen-Synchrotron, DESY, Zeuthen — [2]Technische Hochschule Wildau,Wildau — [3]Charité Universitätsmedizin Berlin, Berlin

Zebrafish (Danio rerio) embryos provide a sensitive model for studying normal tissue responses. This study was conducted within FLASHlab@PITZ, where PITZ delivers electron beams from conventional to ultra-high dose rates up to 10^15 Gy/s. Wild-type AB embryos at 24 hours post fertilization (hpf) received 10 Gy via conventional X-rays (0.04 Gy/s), low dose rate electrons (LDR, 0.05 Gy/s), or ultra-high dose rate electrons (UHDR, 10^5 Gy/s). At 119 hpf, toxicity was assessed through spinal curvature, pericardial edema, eye diameter, and body length. X-rays and LDR increased toxicity (X-rays: 50% medium, 50% none*mild; LDR: 33% severe, 17% mild, 50% normal). UHDR greatly reduced effects, with no medium or severe toxicity and 42% none and 58% mild changes. These results demonstrate a marked tissue-sparing trend under UHDR conditions and provide early evidence for a FLASH-mediated normal tissue sparing effect.

BP 37.3 Fri 10:00 BAR/0106

Holographic vibration spectroscopy - extracting mechanical properties of adherent cells from their vibrational response — •Eric Schneider[1], Bob Fregin[1], Dominic Mokbel[2], Sebastian Aland[2], and Oliver Otto[1] — [1]Institute of Physics, University of Greifswald, Greifswald, Germany — [2]Institute of Numerical Mathematics and Optimization, TU Bergakademie Freiberg, Freiberg, Germany

The mechanical properties of biological cells are closely linked to their pathophysiological state, and high-throughput quantification is essential for using them as biomarkers in basic and translational research. While microfluidic technologies can characterize suspended cells at rates above 1,000 cells per second, no comparable method exists for adherent cells or tissues. Here, based on preliminary experiments with holographic vibration spectroscopy (HVS), developed in our group, we present a theoretical framework to address this gap. In HVS, adherent cells are harmonically oscillated at defined frequencies and amplitudes, and their deformation and phase shift encode their mechanical properties. To validate this concept, we developed a finite-element simulation framework using the open-source library AMDIS, capable of modeling cellular vibration across a broad parameter space. From these simulations, we derive a protocol to solve the inverse problem and show that viscoelastic properties can be uniquely determined using only the amplitude response at two vibration frequencies. Combined with HVS, this framework will next be used to rapidly and non-invasively quantify the viscoelastic properties of adherent cells and tissues.

BP 37.4 Fri 10:15 BAR/0106

Investigating the dynamics of cellular rearrangements in minimal four-cell clusters — •Agathe Jouneau, Tianyi Cao, and Joachim Rädler — Faculty of Physics and Center for NanoScience, Ludwig-Maximilians-Universität, Munich, Germany

Animal cells assemble into tissues that exhibit diverse mechanical responses, from solid-like to liquid-like states. In solid-like states, tissues can withstand mechanical stress, whereas in liquid-like states, they release stress through cellular rearrangements. Recent evidence suggests that the transition between solid and liquid-like states is central to biological processes such as embryogenesis, wound healing and cancer metastasis. However, the way in which local interactions between the constituent cells control the tissue fluidity remains unclear. The process by which cells exchange neighbors is known as a cell intercalation, or a T1 transition in foam physics terminology. Theoretical models have shown that the height of the energy barrier associated with T1 transitions determines tissue fluidity. In our work, we study the dynamics of T1 transitions in a minimal

system of four epithelial cells. We confine the cells onto adhesive micropatterns or in hydrogel microcavities, and use time-lapse microscopy to record the evolution of cell-cell junctions over time. We aim to use this platform to study how perturbations of cell-cell adhesion proteins impact cell rearrangement, as well as to experimentally test existing models for cellular dynamics.

BP 37.5 Fri 10:30 BAR/0106

Collective actuation in solid tissues: Dynamics and mechanics of an oscillating tissue shell during morphogenesis — •Zoë Lange[1], Henrik Jaeschke[1], Lea Möller[1], Mariia Golden[2], Artemiy Golden[2], Marc Pereyra[1], Frederic Strobl[2], Ernst H.K. Stelzer[2], and Franziska Matthäus[1] — [1]Frankfurt Institute for Advanced Studies — [2]Buchmann Institute for Molecular Life Sciences

Morphogenesis relies on coordinated mechanical deformations of embryonic tissues, yet the dynamic material properties that enable these shape changes remain incompletely understood. In the *Tribolium castaneum* embryo, the extraembryonic serosa tissue forms a closed and oscillating epithelial shell, providing a powerful model to study active mechanical processes in vivo. Here, we combine quantitative live imaging with particle image velocimetry, cell-boundary segmentation, cell-boundary tracking, and stress inference methods to characterize the spatiotemporal mechanics of the oscillatory contractions in the tissue shell. We show that the extraembryonic epithelium behaves as an active elastic solid whose global oscillation emerges from synchronizing cellular contraction. By integrating measured deformation with inferred force maps, we identify a cellular program of mechanosensitive remodeling. Our results provide a mechanistic link between active force production at the cellular scale and emergent morphogenetic dynamics at the tissue scale, establishing the *Tribolium* tissue shell as a model system for collective actuation in active elastic materials *in vivo*.

BP 37.6 Fri 10:45 BAR/0106

Plant movement systems enabled by plant hinges: diversity, evolution, form-structure-function relationships and their biomimetic potential — Arooj Sajjad and •Simon Poppinga — Technische Universität Darmstadt, Botanischer Garten, Schnittspahnstraße 2, 64287 Darmstadt, Germany.

Plants are often described as comparatively static systems, yet many species exhibit diverse and mechanically sophisticated forms of movement. In recent decades, such plant movement systems have gained increasing attention due to their remarkable flexibility, versatility, and structural robustness. Plants move in a variety of ways, e.g. to align themselves with sunlight or the earth's gravitational field, to catch prey, to interact with pollinators, and to adhere to nearby structures in the environment. Plant movements are often enabled by joint-like structures, commonly referred to as plant hinges in the literature. Unlike technical hinges, which allow for rigid body movements and are maintenance-intensive and prone to failure, compliant mechanisms as found in plant movement systems fulfil roles analogous to technical joints, albeit fundamentally differing in form, kinematics, and structure. Interestingly, the hinges in most motile plant structures (e.g. motile sepals in orchids or lever mechanisms in sages) have not been investigated regarding their form-structure-function relationships. In this broad research study, we approach these compliant mechanisms in plants from an engineering perspective on kinematic pairs. Our research also aims to understand convergent mechanisms in plants. One aim is to develop future biomimetic actuator design.

15 min. break

BP 37.7 Fri 11:15 BAR/0106

Understanding tissue mechanics through tumour organoids — •Mathilde G. Lettinga[1], Vaibhav Mahajan[1], Raimund Schlüssler[1], Stefanie Hübner[2,3], Valeria Lozovanu[2,3], Franziska Baenke[2,3,4], Daniel E. Stange[2,3,4], and Anna V. Taubenberger[1] — [1]BIOTEC, CMCB, TU Dresden — [2]VTG, University Hospital Carl Gustav Carus, TU Dresden — [3]DKTK, Heidelberg — [4]NCT/UCC, Dresden

Tumours exhibit altered physical properties that manifest across spatial scales. Compared to healthy tissue, solid tumours are typically stiffer, which can partly be attributed to the extracellular matrix. However, the contributions of the epithelial cancer cells to the emergent tissue properties remain unclear.

Aiming to elucidate the role of cells in tissue mechanics, we investigated the mechanical and morphological properties of patient-derived colorectal liver metastasis organoids. Organoids from different patients varied in morphology, displaying either a large central lumen or a multitude of small lumina. We performed bulk compression with AFM and found that single-luminal organoids are stiffer and more elastic than multi-luminal organoids. Concurrently, Brillouin microscopy in situ showed a higher Brillouin frequency shift for single-luminal organoids, indicating lower compressibility. 3D segmentation revealed more elongated, ordered, homogeneous and smaller nuclei in the single-luminal organoids compared to their multi-luminal counterparts. Thus, our data suggest that the mechanical properties of organoids are coupled to the physical properties of their constituent cells.

BP 37.8 Fri 11:30 BAR/0106

A morphoelastic phase field model predicts buckling instability in tumor growth — Luise Zieger[1], Min Wu[3], John Lowengrub[4], and •Sebastian Aland[1,2] — [1]TU Freiberg — [2]HTW Dresden — [3]Worcester Polytechnic Institute, USA — [4]UC Irvine, USA

It is well known that growing tumors generate and respond to stress in their local environment. On the one hand, local cell proliferation and apoptosis lead to complex strain patterns in the tissue. On the other hand, tissue re-arrangements can relax the resulting mechanical shear stresses and make the tissue more fluid-like. To predict the outcomes of these nonlinear visco-elastic interactions, we introduce the framework of morphoelasticity to phase field modeling of a growing tumor embedded in a surrounding host tissue. Coupling this continuum system to diffusible growth-promoting nutrient, our simulations identify a symmetry-breaking instability in 2D and 3D driven by two primary mechanisms: (i) elastic buckling instability generated by tangential stresses along the tumor-host interface and (ii) instabilities generated by local imbalances between cell divisions and cell death. Further, tissue fluidity and compressibility can lead to changes in tumor topologies. Our modeling framework provides a robust methodology for investigating how tissue mechanics and growth factor signaling influence the progression and invasive potential of solid tumors.

BP 37.9 Fri 11:45 BAR/0106

Orientational lineage memory and mechanical ordering during diffusion-limited growth — •Ilias-Marios Sarris[1], Ramin Golestanian[1,2], and Philip Bittihn[1] — [1]MPI for Dynamics and Self-Organization, Göttingen, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, United Kingdom

Growth and shape formation in crowded multicellular assemblies arise from the interplay of chemical gradients, single-cell expansion, and mechanical interactions. Using a particle-based model that resolves nutrient fields and cellular orientations with tunable lineage memory, we study how orientational order emerges in expanding fronts whose morphology is set by nutrient limitation. We find a transition in nematic order controlled by front morphology: under strong orientation inheritance, both thin active layers (fingering fronts) and thick active layers (flat fronts) produce strong alignment, while intermediate cases are less ordered. Velocity, reorientation, and stress statistics reveal a crossover from inheritance-dominated to mechanically driven alignment that progressively overrides lineage memory. As a result, orientational memory yields a fitness advantage only in the diffusion-limited, memory-dominated regime, elucidating how nutrient supply and mechanics jointly shape self-organization during growth.

BP 37.10 Fri 12:00 BAR/0106

Feedback-controlled epithelial mechanics: emergent soft elasticity and active yielding — •Fridtjof Brauns[1,2], Pengyu Yu[3,4], and M. Cristina Marchetti[3] — [1]MPI-PKS, Dresden, Germany — [2]KITP, Santa Barbara, USA — [3]University of California, Santa Barbara, USA — [4]Tsinghua University, Beijing, China

Biological tissues exhibit distinct mechanical and rheological behaviors during morphogenesis. While much is known about tissue phase transitions controlled by structural order and cell mechanics, key questions regarding how tissue-scale nematic order emerges from cell-scale processes and influences tissue rheology remain unclear. Here, we develop a minimal vertex model that incorporates a coupling between active forces generated by cytoskeletal fibers and their alignment with local elastic stress in solid epithelial tissues. We show that this feedback loop induces an isotropic–nematic transition, leading to an ordered solid state that exhibits soft elasticity. Further increasing activity drives collective self-yielding, leading to tissue flows that are correlated across the entire system. This remarkable state, that we dub plastic nematic solid, is uniquely suited to facilitate active tissue remodeling during morphogenesis. It fundamentally differs from the well-studied fluid regime where macroscopic elastic stresses vanish and the velocity correlation length remains finite, controlled by activity. Altogether, our results reveal a rich spectrum of tissue states jointly governed by activity and passive cell deformability, with important implications for understanding tissue mechanics and morphogenesis.

BP 37.11 Fri 12:15 BAR/0106

Neuromechanics of peristalsis — •Sifan Yin[1], Suraj Shankar[2], and Lakshminarayanan Mahadevan[3] — [1]MPI-PKS, Dresden, Germany — [2]University of Michigan, Ann Arbor, MI, US — [3]Harvard University, Cambridge, MA, US

The peristalsis of cylindrical-shaped organisms or organs is driven by the propagation of rhythmic waves of contraction and relaxation along the tube wall. These waves are generated by coupled interactions of neural control, mechanotransduction, and active muscular contraction. Here, we propose a minimal neuromechanical model for spontaneously coordinated peristaltic waves by locally coupling the neuro-muscular dynamics to the mechanics of an active elastic tube, such as the Nematostella body, the gastro-intestinal tract, and the ureters. We analyze our model using a combination of analytical and numerical methods to investigate the nucleation, propagation and extinction of pulse, and the transi-

tions between disordered twitching and coordinated traveling waves. Our theory naturally elucidates how the interactions among mechanics and neural activities can give rise to coordinated peristaltic motion without any center pattern generator (CPG). This work can supplement ways to robustly design robotics with neural feedback and help to understand early peristaltic wave generation before CPG formation, especially in early embryonic development.

BP 37.12 Fri 12:30 BAR/0106

Muscle growth by sarcomere divisions — Clement Rodier[1], Ian D. Estabrook[2,3], Frank Schnorrer[1], and •Benjamin M. Friedrich[2] — [1]IBDM, Marseilles, France — [2]EXC Physics of Life, TU Dresden, Germany — [3]EMBL, Heidelberg, Germany

The sarcomere is the elementary contractile unit of muscles. Sarcomeres are organized into highly regular periodic chains termed myofibrils, which span the millimeter-length of muscle cells. During development, new sarcomeres are added to mechanically tensed myofibrils as muscle cells increase in length. Yet, how muscles add new sarcomeres to facilitate muscle growth remained elusive. Using live imaging and high-throughput image analysis of the Drosophila flight muscle, we identified a new mechanism of tension-driven sarcomere addition where individual sarcomeres divide along the myofibril tension axis into daughter sarcomeres. Thereby, new sarcomeres can be inserted into contractile myofibrils without compromising their mechanical integrity. A similar mechanism may apply in vertebrate muscle development and regeneration.

[1] Rodier et al. Sci. Adv. 11(28), 2025

BP 38: Active Matter VI (joint session DY/BP)

Time: Friday 9:30–12:15 Location: ZEU/0160

See DY 62 for details of this session.

BP 39: Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates III (joint session CPP/BP)

Time: Friday 9:30–11:15 Location: ZEU/0260

Topical Talk BP 39.1 Fri 9:30 ZEU/0260

Data-driven modelling of phase-separating intrinsically disordered regions — •Giulio Tesei[1,2], Fatima Kamal Zaidi[3], Shanlong Li[4], Julian O. Streit[1], Jianhan Chen[4], Tanja Mittag[3], and Kresten Lindorff-Larsen[1] — [1]Department of Biology, University of Copenhagen, Copenhagen, Denmark — [2]Department of Biomedical Science, Malmö University, Malmö, Sweden — [3]Department of Structural Biology, St. Jude Children's Research Hospital, Memphis, U.S.A. — [4]Department of Chemistry, University of Massachusetts, Amherst, U.S.A.

Intrinsically disordered regions (IDRs) constitute about one third of the human proteome and play important roles in biological processes. While lacking well-defined 3D structures, IDRs adopt heterogeneous ensembles influenced by multivalent interactions; these same interactions can promote phase separation and contribute to the formation of biomolecular condensates. I will first present CALVADOS, an efficient one-bead-per-residue model optimized on experimental data reporting on IDR conformational properties and extensively validated on both single-chain and phase behavior across diverse sequences. I will then describe how we used large sets of CALVADOS simulations to train machine-learning models that accurately predict single-chain compaction and homotypic phase-separation propensity directly from sequence. Finally, I will introduce a hybrid-resolution model with an atomistic backbone representation that matches the accuracy of CALVADOS for global dimensions and phase separation while also capturing local structure and backbone hydrogen bonding.

BP 39.2 Fri 10:00 ZEU/0260

Born to Condense: Polysomes Drive Co-Translational Condensation of Biomolecular Condensate Proteins — •Zhouyi He, Jens-Uwe Sommer, and Tyler Harmon — Leibniz Institute of Polymer Research, 01069, Dresden, Germany

Biomolecular condensates formed by protein LLPS are ubiquitous and crucial in cells. While the physics and functions of LLPS are well studied, its interplay with protein synthesis, translation, remains largely unexplored. Here we propose Co-Translational Condensation (CTC), a mechanism in which nascent protein chains of polysomes, multiple ribosomes on one mRNA, interact with condensates, localizing translation to condensate surfaces. Using coarse-grained simulations, we show that protein domain architecture dictates the extend of CTC, consistent with a Langmuir adsorption model. Bioinformatic analysis reveals that most condensate-associated proteins have architectures favoring CTC, with strong interaction regions of nascent chains exposed on polysomes. Dynamically, simulation and reaction-diffusion modeling reveal that CTC is kinetically feasible within typical polysome lifetimes, either through large polysomes nucleating new condensates or via diffusion to pre-existing condensates. As a case study, we demonstrate that CTC enhances post-translational modifications by minimizing unmodified intermediates. More broadly, we anticipate CTC may also influence protein folding, misfolding, and signal-integration latency. Together, our results establish CTC as a general mechanism coupling translation with phase separation, with broad implications for protein evolution, cellular organization, and synthetic biology.

BP 39.3 Fri 10:15 ZEU/0260

Local RNA/protein stoichiometry tunes the electrostatic microenvironment inside reconstituted multicomponent condensates — •Patrick M. McCall — Leibniz Institute for Polymer Research Dresden, Dresden, DE

Biomolecular condensates are demixed phases of biopolymers and, in living cells, commonly form through the associative phase separation of strongly-charged nucleic acids together with protein polyampholytes carrying a weak net charge. While condensates are proposed to offer distinct aqueous environments for the organization of cellular biochemistry, it remains unclear which physical aspects of the microenvironment are relevant and how widely they can vary between condensates. Motivated by the large asymmetry in structural charge between typical condensate components such as RNAs and RNA-binding proteins, we explore here the implications of electroneutrality on the electrostatic environment within model multicomponent condensates. Combining classical Donnan theory with recent measurements of the macromolecular composition of condensates reconstituted from full-length FUS protein and a homopolymeric RNA [McCall et al Nat Chem 2025], we compute the partitioning of salt ions as well as the Donnan potential across the phase boundary. We find that RNA/FUS stoichiometry tunes both co-ion exclusions over a wide range and is coupled to a pH jump across droplet interface. We also find that co-ion exclusion is suppressed by counter-ion condensation and enhanced by non-ideality of un-bound ions. These results provide insight into the range of ionic conditions accessible to a prominent class of biomolecular condensate.

BP 39.4 Fri 10:30 ZEU/0260

Coarse-grained model to study the effects of electric fields on protein interactions — •Agaya Johnson[1], Debes Ray[2,4], Mahnoush Madani[3], Jan Dhont[2,3], Florian Platten[2,3], Kyongok Kang[2], and Sofia Kantorovich[1] — [1]University of Vienna, Kolingasse 14-16, 1090, Vienna, Austria. — [2]nstitute of Biological Information Processing IBI-4, Forschungszentrum Jülich, 52428 Jülich, Germany. — [3]Faculty of Mathematics and Natural Sciences, Heinrich Heine University Düsseldorf, 40225 Düsseldorf, Germany. — [4]Solid State Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400085, India.

Proteins can undergo transition between a wide range of organisational states, from soluble monomers to disordered phases and ordered structures. Experiments have shown that lysozyme in sodium thiocyanate solution can form homogeneous, crystalline, or liquid phases depending on the salt and protein concentrations, and that these phase boundaries can be shifted by applying an electric field. We present a coarse-grained model of lysozyme in sodium thiocyanate solution, representing the protein as an ellipsoid decorated with charged and adhesive surface patches. Counterions and monovalent salt are treated explicitly via excluded-volume repulsion and Coulombic interactions. We investigate (i) how patch size and salt*patch interactions influence ion distributions around a single protein, with and without an external electric field, and (ii) the resulting effective interactions between two proteins as functions of patch properties, salt concentration, and applied electric field.

BP 39.5 Fri 10:45 ZEU/0260

Entropic Clustering of Stickers Induces Aging in Biocondensates — •Hugo Le Roy[1] and Paolo De Los Rios[2] — [1]Department of Civil, Chemical and Environmental Engineering, University of Genoa, Genoa, Italy — [2]Institute of Physics, Ecole Polytechnique Fédérale de Lausanne

Neurodegenerative conditions, such as Parkinson's disease, results from the aggregation of synaptic proteins such as alpha-synuclein. In a healthy presynaptic neuron, effective neurotransmission relies on the spatial organization of synaptic vesicles within phase-separated droplets. These vesicles release neurotransmitters into the synaptic cleft to activate ion-gated channels on the postsynaptic neuron.

In this work, we investigate how this transmission process is impaired during neurodegeneration. Specifically, we focus on the solidification of these phase-separated droplets, a phenomenon described as aging, leading to protein aggregation and associated with the emergence of pathology. We explore the connection between the mechanical properties of the condensates and their microscopic structure using a minimal physical model that treats complex molecules as stickers and spacers. We show that entropy maximization of spacers leads to an effective attractive force between stickers. As a result, our system displays a surprisingly slow relaxation toward equilibrium, reminiscent of glassy systems and consistent with the liquid-to-solid transition observed in aging droplets. By analyzing the clustering dynamics of stickers, we successfully explain the microscopic origin of this glassy relaxation.

BP 39.6 Fri 11:00 ZEU/0260

Biomolecular condensates with a Twist: From Assembly to Arrest — •Mahesh Yadav[1,2] and Lukas Stelzl[2] — [1]Institute of Physics, Johannes Gutenberg University, Mainz — [2]Institute of Molecular Physiology, Johannes Gutenberg University, Mainz

In this work, we investigate the phase behavior of RNA-binding protein Fused in Sarcoma (FUS), whose multivalent and intrinsically disordered regions drive the formation of biomolecular condensates through liquid-liquid phase separation. FUS is a multi-domain protein with arginine-glycine-rich segments (RG-rich domains) that participate in essential cellular proceses. We examine how characteristic sequence motifs such as RGG.. mediate homotypic and nucleic acid binding, and how targeted point mutations (e.g., RtoK, RtoA) disrupt these motifs and impair condensate formation. Using the thermodynamics phase diagram as a benchmark we highlighted the shift in phase separation propensity of the FUS and its variants. Furthermore, we identify the role of key interactions such as electrostatics, π-π and cation-π in nucleic acid binding at atomistic scale. We further characterized the emergent viscoelastic behavior of FUS condensates at multiple scales. We observe that upon mutations the overall dynamics slows down which reflects the gel-like state. Within the condensate interior, protein chains exhibit sub-diffusive dynamics arising from intermittent binding and viscoelastic resistance, mobility at the interface is further suppressed due to anisotropic interactions and interfacial confinement. To quantify these behaviors across relevant scales, we employ multi-resolution simulation models.

BP 40: Cell Mechanics II / Cytoskeleton II

Time: Friday 10:00–11:15 Location: BAR/0205

BP 40.1 Fri 10:00 BAR/0205

The keratin network adapts the nucleus to cellular strain — •Ruben Haag[1], Ruth Meyer[1], Sascha Lambert[2], Hajaani Manoharan[3], Ulrike Rölleke[1], Jens Konrad[3], Bernd Hoffman[3], Rudolf Merkel[3], Stefan Klumpp[2], and Sarah Köster[1] — [1]Institute for X-Ray Physics, University of Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, University of Göttingen, Germany — [3]Institute of Biological Information Processing, Forschungszentrum Jülich, Germany

Intermediate filaments (IFs) comprise one of the cytoskeletal network types and are cell-type specific. In epithelial cells, the keratin IF network connects the desmosomes in the cell membrane with the perinuclear keratin cage, thus forming a mechanical link from the nucleus to the cell membrane. We now ask whether this link transmits mechanical signals from outside the cell to the nucleus. To answer this question, we stretch both epithelial wild type and keratin knockout cells uniaxially and equibiaxially. During stretching, we image cell nuclei and measure their individual deformation to study the influence of the keratin IF network on them. To understand how the keratin network transmits force to the nucleus, we image the keratin network during cell stretching and create a minimal model to mimic how the keratin network deforms the nucleus. Our results suggest that stretching the keratin network is a two-step process: individual keratin bundles are initially pulled straight and are then stretched. Possibly, by this two-step process, the keratin network adapts the nucleus to cellular strain.

BP 40.2 Fri 10:15 BAR/0205

Improving T cell migration and invasion with the Microtubule destabilizing agent Pretubulysin. — •Lukas Schuster[1], Galia Montalvo[1], Reza Shaebani[1], Anna Burgstaller[2], Shweta Nandakumar[1], Rhoda Hawkins[3], Laura Schaedel[1], Bin Qu[4], and Franziska Lautenschläger[1] — [1]Saarland University, Saarbrücken, Germany — [2]Leibniz Institute for New Materials, Saarbrücken, Germany — [3]School of Mathematical and Physical Sciences, University of Sheffield, Sheffield, United Kingdom — [4]Center for Integrative Physiology and Molecular Medicine (CIPMM), Saarland University, Homburg, Germany & Department of Biomedical Sciences, Osnabrück University, Osnabrück, Germany

The immune response depends on the ability of cytotoxic T lymphocytes (CTLs) to migrate and invade into dense 3D environments, such as tumors, and to kill cancer cells. Thus, optimizing the migratory behavior of CTLs is crucial to boost immune response in the treatment against cancer. Here, we focused on the role of destabilized microtubules (MTs) in cell migration. We showed that the disruption of MTs in CTLs with the compound Pretubulysin enhances the infiltration of 3D collagen gels and the killing of target cells. In addition, we confirmed the motile phenotype in 2D and 1D migration assays. We further studied the mechanism of how MT disruption induces cell motility in a theoretical active droplet model. We found enriched actomyosin in the back of CTLs to be linked to a fast and persistent migrating cell.

BP 40.3 Fri 10:30 BAR/0205

Role of mechanics in early immune recognition — •Kheya Sengupta — CINaM, CNRS, Luminy, France.

Our immune system depends on cell scale forces, which are implicated in various phenomena ranging from migration to recognition of pathology or for potentiating diseased cells for killing. Here the focus will be on the first steps of immune recognition which hinges on formation of bonds between specialised receptors and their specific ligands called antigens, where mechanics and forces are thought to be essential to discriminate our own antigens from those indicative of pathology. Intriguingly, unlike for tissue forming cells, the response of T cells is biphasic with the stiffness of their environment when the interaction is mediated through the T-cell receptors (TCRs). However, when the adhesive ligands of integrins are additionally involved, the cellular response becomes monotonic. Based on a mesoscale model, this ligand-specific response can be attributed to molecular properties of a putative link between the ligand/receptor pair and the cytoskeleton. While the molecules linking integrins and actin are known, the equivalent molecules for TCR are yet to be identified. Our model predicts kinetic and mechanical parameters for this putative link, whose existence we prove by mechanical extraction of membrane tubes. We also measure cell scale forces and show that their spatio-temporal patterns depend on chemistry, mechanics and T cell sub-type. Overall, our findings reinforce the proposition that force application provides a general mechanism for immune cells to discriminate mechanosensitive bonds.

BP 40.4 Fri 10:45 BAR/0205

Investigating the interaction between cardiac fibroblasts using ROCS and fluorescence microscopy — •Arash Felekary and Alexander Rohrbach — IMTEK, University of Freiburg, Germany

Cell-cell interaction is essential for cardiac function. Tunneling nanotubes (TNTs), thin actin-based membrane protrusions, mediate long-range interactions by transporting organelles and signaling molecules. To study their role in cardiac fibroblast (FB) interaction, we combined Rotating Coherent Scattering (ROCS) microscopy with fluorescence imaging. ROCS provides label-free, high-contrast recordings at up to 100 Hz and resolves TNTs and lamellipodia across several micrometers above the substrate. Using this approach, we observed a linear correlation between TNT density and lamellipodia motion velocity. Collagen labeling revealed that TNTs frequently align with collagen fibers, suggesting a structural coupling between ECM-linked TNTs and actin-driven protrusions. These observations motivated a spatially resolved simulation of actin filament polymerization and branching, incorporating integrin*collagen interactions and Arp2/3 activation. The model reproduces the experimentally observed increase in lamellipodial velocity with TNT density and supports a mechanism in which TNTs locally amplify integrin-mediated actin remodeling. In this presentation, we discuss how TNTs, lamellipodia, and ECM components cooperatively guide FB interaction, offering new insight into the structural and mechanical coordination underlying cardiac tissue remodeling.

BP 40.5 Fri 11:00 BAR/0205

How to determine cell property distributions from high-throughput experiments via computer simulations — •Stephan Gekle — Biofluid Simulation and Modeling, Theoretische Physik VI, Universität Bayreuth

A central challenge in computer simulations of living cells is the accurate determination of model parameters based on experimental data. This challenge arises since cell properties such as membrane or cytoplasm viscosities are often difficult or impossible to directly measure in an experiment. The current paradigm in the field is to try to find a single "optimal" value for each such property. This approach completely disregards biological heterogeneity and cell-to-cell variability.

Here, we will present a novel inference method which starts from the assumption that *the* optimal value of a cellular property does not exist and that biological reality must rather be reflected by a *distribution* of values for each cell property. We will show how to obtain such property distributions for a realistic and technologically relevant scenario of disease detection via red blood cell membrane alterations.

For this, we will present boundary-integral simulations of red blood cells passing through a microchannel setup corresponding to real-time deformability cytometry (RT-DC) experiments. We will show how the resulting large amounts of scattered experimental data can be combined with our efficient simulations to infer distributions of cytosol and membrane viscosities in a heterogeneous cell population taking full account of cell-to-cell variability.

BP 41: Franco-German Session: Bacterial Biophysics II

Time: Friday 11:30–12:45 Location: BAR/0205

Invited Talk BP 41.1 Fri 11:30 BAR/0205

Probing spatiotemportal electrochemical dynamics on single bacterial cells — Anaïs Biquet-Bisquert[1], Baptiste Carrio[1], Nathan Meyer[1], Thales Fernandes[1], Manouk Abkarian[1], Farida Seduk[2], Axel Magalon[2], •Ashley Nord[1], and Francesco Pedaci[1] — [1]Centre de Biologie Structurale, Université de Montpellier, CNRS, INSERM. Montpellier, France. — [2]Aix Marseille Université, CNRS, Laboratoire de Chimie Bactérienne (UMR7283), IMM, IM2B, 13402 Marseille, France.

Electrochemical gradients across biological membranes are fundamental to cellular bioenergetics. In bacteria, the proton motive force (PMF) drives critical functions such as ATP synthesis and motility. Although historically regarded as temporally and spatially stable, recent studies have revealed dynamic PMF behaviors at single-cell and community levels, which are implicated in processes like intracellular communication and coordination. The bacterial flagellar motor, a rotary nanomachine directly powered by the PMF, provides a unique and sensitive tool for probing these dynamics. By employing light-activated proton pumps and monitoring changes in flagellar motor activity, we perturb and investigate the PMF at the single-cell level. This approach reveals millisecond-scale temporal fluctuations and rapid lateral homogenization of the PMF, reminiscent of the electrotonic potential spread observed in passive neurons.

BP 41.2 Fri 12:00 BAR/0205

Cable Bacteria as Conductive Interfaces: Towards Scalable, Bacteria-derived Electronics — •Hannah Ferenz[1,2], Rakesh Nair[2], and Hans Kleemann[2] — [1]Sächsisches Landesgymnasium Sankt Afra zu Meißen, 01662 Meißen, Germany — [2]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Technische Universität Dresden, 01187 Dresden, Germany.

Cable bacteria (Electrothecera and Electronema spp.) are multicellular filamentous bacteria that perform centimeter-scale electron transport via parallel conductive fibers embedded in their cell envelope, achieving conductivities up to 30 S cm^-1, rivaling synthetic conjugated polymers. We present a robust bioprocess using controlled oxygen-sulfide gradients in natural sediments to produce mechanically coherent, dense biofilms (>10^5 filaments cm^-2). These living conductive networks self-assemble, remain stable for months in-culture, and self-repair via continued growth after damage.

We demonstrate how these bacterial cultures can be used for the development of bio-derived electrodes based on their inherent nickel-sulfur complexes. These results establish cable bacteria as the first genetically tractable, self-growing biological conductor suitable for integration into transient and sustainable electronics, offering a path toward low-cost, environmentally benign bioelectronic interfaces for sensing, energy harvesting, and wearable devices.

BP 41.3 Fri 12:15 BAR/0205

Biophysics of bacterial survival during starvation — •Severin Schink — LMU München, Fakultät für Biologie

Most bacteria live in nutrient-limited states, yet the physical principles that set their lifespan and govern loss of viability during starvation remain poorly understood. I present a framework that links death dynamics, proteome adaptation and competition under starvation in E. coli.

Using time-lapse microscopy, we show that starving cells maintain a plasmolysed state and typically die via a rapid collapse of ion homeostasis. A coarse-grained model of ion transport maps death to a Kramers-like escape process set by nutrient recycling. The model predicts how death rates scale with permeability, ionic strength and cell geometry, and how modified media extend lifespan by lowering maintenance costs.

Proteome-wide analysis reveals that envelope proteins are key for survival: reallocating proteome into the envelope lowers ion permeability and death rate but constrains growth, generating a trade-off between proliferation and starvation survival. Co-cultures of physiologically distinct populations reveal cross-feed feedback: nutrients released by dying cells are recaptured by survivors, amplifying small differences in maintenance and uptake into large fitness advantages. Together, these results identify a minimal set of physical parameters ion gradients, permeability, recycling yield and uptake capacity that control lifespan and selection under starvation.

BP 41.4 Fri 12:30 BAR/0205

Selective inhibition of microbial methanogenesis - a shortcut toward climate change mitigation — •Benedikt Sabass — TU Dortmund — LMU München

In a world that is increasingly affected by climate change, new solutions are urgently needed to reduce greenhouse gas emissions. One of the most effective measures to limit global warming is to reduce methane emissions, a significant proportion of which is produced in the rumen of cattle. Rumen methanogenesis is a complex process that involves various biochemical pathways and cooperation among species from all three domains of life.

A reduction of methane emissions through feed additives has been shown to be feasible in principle, but effective and economical solutions are not yet available. Here, I present an overview of our research on compounds that selectively inhibit methanogenesis. I summarize existing strategies, describe our in-vitro screening assay, and present results from animal tests. Finally, I outline basic open questions regarding the molecular mechanisms of methanogenesis from a biological physics perspective.

BP 42: Closing Talk (joint session CPP/BP/DY)

Time: Friday 13:15–14:00 Location: HSZ/0002

Invited Talk BP 42.1 Fri 13:15 HSZ/0002

Biomolecular Condensates: Challenges for Polymer Physics — •Jens-Uwe Sommer — Leibniz-Insitut für Polymerforschung Dresden, Bereich Theorie der Polymere,Hohe Straße 6, 01069 Dresden, Germany — TU Dresden, Insitut für Theoretische Physik, Zellescher Weg 17, D-01069 Dresden, Germany

Biomolecular condensates (BMCs) constitute an emerging paradigm in the understanding of biological functions. They shift the focus from individual biochemical processes toward the collective behavior of biopolymers, in which phase-separation mechanisms and intrinsically disordered proteins lacking canonical enzymatic roles play central and often decisive functions. Consequently, universal principles of complex (bio)polymer solutions gain relevance, and several classical questions in the physics of living matter can now be revisited from this polymer-physics perspective. In this talk, I will discuss theoretical approaches and concepts that are based on universal principles, with a particular emphasis on current challenges in the field.

Chemical and Polymer Physics Division
Fachverband Chemische Physik und Polymerphysik (CPP)

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The 2026 Meeting of the CPP Division is marked by the 75th anniversary of the Polymer Physics Division, which is celebrated in the Focus Session "75 Years Division Polymer Physics: From Curiosity to Smart Materials". Two Focus Sessions address the topics "Theoretical Modeling and Simulation of Biomolecular Condensates" and "Water: From Atmosphere to Space". To honor the guest country France, we have organized the following French-German sessions: "Membranes and Porous Materials", "Nanomaterials, Composites and Hybrids", "Simulation Methods and Modeling of Soft Matter", "2D Materials, Thin Films and Interfaces" as well as a Round Table Discussion "The Future of Neutrons in France and Germany". Plenary speakers include Peter Müller-Buschbaum, Hugues Chaté, Antony Hyman, and Annabella Selloni. The former chairman of the CPP Division, Kurt Kremer, is this year's awardee of the Max Planck Medal. The CPP Division supports the Symposia "The Sustainability Challenge: A Decade of Transformation" and "Fluids with Broken Time-Reversal Symmetry: Odd/Hall Viscosity between Active Matter and Electron Flows" as well as the French-German Symposium "Soft, Active and Alive: Emergent Properties in Living Matter". The Meeting concludes with a Highlighted Invited Talk given by Jens-Uwe Sommer.

Overview of Invited Talks and Sessions

(Lecture halls ZEU/LICH, ZEU/0255, ZEU/0260, and HÜL/S386; Poster P5)

Invited Talks

CPP 3.1	Mon	9:30–10:00	ZEU/LICH	**Theory and Modeling of Fluid Adsorption and Transport in Nanoporous Materials** — •Benoit Coasne
CPP 4.1	Mon	9:30–10:00	ZEU/0255	**Exploration of Cathode Materials for Li-S Batteries** — •Yan Lu
CPP 5.1	Mon	9:30–10:00	ZEU/0260	**Cleaning of dusty surfaces** — •Doris Vollmer, Franziska Sabath, Abhinav Naga, Stefanie Kirschner, Tarik Karakaya, Rüdiger Berger, Hans-Jürgen Butt, Halim Kusumaatmaja
CPP 6.1	Mon	11:15–11:45	ZEU/LICH	**Hierarchical Porosity Meets Nanoconfined Water: Toward Water-Driven Functional Materials** — •Patrick Huber
CPP 9.1	Mon	15:00–15:30	ZEU/LICH	**Why Polymers Swell or Collapse: Molecular Insights into Cosolute Effects** — •Nico van der Vegt
CPP 12.1	Mon	15:00–15:30	ZEU/0255	**Multifunctional films by tailoring chemistry and morphology of polymer brushes at the nanoscale** — •Petra Uhlmann, Alexander S. Münch
CPP 12.6	Mon	16:30–17:00	ZEU/0255	**Thin-film and interface properties in energy conversion devices unveiled by X-rays** — •Marcus Bär
CPP 13.1	Mon	15:00–15:30	ZEU/0260	**Modelling and simulation of pH-sensitive polyelectrolyte microgels** — •Stefanie Schneider
CPP 16.1	Mon	17:15–17:45	ZEU/0260	**Understanding the Passivation Properties of Solid Electrolyte Interphases (SEIs) in Batteries: Generator-Collector Experiments combined with a Transport and Reaction Model** — •Bernhard Roling, Falk Krauss, Annalena Duncker, Isabel Pantenburg
CPP 21.1	Tue	9:30–10:00	ZEU/0255	**Molecular modelling of gas solubility and free volume trends in Si-functionalized ionic liquids** — •Kateryna Goloviznina, Eduards Bakis, Inês C. M. Vaz, Agilio Padua, Margarida Costa Gomes
CPP 22.1	Tue	9:30–10:00	ZEU/0260	**From Solution to Thin Films: Structure Formation Pathways in Organic Photovoltaic Films** — •Eva M. Herzig
CPP 26.1	Tue	14:00–14:30	HÜL/S386	**Investigating lignin graphitisation depending on botanical source and extraction method** — Lucie Dieval, Phuthiphong Ouitrakoon, Robert Hunter, Sébastien Schaefer, Louis Hennet, Erik Elkaim, Julie Ruellou, Milo S. P. Shaffer, Agnieszka Brandt-Talbot, •Pascale Launois

CPP 30.1	Tue	14:00–14:30	ZEU/0260	**Solvent effects on amphiphile self-assembly in Deep Eutectic Solvents** — •Karen Edler
CPP 31.1	Wed	9:30–10:00	ZEU/0255	**Hydrogels with a Pinch of Embodied Intelligence** — •Andreas Walther
CPP 33.1	Wed	10:00–10:30	ZEU/LICH	**Shape-induced superstructure formation in concentrated ferrofluids** — •Sabrina Disch
CPP 37.1	Wed	15:00–15:30	ZEU/LICH	**Predicting molecular ordering in deposited molecular films** — •Denis Adrienko
CPP 38.1	Wed	15:00–15:30	ZEU/0255	**Engineering, processing and application of recombinant spider silk proteins** — •Thomas Scheibel
CPP 39.1	Wed	15:00–15:30	ZEU/0260	**A polarizable model for atomistic simulations of metals and graphitic material/liquid interfaces** — Krishan Kanhaiya, Hendrik Heinz, •Marialore Sulpizi
CPP 42.1	Wed	17:00–17:30	ZEU/0260	**Mesopores filled with (poly)ionic liquids: phase transitions under confinement, and structure seen by SAXS and SANS** — •Julian Oberdisse, Anne-Caroline Genix
CPP 44.1	Thu	9:30–10:00	ZEU/LICH	**Shedding light on wide bandgap perovskites** — •Michael Saliba
CPP 53.1	Fri	9:30–10:00	ZEU/LICH	**Limits and Prospects of Organic Solar Cells** — •Dieter Neher
CPP 54.1	Fri	9:30–10:00	ZEU/0255	**NMR-based molecular rheology and structural characterization of model gels** — •Kay Saalwächter, Bidit Lamsal
CPP 56.1	Fri	10:45–11:15	HÜL/S386	**Liquid Dynamics at Interfaces** — •Michael Vogel
CPP 61.1	Fri	13:15–14:00	HSZ/0002	**Biomolecular Condensates: Challenges for Polymer Physics** — •Jens-Uwe Sommer

Topical Talks

CPP 19.1	Tue	9:30–10:00	ZEU/LICH	**Surface adsorption and protonation equilibrium of atmospheric organics at the aqueous surface** — •Nønne Prisle
CPP 27.1	Tue	14:00–14:30	ZEU/LICH	**Why water in plants survives negative pressure** — Marin Šako, Emanuel Schneck, Roland Netz, •Matej Kanduč
CPP 32.1	Wed	9:30–10:00	ZEU/0260	**Synchrotron X-Ray Studies on Structural Transitions in Water and Alcohol containing Ice Analogues** — •Christina M. Tonauer
CPP 45.1	Thu	9:30–10:00	ZEU/0260	**Wetting transitions in biomolecular coacervates** — •Susanne Liese, Tiemei Lu, Evan Spruijt, Christoph Weber
CPP 51.1	Thu	15:15–15:45	ZEU/LICH	**The Loops of Life** — Brian Chan, •Michael Rubinstein
CPP 51.2	Thu	15:45–16:15	ZEU/LICH	**Polyelectrolytes and Biological Systems: A Charged Relationship** — •Matthias Ballauff
CPP 51.3	Thu	16:15–16:45	ZEU/LICH	**From block copolymer morphologies to functional polymer membranes** — •Volker Abetz
CPP 51.4	Thu	16:45–17:15	ZEU/LICH	**Molecular electronic materials and devices for solar energy conversion** — •Jenny Nelson
CPP 51.5	Thu	17:15–17:45	ZEU/LICH	**Control of cell and tissue stiffness by biopolymer networks and particle inclusions** — •Paul Janmey
CPP 55.1	Fri	9:30–10:00	ZEU/0260	**Data-driven modelling of phase-separating intrinsically disordered regions** — •Giulio Tesei, Fatima Kamal Zaidi, Shanlong Li, Julian O. Streit, Jianhan Chen, Tanja Mittag, Kresten Lindorff-Larsen

Discussion on Sustainability on Monday during Lunch Break

PSV I	Mon	13:00–13:45	HSZ/AUDI	**Sustainability! And now? – Opportunities for young researchers** — •Roxana Scharpegge, Hiroki Sayama, Thomas Schubatzky, Birte Höcker, Uwe Riedel, John Plane, Pauleo Nimtz, Stefanie Falk

Invited Talks of the joint Symposium SKM Dissertation Prize 2026 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	HSZ/0002	**Stochastic-Calculus Approach to Non-equilibrium Statistical Physics** — •Cai Dieball
SYSD 1.2	Mon	10:00–10:30	HSZ/0002	**Nonuniform magnetic spin textures for sensing, storage and computing applications** — •Sabri Koraltan
SYSD 1.3	Mon	10:30–11:00	HSZ/0002	**Anomalous Quantum Oscillations beyond Onsager's Fermi Surface Paradigm** — •Valentin Leeb

SYSD 1.4	Mon	11:00–11:30	HSZ/0002	**Coherent Control Schemes for Semiconductor Quantum Systems** — •Eva Schöll
SYSD 1.5	Mon	11:30–12:00	HSZ/0002	**On stochastic thermodynamics under incomplete information: Thermodynamic inference from Markovian events** — •Jann van der Meer

Invited Talks of the joint Symposium The Sustainability Challenge: A Decade of Transformation (SYSC)

See SYSC for the full program of the symposium.

SYSC 1.1	Mon	15:00–15:30	HSZ/AUDI	**Open-Endedness and Community-Based Approaches to Sustainability Challenges** — •Hiroki Sayama
SYSC 1.2	Mon	15:30–16:00	HSZ/AUDI	**Education as a Social Tipping Element: Evidence from Climate and Physics Education Research** — •Thomas Schubatzky
SYSC 1.3	Mon	16:00–16:30	HSZ/AUDI	**Mechanistic and Material Perspectives on Enzymatic Hydrolysis of Semicrystalline Polyesters** — •Birte Höcker
SYSC 1.4	Mon	16:45–17:15	HSZ/AUDI	**Decarbonization Options for Industry** — •Uwe Riedel
SYSC 1.5	Mon	17:15–17:45	HSZ/AUDI	**Impacts of Cosmic Dust and Space Debris in the Terrestrial Atmosphere** — •John Plane

Invited Talks of the joint Symposium Fluids with Broken Time-Reversal Symmetry: Odd/Hall Viscosity between Active Matter and Electron Flows (SYBS)

See SYBS for the full program of the symposium.

SYBS 1.1	Tue	9:30–10:00	HSZ/AUDI	**Odd viscosity in three-dimensional fluids: flows, wakes, and eddies** — •Tali Khain
SYBS 1.2	Tue	10:00–10:30	HSZ/AUDI	**Odd viscosity in two-dimensional hydrodynamic electron transport** — •Igor Gornyi, Dmitry Polyakov
SYBS 1.3	Tue	10:30–11:00	HSZ/AUDI	**Odd slip on chiral active surfaces** — •Andrej Vilfan, Yuto Hosaka
SYBS 1.4	Tue	11:15–11:30	HSZ/AUDI	**Parity-odd transport in electron fluids** — •Johanna Erdmenger
SYBS 1.5	Tue	11:30–11:45	HSZ/AUDI	**Curved Odd Elasticity** — Lazaros Tsaloukidis, Yuan Zhou, Jack Binysh, Nikta Fakhri, Corentin Coulais, •Piotr Surówka

Invited Talks of the joint Symposium France: Soft, Active and Alive: Emergent Properties in Living Matter (SYGF)

See SYGF for the full program of the symposium.

SYGF 1.1	Wed	15:00–15:30	HSZ/AUDI	**Liquid crystal geometries in type I collagen-based tissues** — •Nadine Nassif
SYGF 1.2	Wed	15:30–16:00	HSZ/AUDI	**Self-organization of the cytoplasm by physical instabilities** — •Jan Brugues
SYGF 1.3	Wed	16:00–16:30	HSZ/AUDI	**From morphogenesis to space partitioning by microtubules and molecular motors.** — •Manuel Thery
SYGF 1.4	Wed	16:45–17:15	HSZ/AUDI	**More than the sum: how composite interfaces govern function** — •Alba Diz-Muñoz
SYGF 1.5	Wed	17:15–17:45	HSZ/AUDI	**Swimming and Swarming of Intelligent Active Particles** — Segun Goh, Priyanka Iyer, Rajendra Singh Negi, •Gerhard Gompper
SYGF 1.6	Wed	17:45–18:15	HSZ/AUDI	**Perturbing the collective motion of fish with challenging environments** — •Aurélie Dupont

Sessions

CPP 1.1–1.11	Mon	9:30–12:45	BAR/SCHÖ	**Active Matter I (joint session BP/CPP/DY)**
CPP 2.1–2.4	Mon	9:30–10:30	MER/0002	**Sustainability: Challenges and Solutions (joint session UP/CPP/SOE)**
CPP 3.1–3.5	Mon	9:30–11:00	ZEU/LICH	**French-German Session: Membranes and Porous Materials I**
CPP 4.1–4.6	Mon	9:30–11:15	ZEU/0255	**Energy Storage Materials and Devices I**
CPP 5.1–5.5	Mon	9:30–11:00	ZEU/0260	**Wetting, Fluidics and Liquids at Interfaces and Surfaces I (joint session CPP/DY)**
CPP 6.1–6.5	Mon	11:15–12:45	ZEU/LICH	**French-German Session: Membranes and Porous Materials II**
CPP 7.1–7.5	Mon	11:30–12:45	ZEU/0255	**Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods I**

CPP 8.1–8.5	Mon	11:30–12:45	ZEU/0260	**Wetting, Fluidics and Liquids at Interfaces and Surfaces II (joint session CPP/DY)**
CPP 9.1–9.7	Mon	15:00–17:00	ZEU/LICH	**French-German Session: Simulation Methods and Modeling of Soft Matter I**
CPP 10.1–10.13	Mon	15:00–18:30	ZEU/0118	**Droplets, Wetting, and Microfluidics (joint session DY/CPP)**
CPP 11.1–11.12	Mon	15:00–18:30	ZEU/0160	**Active Matter II (joint session DY/BP/CPP)**
CPP 12.1–12.6	Mon	15:00–17:00	ZEU/0255	**French-German Session: 2D Materials, Thin Films and Interfaces I**
CPP 13.1–13.7	Mon	15:00–17:00	ZEU/0260	**Charged Soft Matter, Polyelectrolytes and Ionic Liquids**
CPP 14.1–14.7	Mon	17:15–19:00	ZEU/LICH	**French-German Session: Simulation Methods and Modeling of Soft Matter II**
CPP 15.1–15.7	Mon	17:15–19:00	ZEU/0255	**Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods II**
CPP 16.1–16.6	Mon	17:15–19:00	ZEU/0260	**Energy Storage Materials and Devices II**
CPP 17.1–17.51	Mon	19:00–21:00	P5	**Poster I**
CPP 18.1–18.12	Tue	9:30–12:45	BAR/SCHÖ	**Active Matter III (joint session BP/CPP/DY)**
CPP 19.1–19.5	Tue	9:30–11:00	ZEU/LICH	**Focus Session: Water – from Atmosphere to Space I (joint session CPP/DY)**
CPP 20.1–20.12	Tue	9:30–12:45	ZEU/0160	**Complex Fluids and Soft Matter (joint session DY/CPP)**
CPP 21.1–21.6	Tue	9:30–11:15	ZEU/0255	**French-German Session: Simulation Methods and Modeling of Soft Matter III**
CPP 22.1–22.6	Tue	9:30–11:15	ZEU/0260	**Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics I**
CPP 23.1–23.6	Tue	11:15–12:45	ZEU/LICH	**Focus Session: Water – from Atmosphere to Space II (joint session CPP/DY)**
CPP 24.1–24.5	Tue	11:30–12:45	ZEU/0255	**French-German Session: Simulation Methods and Modeling of Soft Matter IV**
CPP 25.1–25.5	Tue	11:30–12:45	ZEU/0260	**Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics II**
CPP 26.1–26.5	Tue	14:00–15:30	HÜL/S386	**French-German Session: 2D Materials, Thin Films and Interfaces II**
CPP 27.1–27.5	Tue	14:00–15:30	ZEU/LICH	**Focus Session: Water – from Atmosphere to Space III (joint session CPP/DY)**
CPP 28.1–28.5	Tue	14:00–15:30	ZEU/0160	**Active Matter IV (joint session DY/BP/CPP)**
CPP 29.1–29.6	Tue	14:00–15:30	ZEU/0255	**Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods III**
CPP 30.1–30.5	Tue	14:00–15:30	ZEU/0260	**Complex Fluids, Colloids, Micelles and Vesicles I**
CPP 31.1–31.7	Wed	9:30–11:30	ZEU/0255	**Responsive and Adaptive Systems**
CPP 32.1–32.4	Wed	9:30–10:45	ZEU/0260	**Focus Session: Water – from Atmosphere to Space IV (joint session CPP/DY)**
CPP 33.1–33.4	Wed	10:00–11:15	ZEU/LICH	**Complex Fluids, Colloids, Micelles and Vesicles II**
CPP 34.1–34.4	Wed	11:00–12:00	ZEU/0260	**Focus Session: Water – from Atmosphere to Space V (joint session CPP/DY)**
CPP 35.1–35.5	Wed	11:15–12:45	ZEU/0118	**Glasses and Glass Transition (joint session DY/CPP)**
CPP 36.1–36.1	Wed	11:45–12:45	ZEU/LICH	**Round Table Discussion: The Future of Neutrons in France and Germany (joint session CPP/BP)**
CPP 37.1–37.6	Wed	15:00–16:45	ZEU/LICH	**Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics III**
CPP 38.1–38.6	Wed	15:00–16:45	ZEU/0255	**Biopolymers, Biomaterials and Bioinspired Functional Materials I (joint session CPP/BP)**
CPP 39.1–39.6	Wed	15:00–16:45	ZEU/0260	**French-German Session: Nanomaterials, Composites and Hybrids I**
CPP 40.1–40.6	Wed	17:00–18:30	ZEU/LICH	**Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics IV**
CPP 41.1–41.7	Wed	17:00–18:45	ZEU/0255	**Biopolymers, Biomaterials and Bioinspired Functional Materials II (joint session CPP/BP)**
CPP 42.1–42.6	Wed	17:00–18:45	ZEU/0260	**French-German Session: Nanomaterials, Composites and Hybrids II**
CPP 43.1–43.11	Thu	9:30–12:45	BAR/SCHÖ	**Biomaterials and Biopolymers (joint session BP/CPP)**
CPP 44.1–44.6	Thu	9:30–11:15	ZEU/LICH	**Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics V**
CPP 45.1–45.6	Thu	9:30–11:15	ZEU/0260	**Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates I (joint session CPP/BP)**
CPP 46.1–46.66	Thu	9:30–11:30	P5	**Poster II**
CPP 47.1–47.7	Thu	10:15–12:45	BAR/0106	**Focus Session: Controlling Microparticles and Biological Cells by Ultrasound (joint session BP/CPP/DY)**
CPP 48.1–48.5	Thu	11:30–12:45	ZEU/LICH	**Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics VI**
CPP 49.1–49.5	Thu	11:30–12:45	ZEU/0255	**Gels, Polymer Networks and Elastomers I**
CPP 50.1–50.5	Thu	11:30–12:45	ZEU/0260	**Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates II (joint session CPP/BP)**
CPP 51.1–51.5	Thu	15:15–17:45	ZEU/LICH	**Focus Session: 75 Years Polymer Physics Division: From Curiosity to Smart Materials (joint session CPP/BP)**

CPP 52	Thu	18:00–19:00	ZEU/LICH	**Members' Assembly**
CPP 53.1–53.6	Fri	9:30–11:15	ZEU/LICH	**Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics VII**
CPP 54.1–54.6	Fri	9:30–11:15	ZEU/0255	**Gels, Polymer Networks and Elastomers II**
CPP 55.1–55.6	Fri	9:30–11:15	ZEU/0260	**Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates III (joint session CPP/BP)**
CPP 56.1–56.4	Fri	10:45–12:00	HÜL/S386	**Molecular and Polymer Dynamics, Friction and Rheology I**
CPP 57.1–57.6	Fri	11:30–13:00	ZEU/LICH	**Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics VIII**
CPP 58.1–58.6	Fri	11:30–13:00	ZEU/0255	**Gels, Polymer Networks and Elastomers III**
CPP 59.1–59.6	Fri	11:30–13:00	ZEU/0260	**Crystallization**
CPP 60.1–60.3	Fri	12:15–13:00	HÜL/S386	**Molecular and Polymer Dynamics, Friction and Rheology II**
CPP 61.1–61.1	Fri	13:15–14:00	HSZ/0002	**Closing Talk (joint session CPP/BP/DY)**

Members' Assembly of the Chemical and Polymer Physics Division

Thursday 18:00–19:00 Raum ZEU/LICH

- Report of the current speakers
- Election of the second deputy speaker
- Award of the poster prize of the CPP Division
- Miscellaneous

Sessions

– Invited, Topical, Contributed Talks, Discussions, and Posters –

CPP 1: Active Matter I (joint session BP/CPP/DY)

Time: Monday 9:30–12:45 Location: BAR/SCHÖ

CPP 1.1 Mon 9:30 BAR/SCHÖ

Bayesian inference of magnetosensing in a magnetotactic bacterium — •Sascha Lambert[1], Emilie Gachon[2], Damien Faivre[2], and Stefan Klumpp[1] — [1]University of Göttingen, Institute for the Dynamics of Complex Systems, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany. — [2]Aix Marseille Université, CEA, CNRS, BIAM, 13115 Saint-Paul-Lez-Durance, France.

Magnetotactic bacteria are often assumed to align only passively with external magnetic fields, yet recent observations of the magnetotactic bacterium SS-5 reveal a pronounced increase in swimming speed under geomagnetic conditions. Because flagellated microorganisms typically follow helical paths, magnetic torques could, in principle, straighten their trajectories and create an apparent increase in speed, offering a purely mechanical explanation. We test this hypothesis using a physical swimming model based on Active Brownian Particles that incorporates magnetic torques, rotational propulsion, and helical motion, and we explore the relevant parameter space using Bayesian inference constrained by three-dimensional trajectory data. Posterior predictive simulations demonstrate that the mechanically induced increase in apparent speed is far too small to account for the experimental observations, even under extreme parameter choices. The results quantitatively rule out swaying as a sufficient explanation for the behaviour of SS-5 and instead support the presence of an active magnetic sensing mechanism.

CPP 1.2 Mon 9:45 BAR/SCHÖ

Vorticity-induced surfing and trapping in porous media — •Pallabi Das[1], Mirko Residori[1], Axel Voigt[2,3,4], Suvendu Mandal[5], and Christina Kurzthaler[1,3,4] — [1]Max Planck Institute for the Physics of Complex Systems, Germany — [2]Institute of Scientific Computing, TU Dresden, Germany — [3]Center for Systems Biology Dresden, Germany — [4]Cluster of Excellence, Physics of Life, TU Dresden, Germany — [5]TU Darmstadt, Germany

Microorganisms often encounter strong confinement and complex hydrodynamic flows while navigating their habitats. Combining finite-element methods and stochastic simulations, we study the interplay of active transport and heterogeneous flows in dense porous channels. We find that swimming always slows down the traversal of agents across the channel, giving rise to robust power-law tails of their exit-time distributions. These exit-time distributions collapse onto a universal master curve with a scaling exponent of $\approx 3/2$ across a wide range of packing fractions and motility parameters, which can be rationalized by a scaling relation. We further identify a new motility pattern where agents alternate between *trapping* along fast streams and extended *surfing* phases, the latter determining the power-law exponent. Unexpectedly, trapping occurs in the flow backbone itself – not only at obstacle boundaries – due to vorticity-induced reorientation in the highly-heterogeneous flow environment. These findings provide a fundamentally new active transport mechanism with direct implications for biofilm clogging and the design of novel microrobots capable of operating in heterogeneous media.

CPP 1.3 Mon 10:00 BAR/SCHÖ

Adhesion Patterns in Gliding Filamentous Cyanobacteria — •Elias Fischer[1], Paul Nieschwitz[2], Stefan Karpitschka[2], and Holger Stark[1] — [1]Institute of Physics and Astronomy, TU Berlin, Germany — [2]Department of Physics, Universität Konstanz, Germany

Filamentous cyanobacteria play an important role in many ecosystems and the carbon cycle of our planet. They exhibit gliding motility when in contact with solid surfaces or each other. Despite their ecological relevance and increased use in biotech applications, the exact nature of the force-generating process remains not fully understood.

Our recent measurements of filamentous cyanobacteria gliding across flat surfaces and visualized in kymographs show spatio-temporal adhesion regions along the filament, indicating an intrinsic helical shape. Based on our a novel approach for modeling the mechanical aspects of individual cyanobacteria filaments, we are able to interpret the complex kymograph patterns. Each filament is modeled as a helical chain of thin cylindrical segments in 3D with bending and twisting elasticity. The filaments interact with nearby surfaces and filaments via a hard-core repulsion and an exponentially decaying adhesion force. Importantly, the propulsion forces that push the filament forward are only applied locally at surface-contacting segments.

Our simulated kymographs reveal how both the helical shape and the adhesion strength strongly influence the filament's gliding speed and the dynamics of the surface-attachment regions. Thereby, we crucially contribute to the understanding of how real filamentous cyanobacteria generate their propulsion forces.

CPP 1.4 Mon 10:15 BAR/SCHÖ

The 3D chirality of malaria parasites determines their motion patterns in 2D and originates at the apical pole — •Leon Lettermann[1], Mirko Singer[2], Smilla Steinbrück[2,3], Falko Ziebert[1], Sachie Kanatani[3], Photini Sinnis[3], Friedrich Frischknecht[2], and Ulrich Schwarz[1] — [1]Institute for Theoretical Physics & BioQuant, Heidelberg University — [2]Parasitology, Center for Infectious Diseases, Heidelberg University — [3]School of Public Health and Malaria Research Institute, Johns Hopkins University

Plasmodium sporozoites, the slender forms of the malaria parasite injected by mosquitoes into the skins of their vertebrate hosts, provide a medically highly relevant model system for active chiral particles. Using 3D tracking in synthetic hydrogels, we show that sporozoites consistently move on right-handed helical trajectories. When they encounter a two-dimensional substrate, they switch to clockwise circular motion, whereas circling on glass in medium occurs with the opposite sense of rotation, suggesting on glass they try to invade the medium above. Using a sandwich assay, we demonstrate that chirality also determines the reverse transition from two-dimensional to three-dimensional motion. Combining these measurements with a theory for gliding motility allows us to identify the likely origin of chirality, namely an asymmetric distribution of adhesins. After confirming this via two-sided traction force microscopy, we finally use STED super-resolution microscopy to reveal a corresponding tilt in the apical ring complex. In summary, our analysis thus uncovers both the biological relevance and the molecular basis of chirality in the movement of malaria parasites.

CPP 1.5 Mon 10:30 BAR/SCHÖ

Squirmer dynamics in porous environments — •Mirko Residori[1], Christina Kurzthaler[1], and Sebastian Aland[2] — [1]Max Planck Institute for the Physics of Complex Systems — [2]TU Freiberg

We introduce a computational framework for simulating the dynamics of microswimmers in complex porous environments. Specifically, we adopt a diffusive domain approach to represent the surface of a micro-swimmer, modeled as a squirmer. This method ensures accurate and stable finite-element simulations, even in highly confined geometries. Validation against analytical and numerical benchmarks confirms the model*s accuracy and robustness. We then apply it to explore squirmer motion in heterogeneous porous media, revealing how hydrodynamic interactions lead to behaviors such as dynamic trapping due to hydro-dynamically induced re-orientations. Moreover, we demonstrate that the squirmer parameter and the repulsive potential critically influence a squirmer's ability to navigate and escape confinement. The proposed framework offers a versatile and efficient tool for studying active motion in complex fluids and provides new insights into micro-swimmer transport and control in natural and engineered systems.

CPP 1.6 Mon 10:45 BAR/SCHÖ

Dynamics of passive tracers in active dumbbell suspension — •Chandranshu Tiwari and Sunil P. Singh — Department of Physics, Indian Institute of Science Education and Research, Bhopal 462066, India.

The transport of passive tracers in active fluids exhibits rich dynamics arising from persistent interactions between active agents and the tracer. In our work, we employ Brownian dynamics simulations to investigate the dynamical behaviour of both isotropic(circular) and anisotropic(elliptical) tracers in active dumbbell suspension, considering only steric interactions. For circular tracers, we find that the speed shows a crossover from monotonically decreasing to increasing with tracer size as the dumbbells' speed is increased. The tracer's effective diffusion also displays a non-monotonic dependence on area fraction: the diffusivity first increases and then decreases at higher area fractions.

For anisotropic tracers, the characteristic non-monotonic trend persists. Moreover, their motion along the major and minor axes differs significantly. Anisotropic accumulation of active particles around the tracer generates direction-dependent forces and fluctuations, favouring motion along the major axis. Consequently, both the speed and diffusivity along the major axis exceed those along the minor axis.

15 min. break

Invited Talk CPP 1.7 Mon 11:15 BAR/SCHÖ

Modeling and inference of magnetotactic motility in complex environments — •Stefan Klumpp — Institute for the Dynamics of Complex Systems, University of Göttingen, Göttingen, Germany

Magnetotactic bacteria orient themselves and swim along field lines of the geomagnetic field. Their magnetically directed self-propelled motion makes them an instance of dipolar active matter. Here we focus on the interaction of these bacteria with walls or obstacles. Experiments in microfluidic systems show that interactions with walls result in (possibly transient) alignment parallel to the wall, which may compete with the alignment with the magnetic field. The dynamic behavior arising from the competition of the two alignments includes U-turn trajectories in circular chambers and trapping and escape dynamics in channels with overlapping cylindrical obstacles. In a phenomenological picture, the resulting motion can be described in an Active Brownian Particle model by introducing a wall torque that competes with the magnetic torque, which results in good agreement with experimental observations. Systematic Bayesian inference of the wall torque from observations shows that only a part of the torque function (dependence on incident angle) can be learned reliably from the data.

CPP 1.8 Mon 11:45 BAR/SCHÖ

Quantifying aggregation behaviour of filamentous cyanobacteria — •Elias Illing and Stefan Karpitschka — Fachbereich Physik, Universität Konstanz

Cyanobacteria are ubiquitous in nature, frequently causing ecological and economic harm by explosive growth, so called blooms.

We investigate the collective dynamics of entangled filamentous cyanobacteria in open liquid media, reminiscent of their aggregates found during later stages of blooms. We investigate the impact of illumination on the clustering and spreading of the bacteria and quantify the morphology of the bacterial aggregates by image analysis. We determine the critical density necessary for initial clustering and track the evolution of the subsequent stages, ranging from stable clusters to spreading mats. These states can be modulated by light intensity variations, potentially allowing for control of the morphological evolution of cyanobacterial aggregates.

CPP 1.9 Mon 12:00 BAR/SCHÖ

Dynamically Induced Spatial Segregation in Multi-Species Bacterial Bioconvection — •Mingqi Yan[1,2], Chenxi Wang[3], Oscar Gallardo-Navarro[4], Rinat Arbel-Goren[4], Joel Stavans[4], and Erwin Frey[1,2] — [1]Department of Physics, Ludwig-Maximilians-Universität München, Theresienstraße 37, 80333 München, Germany — [2]Max Planck School Matter to Life, Hofgartenstraße 8, 80539, München, Germany — [3]School of Science, Harbin Institute of Technology, 518055, Shenzhen, China — [4]Department of Physics of Complex Systems, Weizmann Institute of Science, 7610001, Rehovot, Israel

Bacterial bioconvection is a classic example of collective behavior in active matter, where upward-swimming bacteria create density instabilities leading to large-scale fluid flows. While this phenomenon is well-studied in single-species suspensions, natural environments are typically inhabited by diverse microbial communities. Here, we investigate the collective dynamics of multi-species bacterial suspensions. Combining experiments with a continum model, we show that different bacterial species can spontaneously segregate into stable, spatially interlocked domains. Our theoretical analysis reveals that this segregation is not driven by biochemical antagonism but rather by the interplay between species-specific motility characteristics and the self-generated hydrodynamic flows. This work provides new insights into how physical interactions alone can drive the spatial organization of complex microbial communities.

CPP 1.10 Mon 12:15 BAR/SCHÖ

Light-switchable microbial rafts at air-liquid interfaces — •Gustav F. Nolte, Alexandros A. Fragkopoulos, Timo Völkl, Mechthild Rappold, and Oliver Bäumchen — University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany

In biological active matter, clustering occurs across a wide range of time and length scales, from molecular assemblies such as actomyosin networks to macroscopic systems like fire ant rafts. Here, we report on a fast, light-switchable, and fully reversible clustering phenotype on the microscale, observed at air-liquid interfaces: the raft formation of the biciliated microalga *Chlamydomonas noctigama*.

C. noctigama is a relative of the model organism *Chlamydomonas reinhardtii*, which exhibits light-switchable adhesion and subsequent clustering at solid-liquid interfaces [1,2]. We show how the cluster morphology depends on cell density and discuss potential growth mechanisms by analyzing dynamics of individual clusters. Furthermore, we characterize the dependence of raft formation on the light spectrum and interfacial free energy. Using micropipette force spectroscopy [3], we show that single cells exploit capillary forces for light-switchable ciliary adhesion to the air-liquid interface, enabling raft formation. In their natural habitats, reversible clustering may provide an advantage by allowing cells to accumulate in locations optimal for photosynthesis while increasing resilience to environmental stress.

[1] C. T. Kreis, et al., *Nat. Phys.* **14**, 45 (2018).
[2] S. Till, et al., *Phy. Rev. Res.* **4**, L042046 (2022).
[3] M. Backholm and O. Bäumchen, *Nat. Protoc.* **14**, 594-615 (2019).

CPP 1.11 Mon 12:30 BAR/SCHÖ

Circadian gravitaxis: Photosynthetic microswimmers remodel local pH to actively tune vertical migration — Arkajyoti Ghoshal[1], Soumitree Mishra[1], Jayabrata Dhar[2], Hans-Peter Grossart[3,4], and •Anupam Sengupta[1,5] — [1]Physics of Living Matter, Department of Physics and Materials Science, University of Luxembourg, Luxembourg — [2]Department of Mechanical Engineering, National Institute of Technology Durgapur, India — [3]Department of Plankton and Microbial Ecology, Leibniz Institute of Freshwater Ecology and Inland Fisheries, Stechlin, Germany — [4]Institute of Biochemistry and Biology, Potsdam University, Germany — [5]Institute for Advanced Studies, University of Luxembourg, Luxembourg

Motile phytoplankton shuttle between bright surface waters and deeper nutrient rich layers, usually controlled by internal circadian clocks. Yet many species show irregular movements, defying the expected circadian rhythm. Studying a bloom forming photosynthetic species, we found that cells adjust their vertical migration by altering local pH, mediated by a shift in their gravitactic behavior. This self-modulation of pH generates sub-populations which are physiologically similar but swim differently, remaining vertically separated even under uniform conditions. Supported by a cell-level analysis and mathematical model, we confirm that the pH-mediated circadian shift is underpinned by morphological adjustments. Our results support a circadian gravitactic model in which diurnal pH control drives diversified migration, enhancing fitness particularly in acidifying oceans.

CPP 2: Sustainability: Challenges and Solutions (joint session UP/CPP/SOE)

Accompanying session to Symposium SYSC

Time: Monday 9:30–10:30 Location: MER/0002

CPP 2.1 Mon 9:30 MER/0002

Making a university climate neutral: First experiences from implementing a Climate Protection Strategy at the University of Greifswald — •Christoph G. Hoffmann, Tiemo Timmermann, and Christian von Savigny — University of Greifswald, Greifswald, Germany

With a resolution of its Academic Senate, the University of Greifswald has in 2021 set the goal to achieve climate neutrality by the end of the decade.

While the aim of achieving climate neutrality within a few years is expectedly ambitious, a university as a bigger research institution has also a unique combination of knowledge to achieve it. This has already led to synergies from which particularly the teaching in the environmental subjects can benefit due to "home-made" practical experiences. This makes the whole University a living lab, in which the opportunities but also challenges of necessary transformations can be explored in an assessable setting.

Therefore, also the environmental physics group aims at contributing to and benefiting from this process. While our group is originally focused on basic atmospheric research, we cover a broader range of environmental physics topics in teaching, which overlap with the needs of the transformation process.

In this talk, we will give a short overview of the Climate Protection strategy of the University of Greifswald before we show some examples from our own work regarding the energy consumption of buildings.

CPP 2.2 Mon 9:45 MER/0002

Life Cycle Assessment practices for PV technologies: systematic literature review — •Zeena Patel — Technische Universität Ilmenau

In response to the growing importance of sustainability in solar energy development, this study addresses critical gaps in the application of Life Cycle Assessment (LCA) to photovoltaic (PV) technologies. A systematic review of 48 recent LCA studies across first-, second-, and third-generation PV systems was conducted to evaluate current practices, identify methodological inconsistencies, and highlight emerging trends. Despite increasing research interest and technological diversification, substantial variability exists in the definition of functional units, system boundaries, and impact categories, which hinders comparability and reproducibility. The widespread reliance on secondary databases and the limited use of primary, site-specific data further constrains the accuracy of environmental impact assessments. Additionally, the underutilization of Life Cycle Costing (LCC) and inconsistent application of sensitivity analyses reveal significant gaps in comprehensive sustainability evaluation. To advance the

field, this study proposes standardization of LCA methodologies, improved data transparency, and expansion of impact categories beyond global warming potential to include toxicity and resource depletion. These measures are essential for enhancing the robustness, reliability, and policy relevance of PV LCA studies, thereby supporting sustainable innovation and deployment in the solar energy sector.

CPP 2.3 Mon 10:00 MER/0002

Electrochemical Modeling of SOFCs with Emphasis on Microkinetic and Anode Overpotential — •Iram Gul[1], Gabriela Soffiati[2], and Thiago Lopes[3] — [1]Research Center for Greenhouse Gas Innovation, University of São Paulo (USP), 05508-030, São Paulo * SP, Brazil — [2]Institute of Physics (IFUSP), University of São Paulo, Universidade, R. do Matão, 1371 - Butantã, São Paulo - SP, 05508-090 — [3]Research Center for Greenhouse Gas Innovation, University of São Paulo (USP), 05508-030, São Paulo * SP, Brazil

This study investigates Solid Oxide Fuel Cells (SOFCs) using a CO/H fuel mixture, focusing on thermodynamics, mass transport, and electrochemical kinetics. Thermodynamic properties such as heat capacity, enthalpy, entropy, and Gibbs free energy were analyzed across 600-800°C using MATLAB simulations. The Dusty Gas Model (DGM) revealed key mass transport behaviors in the anode, while Density Functional Theory (DFT) using VASP provided insights into surface reaction mechanisms. A microkinetic model examined the impact of anode overpotential on reaction kinetics and cell performance. Results show that higher temperatures improve mass transport and reduce Ohmic losses but slightly decrease the thermodynamic driving force. This multi-scale model enhances our understanding of SOFC behavior and offers a basis for improving fuel cell efficiency and material performance.

CPP 2.4 Mon 10:15 MER/0002

Thermal stability of ceria-zirconia oxides(CeZrO4) nanoparticles using combustion synthesis for the CO oxidation and NOx reduction — •Hamza Mohamed — IMMM, UMRS 6283 CNRS, Le Mans Université, Bd O. Messiaen, 72085 Le Mans Cedex 09, France

The study presents a green synthesis approach for fabricating ceria-zirconia oxide nanoparticles (CeZrO4 NPs) using the solution combustion synthesis method. The synthesized CeZrO4 nanoparticles were characterized using various sophisticated instruments and methods to determine their detailed properties. The UV-Vis spectra showed a characteristic absorbance peak at 242 nm and a band gap (Eg) of 3.05 eV. Simultaneously, Fourier transform infrared spectra of CeZrO4 NPs displayed bands at 418 cm-1, 991 cm-1, 1382 cm-1, 1658 cm-1, 2306 cm-1, 3288 cm-1, and 3643 cm-1, which indicates the presence of phytochemicals that facilitate the reduction and stabilization of CeZrO4 NPs. The major peaks for cubic CeZrO4 NPs were obtained with a crystalline size of 9.6 nm by X-ray diffraction. The microscopic analyses revealed irregular, ovoid, and aggregated morphologies with sizes ranging from 3 to 10 nm. The XPS analysis revealed the existence of Ce3d, Zr3d, C1s, and O1s states with their corresponding atomic percentages. Therefore, this investigation focuses on synthesizing catalysts that demonstrate both thermal stability and high catalytic activity for the oxidation of CO and the reduction of NOx.

CPP 3: French-German Session: Membranes and Porous Materials I

Time: Monday 9:30–11:00 Location: ZEU/LICH

Invited Talk CPP 3.1 Mon 9:30 ZEU/LICH

Theory and Modeling of Fluid Adsorption and Transport in Nanoporous Materials — •Benoit Coasne — CNRS/University Grenoble Alpes, Grenoble, France — Institut Laue-Langevin, Grenoble, France

Nanoporous materials are at the heart of numerous important applications: adsorption (gas sensing, chromatography), energy (hydrogen storage, fuel cells and batteries), environment (phase separation, water treatment, nuclear waste storage), etc. Among these materials, nanoporous solids which have pores of the order of nm (e.g. active carbons, zeolites), are particularly interesting as ultra-confinement in their porosity leads to novel adsorption and transport phenomena. In this talk, we will present how molecular simulation and statistical physics allows developing models for adsorption and transport in these extremely confining materials. We will see how simple thermodynamic modeling allows rationalizing adsorption by considering reminiscent capillarity at vanishing length-scales. Then, we will show how transport in nanoporous media can be described without having to rely on macroscopic concepts such as hydrodynamics. In particular, using parameters and coefficients available to experiments, we will see how transport coefficients can be rigorously upscaled using simple models such as intermittent brownian motion and free volume theory.

CPP 3.2 Mon 10:00 ZEU/LICH

Optimizing the Fabrication of Isoporous Block Copolymer Membranes by Concurrent Multi-fidelity Simulations — •Gregor Häfner and Marcus Müller — Institute for Theoretical Physics, University of Göttingen, Germany

Integral-asymmetric copolymer membranes promising promising class of functional macromolecular systems with diverse potential applications, including water purification and protein separation. Their fabrication is a two-step process: solvent evaporation and subsequent nonsolvent-solvent exchange to create an isoporous top-layer, and a spongelike substructure. We model the process using two complementary schemes – a highly coarse-grained, particle-based model that treats the polymer chains directly, and a continuum model, describing the system only by its concentration fields. To exploit the accuracy of the former while retaining the efficiency of the latter, we couple these for a concurrent multi-fidelity simulation. The continuum simulation treats the whole system, spawning a particle-based simulation in the region of its lowest accuracy. For this, a neural network is employed to estimate the future error and guide the decision of the subdomain position. We achieve a tenfold increase in computational efficiency compared to pure particle-based simulations, enabling us to investigate large film depths. Our simulations delineate a process window for successful membrane fabrication, which fully match the experimentally accessible parameters, showing an isoporous top layer, a porous substructure and finger-like macrovoids, allowing us to guide experimental membrane optimization.

CPP 3.3 Mon 10:15 ZEU/LICH

In situ monitoring of relaxation dynamics in polyethylenimine during CO2 absorption and desorption — •Martin Tress — Peter Debye Institute for Soft Matter, Leipzig University

Chemical reactions between carbon dioxide (CO2) and amine have been extensively characterized, however, their influence on the dynamics of polyamines remains largely unexplored. In this work, we compare the dynamics of polyethylenimine (PEI) before and after CO2 absorption through broadband dielectric spectroscopy (BDS) [1]. Upon CO2 absorption, thin film PEI shows a slower dynamics, which is consistent with an elevated glass transition temperature revealed in complementary differential scanning calorimetry measurements. In-situ kinetics measurements in thin film samples as well as PEI-infused porous silica demonstrate complex changes in the overall permittivity as well as relaxation times and relaxation amplitudes of some processes during CO2 sorption or desorption. This suggest an intriguing interplay between physical and chemical CO2-sorption, diffusion and the dynamics of PEI. Finally, a tentative model will be presented to describe the observed curves qualitatively. These results demonstrate that BDS is a powerful in-situ-platform to resolve the temporal dynamical changes of polyamines and their impact on sorption kinetics, and may inform specific system adjustments to improve CO2 capture performance.

[1] M. Tress, S. Ahmadi and S. Cheng, AIChE J. 71 (2025) e18627

CPP 3.4 Mon 10:30 ZEU/LICH

Scalable and Tunable Carbon Nanomembranes for Selective Molecular Transport — •Zhen Yao[1], Jan Biedinger[1], Martin Wortmann[1], Nikolaus Meyerbröker[2], Yang Yang[1], Andreas Hütten[1], Günter Reiss[1], and Armin Gölzhäuser[1] — [1]Bielefeld University, Bielefeld, Germany — [2]bCNM Technologies GmbH, Bielefeld, Germany

Carbon nanomembranes (CNMs), molecularly thin two-dimensional materials with intrinsic sub-nanometer pores, provide a versatile platform for nanofluidics. Their ultrathin structure enables fast molecular flux, while surface chemistry and pore architecture can be tailored for selective transport. We present a scalable synthesis route based on electron-induced crosslinking of spin-coated poly(4-vinylbiphenyl) films, combined with atomic layer deposition (ALD) for pore and surface functionalization. This strategy enables precise tuning of pore dimensions and hydrophilicity, yielding CNMs with water vapor permeance as high as 1.9×10^{-5} mol s^{-1} m^{-2} Pa^{-1} and H_2O/N_2 selectivity above 10000, outperforming state-of-the-art polymer and graphene oxide membranes. These results establish CNMs as promising candidates for energy-efficient dehumidification and gas separation. Together, these studies demonstrate how scalable fabrication and nanoscale interface engineering translate into tunable nanofluidic transport, highlighting CNMs as a versatile materials platform for separations, sensing, and controlled molecular flow.

CPP 3.5 Mon 10:45 ZEU/LICH

Is it possible to use nano-confined water for cloaking or magnifying of static electric fields? — •Kira Fischer[1], Julia Brandt[1], Philipp Stärk[2], Alexander Petrov[1], and Alexander Schlaich[1] — [1]Hamburg University of Technology — [2]University of Stuttgart

Assuming radial anisotropy in the dielectric response of water in cylindrical or spherical confinement, Kettunen et al., have shown that for certain ratios of per-

mittivity contrast it is possible to cloak the interior sample, or to magnify the response of an inner cylinder. Indeed, water at interfaces and in confinement shows a strongly anisotropic dielectric response, with high dielectric permittivity in parallel and low permittivity perpendicular to the interface, as observed experimentally by Fumagalli et al.

Here, we probe the radial and azimuthal dielectric response of water in cylindrical confinement. We do so by calculating the dielectric permittivity profile from molecular dynamics simulations, both using a Green-Kubo relation as well as applied fields. Near the interface, we observe a high dielectric permittivity in the azimuthal direction and a low dielectric permittivity in the radial direction of the cylinder, supporting the concept of radial anisotropy.

Applying a static, homogenous external field we then analyse the resulting water polarization. The observed effective response of water inside a cylinder is almost bulk like, and no significant cloaking effect is observed. We use effective medium theory to rationalize this behavior and discuss possible applications of cloaking in model fluids.

CPP 4: Energy Storage Materials and Devices I

Time: Monday 9:30–11:15 Location: ZEU/0255

Invited Talk CPP 4.1 Mon 9:30 ZEU/0255

Exploration of Cathode Materials for Li-S Batteries — •Yan Lu — Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Recently, a lot of efforts have been devoted into lithium-sulfur (Li-S) battery system due to its high theoretical capacity (1675 mAh g-1) and low cost, which could be a competitive candidate for the next-generation batteries in the future. However, it suffers from a poor cycling stability during charging-discharging, which is blamed to the "shuttle effects" of lithium polysulfides. Fundamental understanding of the formation and dissolution processes of both solid phases, S8 and Li2S, is necessary for the development of advanced cathode materials (both organosulfur and metal compound-based sulfur host) with improved electrochemical performance. Synchrotron-based operando high-resolution X-ray imaging has been successfully used for the detailed morphology study of sulfur particles during cycling of the battery cells. Using colloidal route, complex hybrid carbon nanostructures have been synthesized using colloidal polymeric particle as soft template, which have been applied as cathode materials for Li-S batteries.

CPP 4.2 Mon 10:00 ZEU/0255

Temperature-dependent Crystal Structure of Dimethyl Carbonate — •Lea Westphal[1,2], Peter Müller-Buschbaum[1], and Anatoliy Senyshyn[2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]MLZ, TUM, Garching, Germany

The performance and safety/stability of Li-ion batteries (LIBs) can be enhanced by optimizing the charge-storing electrode materials and/or the charge-mediating liquid electrolytes. In LIB research, the major focus has been on the electrode subsystem, while liquid electrolytes are studied much less. Upon cooling of LIBs to investigate their performance at low temperatures, a series of Bragg reflections has been observed, which was assigned to the freezing of liquid electrolyte. Further measurements reveal the development of long-range order in the model electrolyte mixture LP30. To better understand this emerging order, it is essential to investigate the system's individual components, especially under conditions near room temperature relevant to in situ sub-ambient LIB studies.

This contribution outlines our efforts to crystallize Dimethyl Carbonate with minimized preferred orientation, in order to study the unit cell across the entire solid temperature range using neutron- and synchrotron-based powder diffraction. The datasets are complemented by synchrotron single-crystal diffraction experiments. Additionally, the liquid state is investigated by Total Scattering and Pair Distribution Function analysis.

CPP 4.3 Mon 10:15 ZEU/0255

Electron Energy Loss Spectroscopy for oxidation state analysis on ammonia synthesis catalysts — •Daniela Ramermann, Michael Poschmann, Elisabeth H. Wolf, Holger Ruland, and Walid Hetaba — Max-Planck-Institut für Chemische Energiekonversion, Mülheim (Ruhr)

Electron energy loss spectroscopy (EELS) is a powerful technique, not only for the determination of elemental compositions, but also for the investigation of chemical bonding and oxidation states. For the analysis of EELS data, the use of cross-section models is quite common, but the use of reference spectra improves the quantification results. In addition, it allows for the fitting of the edge shapes to investigate oxidation states with the spatial resolution of the electron microscope.

Because the available databases for EELS references [1] are not exhaustive, reference materials are obtained from acquired commercial materials of well-known and defined properties. It is crucial to thoroughly characterize these materials before measuring the reference spectra, as the materials may have local impurities or differ from the desired oxidation state. For the Fe-based catalyst system some reference materials are of mixed oxidation state, presenting an additional challenge.

We show the process of acquiring suitable EELS references for materials used in catalysis and the application of mapping the oxidation state and phase composition on a Fe based ammonia synthesis catalyst.

[1] https://eelsdb.eu, https://eels.info/atlas

CPP 4.4 Mon 10:30 ZEU/0255

Investigating the Conversion Reaction of the Cathode Active Material FeS_2 in Solid-State Batteries via Transmission Electron Microscopy — •Franziska Hüppe[1], Matilde Pavan[2], Shamail Ahmed[1], Jürgen Belz[1], Jürgen Janek[2], and Kerstin Volz[1] — [1]Philipps-Universität Marburg, Department of Physics and mar.quest, Hans-Meerwein-Straße, 35043, Marburg, Germany — [2]Justus-Liebig-Universität Gießen, Institute of Physical Chemistry and Center for Materials Research, Heinrich-Buff-Ring, 35392, Gießen, Germany

Solid-state batteries are particularly promising for high-energy storage, as they potentially allow for the use of electrode materials with higher specific capacities. In the case of FeS_2 as cathode active material, also the cost effectiveness and the environmental impact would be drastically enhanced. However, FeS_2 is a conversion-type material that undergoes continuous compositional and structural changes during cycling that is not yet fully understood at the micro- and nanoscale.

Scanning transmission electron microscopy (STEM) offers structural insights at high resolution and is combinable with deepening investigation methods like energy dispersive X-ray spectroscopy (EDX) and electron energy loss spectroscopy (EELS) to identify the different compounds forming during different depth of discharge (lithiation).

The pristine, uncycled cathode sheet contains FeS_2 particles with cubic structure. With increasing depth of discharge, the particles react from the outside in, forming core-shell structures. The multimodal STEM analysis will be discussed in detail during the presentation.

CPP 4.5 Mon 10:45 ZEU/0255

Dual-cation pre-intercalated hydrated vanadium oxide for ultralong cycling stability in aqueous zinc-ion batteries — •Yan Ran, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

In this work, hydrated vanadium oxide with pre-intercalated K and Mn ions (K0.07Mn0.13V2O5*1.47H2O) was synthesized via a one-step hydrothermal method, demonstrating an excellent specific capacity of 524.7 mA h g-1 at 0.1 A g-1, and outstanding stability with 82.47% capacity retention after 20,000 cycles at 5 A g-1. The co-intercalation of dual cations increases the interlayer spacing while stabilizing the material structure, expanding the ion transport channels, and improving both the specific capacity and long-cycle stability. Moreover, the Zn2+/H+ co-intercalation mechanism was confirmed by ex-situ characterization. This work will provide insights for the development of competitive cathodes in high-performance aqueous batteries.

CPP 4.6 Mon 11:00 ZEU/0255

Unveiling the Interfacial Behavior of Lithium Batteries by Operando X-ray Scattering — •Yuxin Liang[1], Fabian Apfelbeck[1], Kun Sun[1], Yingying Yan[1], Lyuyang Cheng[1], Guangjiu Pan[1], Tianle Zheng[1], Yajun Cheng[2], Anton Davydok[3], Christina Krywka[3], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]College of Renewable Energy, Hohai University, Changzhou, China — [3]Helmholtz-Zentrum Hereon, Geesthacht, Germany

Poly(ethylene oxide) based solid composite electrolytes suffer from poor conductivity and lithium dendrite growth, especially toward the metallic lithium metal anode. In our recent work, we focus on the fabrication and comprehensive characterization of performance-enhanced PEO-based composite electrolytes for lithium batteries. Advanced nano-focus X-ray scattering techniques were used to investigate the interfacial behavior within the lithium metal battery, as well as its failure mechanisms. With the modification of plasticizer, the electrolyte exhibit good electrochemical performance and interfacial compatibility. However, the reference electrolyte exhibit early dendrite formation from the lithium surface into the electrolyte, leading to persistent structures that degrade performance. The results highlight the potential of these fabrication and analysis methods, demonstrating their application in advancing lithium battery technologies and contributing to the development of cutting-edge characterization techniques.

CPP 5: Wetting, Fluidics and Liquids at Interfaces and Surfaces I (joint session CPP/DY)

Time: Monday 9:30–11:00 Location: ZEU/0260

Invited Talk CPP 5.1 Mon 9:30 ZEU/0260

Cleaning of dusty surfaces — •Doris Vollmer[1], Franziska Sabath[1], Abhinav Naga[2], Stefanie Kirschner[1], Tarik Karakaya[1], Rüdiger Berger[1], Hans-Jürgen Butt[1], and Halim Kusumaatmaja[2] — [1]Max Planck Institute for Polymer Research, 55128 Mainz, Germany — [2]Ackermannweg 10

The accumulation of dust, sand or other contaminants on solar modules leads to significant efficiency losses. Billions of litres of water are used annually to clean solar modules, and other natural or man-made surfaces. However, the complex interplay between capillary and frictional forces, which determines successful removal or unwanted redeposition, is still poorly understood. By combining confocal microscopy and Boltzmann lattice simulations, we observe and quantify the removal of particles from smooth and rough surfaces by a water droplet, varying the hydrophobicity of the surface and the particles. Hydrophilic particles aquaplane, resulting in negligible friction and easy particle removal. For hydrophobic particles, the tangential component of the capillary force promotes or counteracts particle removal. Undesirable redeposition depends on the number and wettability of the particles. On superhydrophobic surfaces, the small contact area facilitates easy removal. For individual particles, we propose a phase diagram for particle removal.

CPP 5.2 Mon 10:00 ZEU/0260

Marangoni contracted droplets on Textured Surfaces: Insights from Lubrication Theory — •Raphael Saiseau, Ze Xu, and Stefan Karpitschka — Fachbereich Physik, Universität Konstanz, 78464 Konstanz, Germany

Wetting and evaporation of droplets on micropatterned surfaces are central to both natural processes and technological applications, from anti-icing and spray cooling to inkjet printing and semiconductor processing. Droplet behavior on such surfaces is set by surface chemistry and topography, and most control strategies traditionally rely on specific materials or designs, limiting their versatility.

By depositing droplets on top of a pillars-decorated substrate in a vapor-controlled chamber, we show that the spreading and wicking can be controlled, and even temporarily suppressed, by using the vapor of a second, low-surface tension liquid, generating Marangoni stresses through its condensation near the droplet edge. We present numerical and semi-analytical solutions of the thin film equation coupled to a composition evolution equation, and diffusion-limited evaporation. The wicking effect of the texture is implemented through an effective height-dependent pressure, analogous to classical hemiwicking models. The emerging Marangoni flows oppose the prevailing capillary flows, leading to a quasi-stationary rather than a spreading or wicking drop. We derive a predictive relation between material parameters and drop shape, opening the way for designing controlled coating, cleaning and drying strategies on textured surfaces.

CPP 5.3 Mon 10:15 ZEU/0260

Photoswitchable Arylazopyrazole Monolayers on Aluminum Oxide for Tunable Wettability — •Tim Blinzer, Christian Honnigfort, and Björn Braunschweig — Institute of Physical Chemistry and Center of Soft Nanoscience, University of Münster, Corrensstraße 28-30, Münster 48149, Germany

Smart surfaces that can change their wettability on demand are interesting for applications such as self-cleaning or microreactors. To tune the surface wettability, we functionalized aluminum oxide surfaces with arylazopyrazole (AAP) phosphonic acids using a Langmuir-Blodgett transfer. AAP molecules in the deposited monolayers undergo reversible E/Z photoisomerization driving changes in surface wettability. This was investigated as a function of surface coverage, where the responsiveness—i.e. the changes in molecular structure and in the apparent contact angle—was studied in detail. Here time-dependent sum-frequency generation (SFG) was used to obtain in situ information on the dynamic changes in monolayer upon E/Z switching with 520 nm green and 365 nm UV light. Furthermore, we show that increasing surface roughness by depositing nanoaggregates of the AAP phosphonic acid leads to a drastic increase in the change of the contact angle when switching from the E to the Z isomer. Indeed, the change in contact angle increased from only 7° for homogeneous monolayers to about 20° for nanostructured surfaces using AAP aggregates.

CPP 5.4 Mon 10:30 ZEU/0260

Motion and interaction of Marangoni contracted droplets on micropatterned surfaces — •Ze Xu, Raphael Saiseau, and Stefan Karpitschka — Fachbereich Physik, Universität Konstanz, Konstanz, Germany

Wetting of micropatterned surfaces is ubiquitous in nature and key to many technological applications like inkjet printing and semiconductor processing. Overcoming the intrinsic, chemistry- and topography-governed wetting behaviors often requires specific materials, leading to contradicting requirements between the processing strategy and the final product. Here, we demonstrate that droplet spreading and wicking on hydrophilic patterns can be controlled by the vapor of a lower-surface-tension liquid. Condensation of the vapor induces Marangoni forces that delay capillary wicking and contract liquid into a droplet on top of the imbibed film. Consequently, a Marangoni-contracted droplet coexists with a finite imbibition film for prolonged times. We demonstrate how these droplets interact with each other, both by their vapor cloud, and by the imbibed liquid film that surrounds them. Modulating the ambient vapor, also these interactions can be modulated, devising new strategies for coating, cleaning, and drying functional surfaces.

CPP 5.5 Mon 10:45 ZEU/0260

Wetting of Swelling Polyelectrolyte Surfaces on a Macroscopic and Nanoscopic Scale — •Mona Meltschoch and Regine von Klitzing — Soft Matter at Interfaces, Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 8, D-64289 Darmstadt, Germany

Wetting on adaptive polymer interfaces plays an important role in soft matter physics, particularly when spreading is affected by substrate hydration. Polyelectrolyte multilayers (PEMs) are suitable model systems because they absorb water and evolve across multiple time scales, creating a link between nanoscale polymer mobility and macroscopic contact line motion. PEM films were prepared by the layer-by-layer method, and their wetting behaviour was examined at different scales. Nanoscale morphology and hydration were characterised by atomic force microscopy (AFM), while macroscopic wetting was followed via optical contact angle (CA) measurements. Previous studies report a decrease in water CA on PSS-terminated PEMs under humid atmosphere. To assess how film architecture affects wetting, PEMs with varying bilayer numbers and terminal charge (PSS vs. PAH) were fabricated, showing smooth surfaces and a linear thickness increase. Current work explores AFM beyond static surface imaging by applying it directly to droplets on PEM films. This approach aims to track local swelling, interface deformation and contact line behaviour under liquid exposure. Measurements with different droplet liquids are being established, with the long-term goal to link nanoscale hydration dynamics to macroscopic changes in contact angle and wetting evolution.

CPP 6: French-German Session: Membranes and Porous Materials II

Time: Monday 11:15–12:45 Location: ZEU/LICH

Invited Talk CPP 6.1 Mon 11:15 ZEU/LICH

Hierarchical Porosity Meets Nanoconfined Water: Toward Water-Driven Functional Materials — •Patrick Huber — Hamburg University of Technology — Deutsches Elektronen-Synchrotron DESY

Natural materials achieve remarkable functionality using only simple chemical building blocks, relying on architectures that span multiple length scales. A key feature of many biological systems is their hierarchical porosity, which guides fluid transport from large channels down to nanopores where water acts as a nanoscale working fluid. In such confined spaces, water displays distinct structural dynamics and interfacial behaviour that strongly influence mechanical, transport, and optical responses. This contribution introduces a new class of sustainable water-driven materials whose active behaviour originates from the interplay between hierarchically porous solid networks and interfacial or nanoconfined water. These Blue Materials exploit water-mediated processes such as humidity-responsive actuation, capillary-driven transport, and pore-structure controlled optical effects. Their functionality is rooted in the precise design of their pore architecture, especially at the nanoscale where confined water governs dynamic material behaviour. Beyond emulating natural processes, these principles open pathways for harvesting electrical energy from environmental wetting-drying cycles, offering a sustainable approach to energy generation in porous materials.

CPP 6.2 Mon 11:45 ZEU/LICH

Accessing topological properties of mesoporous materials via SDGW model — •Georgiy Baroncha[1], Rustem Valiullin[1], and Eustathios Kikkinides[2] — [1]Felix Bloch Insitute for Solid State Physics, Leipzig University, Leipzig, Germany — [2]Department of Chemical Engineering, Aristotle University of Thessaloniki, Thessaloniki, Greece

Gas sorption is commonly used to characterize mesoporous materials, but its ability to reveal how pores are interconnected remains limited due to an incom-

plete understanding of network effects on phase behavior. In this work, we represent mesoporous structures using statistically disordered Bethe, and apply a statistical-thermodynamic approach to interpret adsorption/desorption or melting/freezing phase transitions. We demonstrate that gas sorption analysis can be used not only to determine pore size distributions, but also to quantitatively infer the average interpore connectivity and correlations between pore diameters in the material. At the same time, we find that sorption isotherms are largely unaffected by other aspects of pore network topology. These results identify the key structural factors shaping sorption behavior and broaden the capabilities of gas sorption for simultaneous assessment of pore size distribution and mean connectivity in mesoporous materials.

CPP 6.3 Mon 12:00 ZEU/LICH

2D Water in Clay Nanoconfinement: Tiny Space for Large Implications — •Vasily Artemov — Hamburg University of Technology

This talk presents recent advances in understanding the behavior of two-dimensional water in clay nanoconfinement, with a focus on its dielectric properties. Although clays are abundant, their crystal particles typically lack directional alignment. I will discuss an approach for self-assembling clay particles into large, scalable membranes in which the flakes are oriented parallel to each other, enabling a controlled and reproducible platform for studies of confined water at the nanoscale. Using this self-assembled nanofluidic platform, I will present experimental evidence of confinement-induced charge-separation effects that support electricity storage in water channels of 1 nm wide [1]. By combining insights from nanoscale physics, electrochemistry, and materials science, I will highlight how confinement within clay interlayers can influence ion transport, energy-storage phenomena, and our broader understanding of water at the interfaces.

[1] V. Artemov, S. Babiy, Y. Teng, J. Ma, A. Ryzhov, T.-H. Chen, L. Navratilova, V. Boureau, P. Schouwink, M. Liseanskaia, P. Huber, F. Brushett, L. Laloui, G. Tagliabue, A. Radenovic, Bulk electricity storage in 1-nm water channels, arXiv:2410.11983 (2024)

CPP 6.4 Mon 12:15 ZEU/LICH

Two coexisting populations of sorbed DMSO drive distinct structural changes in a swelling porous material — Raimund Teubler[1,3], Alexandra Serebrennikova[1,2,3], Maximilian Fuchs[1,3], Eduardo Machado Charry[1], Robert Saf[1], Erich Leitner[1,3], and •Karin Zojer[1,3] — [1]Graz University of Technology, Graz, Austria — [2]Wood Kplus Competence Center, Linz, Austria — [3]CDL for mass transport through paper, Graz, Austria

Understanding the swelling of cellulose-lignin-based fibers is essential for describing the mechanisms governing water and volatile uptake in porous materials such as paper. We reveal the dynamics of dimethyl sulfoxide (DMSO) uptake and quantify the resulting changes in fiber and sheet structure by combining three recently developed techniques based on concentration determination in coupled uptake/release experiments, microcomputed tomography (μ-CT), and optical microscopy. DMSO interacts with the fibers in a manner similar to water. We show that DMSO is incorporated into the paper sheet in two distinct populations, each contributing differently to the structural evolution of the material. The first population consists of DMSO molecules incorporated into the fibers, leading to fiber swelling. The second population accumulates at the fiber surfaces; although these molecules bind to and are released from the surface rapidly, they gradually modify the fiber surface [1]. As a consequence, built-in stresses within the fiber network are released, causing structural changes that persist long after fiber swelling has ceased.

[1] R. Teubler et al., DOI: 10.1007/s10450-025-00656-x.

CPP 6.5 Mon 12:30 ZEU/LICH

Electrochemical control of photoluminescence emission by a porous silicon membrane — •Manuel Brinker[1] and Patrick Huber[1,2] — [1]Institute for Materials and X-ray Physics, Hamburg University of Technology, Denickestr. 15, Hamburg 21073, Germany — [2]Centre for X-ray and Nano Science CXNS, Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, Hamburg 22607, Germany

Porous silicon is a highly versatile porous material with a broad range of exceptional properties. Due to the geometrical confinement of the pore walls, the band structure is strongly altered and the pore walls effectively act as quantum wires. Thus, photons are emitted in the visible range when the membrane is excited by a UV source. This optical effect has been widely researched and is the foundation for porous silicon to be applied, e.g., as a sensor material in the life sciences. Here, we study the influence of electrochemo-mechanical coupling on the photoluminescence performance. Thereby, charge carriers are accumulated in the electric double layer of a porous silicon electrode by charging it in an electrolyte solution. A change in surface stress at the interface with the porous material is induced and results in an overall mechanical reaction of the porous material. The strain acting on the pore walls consecutively influences the emission characteristics of the photoluminescence emission. An extensive in-situ study ascertains a highly linear dependence of the emission peak's wavelength on the charging state of the electrode. This research establishes the groundwork for porous silicon electrodes to be utilized as mechano-optical sensors.

CPP 7: Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods I

Time: Monday 11:30–12:45 Location: ZEU/0255

CPP 7.1 Mon 11:30 ZEU/0255

Exploration of quantum-mechanical space towards olfactorial receptor and body odor volatilomes interaction — •Li Chen[1], Leonardo Medrano Sandonas[1], Shirong Huang[1], and Gianaurelio Cuniberti[1,2] — [1]Institute for Materials Science and Max Bergmann Center for Biomaterials, TUD Dresden University of Technology, 01062 Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCMS), TUD Dresden University of Technology, 010628 Dresden, Germany

We present the MORE-QX dataset generated from quantum-mechanical (QM) simulations of atomistic systems spanning diverse design stages for gas sensing. The dataset contains 23,838 and 10,441 BOV*receptor dimer systems in the gas phase and on graphene surfaces, respectively, to obtain sensing-related binding features. By analyzing the property space spanned by MORE-QX, we observe substantial flexibility in identifying interaction configurations with desired electronic binding characteristics, owing to the weak correlations among the properties. To gain insights into the complex interplay between these sensing properties, we construct tree-based machine-learning models for fast evaluation of binding features using only QM molecular properties, and combine them with an explainability framework to identify the key design factors of BOV*receptor systems that govern sensing performance. Our work provides valuable insights into the sensing mechanism and design principles of olfactorial receptors for BOV sensing.

CPP 7.2 Mon 11:45 ZEU/0255

Non-local diffusion model as a description for non-Gaussian diffusion in scattering experiments — •Harish Srinivasan[1,2], Veerendra Kumar Sharma[2], and Subhankur Mitra[2] — [1]Institute of Applied Physics, University of Tübingen, Tübingen, Germany — [2]Solid State Physics Division, Bhabha Atomic Research Centre, Mumbai, India

We introduce a non-local diffusion (NLD) model that provides a unified theoretical framework for describing non-Gaussian diffusive dynamics in fluids. The NLD formulation generalizes conventional diffusion by incorporating a jump kernel, enabling analytical characterization of van-Hove self-correlation functions with exponential tails. This framework naturally connects two major classes of anomalous transport observed in scattering experiments: non-Gaussian fractional Brownian motion (nGfBm) in sub-diffusive glass-formers, and Fickian yet non-Gaussian diffusion (FnGD) in cage-jump dominated liquids. In the nGfBm regime, the NLD description captures the crossover from non-Gaussian to Gaussian sub-diffusion seen in molecular and polymeric glass-formers [1]. In the FnGD regime, the NLD model predicts the exponentially fast approach to Fickianity and the much slower algebraic restoration of Gaussianity [2]. Comparison with incoherent quasielastic neutron scattering data across multiple systems demonstrates the universal applicability of the NLD model and establishes non-local diffusion as the common physical origin of non-Gaussian signatures in molecular fluids. [1] H. Srinivasan et. al., Phys. Rev. Lett. 132, 058202 (2024) [2] H. Srinivasan et. al., arXiv:2504.15020 (2025)

CPP 7.3 Mon 12:00 ZEU/0255

Optimizing EquiDTB potentials for large-scale molecular simulations — •Zekiye Erarslan, Gianaurelio Cuniberti, and Leonardo Medrano Sandonas — Chair of Materials Science and Nanotechnology, TUD Dresden University of Technology, 01062 Dresden, Germany

Density Functional Tight-Binding (DFTB) is a semi-empirical method that enables efficient large-scale simulations at moderate computational cost compared to first-principles quantum-mechanical methods. However, its generalizability is limited by the use of parameterized pairwise repulsive potentials. The recently developed EquiDTB framework [chemRxiv, 10.26434/chemrxiv-2025-z3mhh] has shown that replacing this repulsive term with a many-body ΔTB potential—trained using equivariant neural networks—significantly improves both the accuracy and transferability of the DFTB method. As a result, EquiDTB achieves hybrid DFT-PBE0 level accuracy across diverse electronic, structural, and vibrational properties of large molecules and molecular dimers containing C, N, O, and H atoms. In this work, we extend the EquiDTB framework by training a more general ΔTB potential on the chemical space covered by the newly gen-

erated QCML dataset. This expansion broadens EquiDTB beyond its original four-element scope and enables accurate simulations of neutral molecular systems containing C, N, O, H, P, S, Na, and Cl. We validate the performance of the optimized EquiDTB model through extensive calculations on large molecular dimers, RNA systems, and organic periodic materials.

CPP 7.4 Mon 12:15 ZEU/0255

MolecuTas: an ML platform for refining quantum properties and bioactivity of complex molecules — •Álvaro Vallejo Bay[1], Jannis Krüger[2], Thomas Hellweg[2], Gerardo Prieto[1], and Vicente Domínguez Arca[2,3] — [1]Applied Physics, University of Santiago de Compostela, Spain — [2]Physical and Biophysical Chemistry, Bielefeld University, Germany — [3]Biosystems and Bioprocesses Engineering, IIM-CSIC, Spain

This work introduces MolecuTas, a neural architecture designed for the ultra-fast prediction of atomistic and molecular properties with accuracy approaching density functional theory, yet at negligible computational cost. The project tackles core challenges in computational chemistry, particularly the size dependence of predictive models and the loss of structural detail in conventional representations. To overcome these limitations, we develop a custom data extraction and molecular fragmentation pipeline based on large quantum datasets, ensuring the preservation of essential information such as connectivity, symmetries, chemical environments, and electronic features.

Building on this foundation, we propose a family of advanced Graph Neural Networks that explicitly integrate physicochemical principles and disentangle local from global information, enabling robust generalization across diverse molecular systems. Ultimately, MolecuTas aims to provide a reliable tool for molecular dynamics, enabling precise and fast prediction of partial charges and other key descriptors required for accurate simulations and next-generation chemical design.

CPP 7.5 Mon 12:30 ZEU/0255

Property-guided diffusion modeling for efficient exploration of chemical spaces — •Leonardo Medrano Sandonas[1], Michael Hanna[1], Julian Cremer[2], and Gianaurelio Cuniberti[1] — [1]TUD Dresden University of Technology, Germany. — [2]Pfizer Worldwide R&D, Germany.

The rational in silico design of chemical compounds requires a deep understanding of both structure-property and property-property relationships across chemical compound space, as well as efficient methodologies for defining inverse property-to-structure mappings. In this presentation, I will discuss our recent efforts to leverage the "freedom of design" concept [Chem. Sci. 14, 10702 (2023)] in the chemical space of drug-like molecules to develop an efficient generative AI framework capable of designing molecular compounds with targeted quantum-mechanical (QM) properties. To this end, we have implemented a property-guided active learning approach that optimizes the performance of equivariant diffusion models within each property space. Generated molecules and their associated QM properties are validated through exhaustive DFT calculations at the PBE0+MBD level using the FHI-aims code. Our findings reveal a consistent improvement in property accuracy when guiding the diffusion model to explore less populated regions of the target property space. This performance is further enhanced by incorporating molecular building blocks into the initial training set. We expect our work to advance the development of sustainable generative AI frameworks for identifying molecules tailored to specific chemical processes.

CPP 8: Wetting, Fluidics and Liquids at Interfaces and Surfaces II (joint session CPP/DY)

Time: Monday 11:30–12:45 Location: ZEU/0260

CPP 8.1 Mon 11:30 ZEU/0260

Do the particle number and wettability affect their removability by a single water drop? — •Franziska Sabath[1], Abhinav Naga[2], Halim Kusumaatmaja[2], and Doris Vollmer[1] — [1]Max Planck Institute for Polymer Research, 55128 Mainz, Germany — [2]Institute for Multiscale Thermofluids, School of Engineering, University of Edinburgh, United Kingdom

The accumulation of dust on surfaces, *e.g.* windows and solar panels, is a well-known phenomenon in everyday life. The ratio of the capillary force between particles and drop and the resistive forces between particles and surface, *i.e.* friction and adhesion, determine whether the particles can be removed by a water drop. The likeliness of particle removal depends on both particle and surface wettability. It is still questionable how the particle arrangement, the total resistive force acting and the unwanted redeposition of particles depend on the number and wettability of the particles. Here, we investigate the removal of hydrophobic and hydrophilic spherical particles from a flat surface. As the number of hydrophobic particles increases, the total resistive force increases, but not linearly, and overcomes the capillary force, causing particle redeposition. In contrast, the hydrophilic particles slide on a thin water film, reducing the particle-surface friction and no resistive force is measured within our experimental resolution.

CPP 8.2 Mon 11:45 ZEU/0260

Modelling and simulation of capillary adhesion between rough surfaces — •Yizhen Wang, Martin Ladecký, and Lars Pastewka — University of Freiburg, Freiburg, Germany

At a small enough length scale, surfaces are always rough, regardless whether they are generated by nature or via artificial process. When two such surfaces are placed close enough, the water molecules in the humid air are adsorbed and hence form capillary bridges. Theories for adhesive interactions typically use simple cohesive laws, which are good models for Van-der-Waals interactions but may not be appropriate for capillary adhesion. We here construct a phase-field model that explicitly represents water present between two contacting rough interfaces. We show results obtained with this model on synthetic, computer-generated, self-affine rough interfaces. In quasi-static simulation, we observe the merging and splitting of droplets under the normal and shear movement of the interfaces. The overall force is dominated by the perimeter of the droplet, indicating the importance of a detailed understanding of droplet morphology.

CPP 8.3 Mon 12:00 ZEU/0260

Impact of surface wettability on the removal of montmorillonite aggregates by water drops How natural dirt is removed from various surfaces — •Stefanie Kirschner, Franziska. Sabath, Azadeh Sharifi-Aghili, Tarik Karakaya, and Doris Vollmer — Max Planck Institute for Polymer Research, 55128 Mainz, Germany

Natural dust on photovoltaic modules or windows, is a critical factor that reduces their performance. Previous experiments focused on the removal on single or many spherical particles. The removal of aggregates of natural particles, is not yet understood. Here, we focus on minerals, commonly present in desert dust. Using confocal laser scanning microscopy the detachment behavior upon contact with a water drop is measured on surfaces with different wettability. In addition, the force required to remove the aggregate by a sliding water drop was investigated. During drying on a hydrophilic surface, the dispersed particles cover a larger area. This increases the total contact area, resulting in higher adhesion and reduced detachment. In contrast, hydrophobic surfaces promoted more compact aggregates with improved removability. Finally, I will compare the detachment forces and the removal behavior of different natural aggregates, e.g. soot, salt and humic acid.

CPP 8.4 Mon 12:15 ZEU/0260

Equilibrium droplets on deformable substrates exhibit cloaking and demixing at the three-phase contact line — •Khalil Remini[1], Ralf Seemann[1], Dirk Peschka[2], and Barbara Wagner[2] — [1]Universität des Saarlandes — [2]Weierstrass Institute for Applied Analysis and Stochastics

This work examines the equilibrium shape of liquid droplets on viscoelastic PDMS substrates with varying elasticities. By combining atomic force microscopy (AFM) with an initial lift-off step, we reveal not only the top contour of the droplets but also the buried droplet*substrate interface. A second lift-off step provides additional structural details near the three-phase contact line (TPCL), where the interfacial tensions adopt a Neumann balance. Quantitative analysis of the reconstructed 3D droplet shapes shows that non-crosslinked, liquid PDMS molecules are extracted from the elastic network under stress and accumulate as a liquid rim around the droplet base, thereby altering both the droplet shape and the substrate profile close to the TPCL. These liquid molecules also cloak the droplets with a thin film, modifying the effective surface tensions. Furthermore, dewetting experiments demonstrate that this demixed liquid already appears at an early stage of dewetting and remains at an approximately constant amount throughout the process.

CPP 8.5 Mon 12:30 ZEU/0260

Tuning Sliding Drop Shape — •Fiona Berner, Chaurasia Rishi, Sajjad Shumaly, Chirag Hinduja, Hans-Jürgen Butt, and Rüdiger Berger — Max-Planck-Institut für Polymerforschung

The understanding of wetting phenomena plays a crucial role in many daily processes. For example, dirt repelling glasses can be achieved by a hydrophobic coating. Recently, Hinduja et al, reported on a scanning drop friction force instrument (sDoFFI) to analyse friction forces of drops on surfaces. A drop is fixated to an elastic force sensor with spring constant κ. The sample underneath the drop is moved with a constant speed u leading to sliding of the drop at a defined trajectory along surfaces. The deflection of the capillary,d, provides information

about the friction force between the drop and the surface, $F_{meas} = \kappa \cdot d$ Forces arising from CAH are given by the Furmidge equation, where the drop*s sliding force F_{CAH} corresponds to

$$F_{CAH} = k \cdot \gamma \cdot w \cdot \Big(cos(\theta_{rec}) - cos(\theta_{adv}) \Big) \quad (1)$$

where k is a geometrical factor, γ is the liquid surface tension, w the width of the drop and θ_{rec} and θ_{adv} are the receding and advancing contact angles, respectively. For small u we assume $F_{meas} = F_{CAH}$. The parameters γ, w, θ_{rec} and θ_{adv} are known or can be measured optically. Thus, the geometrical factor k can be calculated. We realize different geometries of the drop by glueing metal rings to the elastic glass capillary. Shaping the metal rings forces the drop to shape. We discuss experiments where we shape the drop into different width and length and discuss dependence of the geometrical factor k.

CPP 9: French-German Session: Simulation Methods and Modeling of Soft Matter I

Time: Monday 15:00–17:00 Location: ZEU/LICH

Invited Talk CPP 9.1 Mon 15:00 ZEU/LICH

Why Polymers Swell or Collapse: Molecular Insights into Cosolute Effects — •Nico van der Vegt — Department of Chemistry, Technical University of Darmstadt

Water-soluble amphiphilic polymers are widely used as stimuli-responsive materials. Their performance is governed by the coil-globule transition, characterised by the theta temperature, which can be tuned by adding small organic molecules (cosolutes). Although related phenomena - such as cononsolvency and salting-out - are well understood at a phenomenological level, their underlying molecular mechanisms remain unclear. This talk explores the solvation physics that determine how different classes of cosolutes influence the coil-globule transition of both generic hydrophobic polymers and realistic systems such as poly(N-isopropylacrylamide), using computer simulations. We identify two distinct molecular driving forces that regulate cosolute-induced hydrophobic interactions, leading to either polymer swelling or collapse. These driving forces depend sensitively on the relevant length scales and expose the interplay between microscopic and macroscopic solvation physics, underscoring the key role of solvent entropy in determining the properties of responsive soft-matter systems. [1] Comm. Chem. 3, 165 (2020), [2] PCCP 24, 2080-2085 (2022), [3] J. Chem. Phys. 160, 164902 (2024)

CPP 9.2 Mon 15:30 ZEU/LICH

THz Pump Pulse Drives Nonlinear H-bond Dynamics in Liquid Water — •Philipp Schienbein — Lehrstuhl für Theoretische Chemie II, Ruhr-Universität Bochum, 44780 Bochum, Germany — Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, 44780 Bochum, Germany

Light-matter interactions are central to processes in nature, chemical engineering, and fundamental research. Of particular interest is the frequency-dependent excitation of molecular systems by incident light. Here, we present machine-learning-accelerated molecular dynamics simulations of water subjected to an intense, monochromatic THz pump pulse, generating a total of 32 ns of trajectory data. The light pulse is explicitly modeled via a time-dependent external electric field, extending our previous framework for field-driven machine learning MD simulations, allowing us to observe the excitation in realtime. Our simulations reproduce key experimental observables, including transient dichroism and birefringence, and reveal that the pulse transiently modulates hydrogen-bond dynamics: H-bonds become markedly shorter-lived compared to unperturbed bulk water. This response is nonlinear, ruling out pure heating and resolving the experimental controversy. These results demonstrate that our machinery to incorporate electric fields in machine learning MD simulations can directly connect microscopic dynamics with measurable observables, further paving the way to controlling water dynamics - and potentially chemical reactivity - through tailored light pulses, a long-standing goal in chemistry.

CPP 9.3 Mon 15:45 ZEU/LICH

Fluctuating Solvent Fields and Vibrational Shifts Revealed by Machine Learned Force Fields — •Florian Brünig and Alexandre Tkatchenko — Department of Physics and Materials Science, University of Luxembourg, Luxembourg

Fluctuating solvent fields is one of the driving mechanism behind vibrational shifts observed in solvatochromic experiments [1]. Previously, experimental infrared spectra have been correlated with mean electric fields obtained from empirical force field molecular dynamics simulations [2]. However, vibrational dynamics of these force fields are insufficient to reproduce the experimental line shape properties.

Here, machine learned force fields (MLFFs) offer multiple opportunities: they are highly accurate, efficient, and can be interpretable if based on physical models. We explore the capabilities of modeling solvatochromism of vibrational probes in solvent and protein environments employing the SO3LR [3] MLFF. SO3LR combines the SO3krates architecture with pairwise analytical electrostatic and dispersion potentials in the long range, and was pretrained on a diverse data set of molecular complexes. We show how fluctuating solvent electrostatic and dispersion fields can be related to vibrational bands in a self consistent manner due to the versatility of MLFFs.

[1] Brünig, FN, Netz, RR, et al. JPCB 126, 1579 (2022).

[2] Weaver, JB, Kozuch, J, Kirsh, JM & Boxer, SG. JACS 144, 7562 (2022).

[3] Kabylda, A, Frank, JT, Müller, KR, Tkatchenko A, et al. JACS 147, 33723 (2025).

CPP 9.4 Mon 16:00 ZEU/LICH

Machine learning potentials for redox chemistry in solution — •Redouan El Haouari[1,2], Emir Kocer[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

Most Machine-Learning Potentials (MLPs) currently in use are local, which prevents the construction of accurate potentials for systems in which long-range charge transfer is important. One example is the distinction of different oxidation states of transition metal ions such as ferrous (Fe^{2+}) and ferric (Fe^{3+}) ions in aqueous solution. In this case the near-sightedness of local MLPs cannot account for distant counter ions or non-local charge transfer. We show that 4th-Generation High-Dimensional Neural Network Potentials (4G-HDNNPs), which employ atomic charges obtained from charge equilibration as globally-determined descriptors, do not suffer from this short-coming. For aqueous ferric and ferrous chloride, the model predicts iron oxidation states correctly matching the total number of chloride ions in the system demonstrating that physical knowledge about the system of interest remains essential to construct reliable MLPs.

CPP 9.5 Mon 16:15 ZEU/LICH

Bridging Accuracy and Sampling: Insights into dAMP Solvation from ML-potentials — •Laurie Stevens[1,2], Riccardo Martina[2], Alberta Ferrarini[2], and Marialore Sulpizi[1] — [1]Chair of Theoretical Physics of Electrified Liquid-Solid Interfaces, Faculty of Physics and Astronomy, Ruhr-Universität Bochum, Germany — [2]Department of Chemical Sciences, Università degli Studi di Padova, Italy

Although nucleotides are essential biomolecular building blocks, key aspects of their structure and interactions, in particular the steps enabling their assembly and polymerization, remain unclear. Here, we investigate the conformational behavior of deoxyadenosine monophosphate (dAMP) in solution using a combined computational-experimental approach. We developed a highly accurate machine-learning potential via active learning that thoroughly samples the free-energy landscape, capturing critical conformational degrees of freedom with near-chemical accuracy. This potential enables nanosecond-scale simulations of water and nucleotides at a level previously inaccessible with hybrid DFT methods. We find that, in solution, dAMP accesses both anti and syn glycosidic conformations. We identify the anti and high anti conformers as the most stable ones, we show that they underlie the intensity variations observed in mid-IR experimental spectra.

CPP 9.6 Mon 16:30 ZEU/LICH

Fine-Tuning Unifies Foundational Machine-learned Interatomic Potential Architectures at ab intio Accuracy — •Christian Dressler, Jonas Hänseroth, Nawaz Qaisrani, and Aaron Flötotto — TU Ilmenau, Institute of Physics, Germany

Machine-learned force fields (MLFFs) have enabled ab initio quality molecular dynamics at speedups of several orders of magnitude. Foundation-model MLFFs, trained on extremely large and diverse datasets, aim to provide broadly transferable force predictions, yet their accuracy remains system-dependent. We investigate five state-of-the-art foundation models (MACE, GRACE, ORB, MATTERSIM, SEVENNET) and fine-tune them for seven chemically diverse systems.[1] Our results show that foundation models provide a useful baseline but still deviate significantly from AIMD. Fine-tuning consistently improves accuracy across all frameworks and yields predictions that closely match AIMD reference data, while also reducing performance differences between models. The final accuracy is largely independent of the underlying architecture. These findings suggest that, after fine-tuning, model choice is no longer the main bottleneck. Prioritizing inference speed and computational efficiency may therefore offer the greatest benefit for accelerating the practical use of ML-based interatomic potentials in materials modeling.

[1] Hänseroth, ... , Dreßler, Fine-Tuning Unifies Foundational Machine-Learned Interatomic Potential Architectures at ab initio Accuracy, https://doi.org/10.48550/arXiv.2511.05337

CPP 9.7 Mon 16:45 ZEU/LICH

NMR crystallography at finite temperatures — •Matthias Kellner and Michele Ceriotti — Laboratory of Computational Science and Modeling, Institut des Matériaux, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

In this talk I will present our latest developments in machine-learning models for predicting NMR chemical shieldings in organic molecular solids. NMR shielding-driven structure determination protocols rely on comparing experimental solid-state NMR shifts with simulations whose accuracy is often limited by computational cost. We address these limitations by combining ensembles of transformer-based shielding predictors with molecular dynamics simulations using a novel, broadly applicable machine-learning interatomic potential. This framework systematically improves agreement with experiment across many benchmark systems, removes the need for empirical corrections and makes it applicable also to disordered and amorphous materials. I will conclude by showing applications of this framework to the structure determination of amorphous active pharmaceutical ingredients.

CPP 10: Droplets, Wetting, and Microfluidics (joint session DY/CPP)

Time: Monday 15:00–18:30 Location: ZEU/0118

CPP 10.1 Mon 15:00 ZEU/0118

Rayleigh instability in the presence of elastocapillarity — •Niphredil Klint and Andreas Isacsson — Chalmers University of Technology, Gothenburg, Sweden

A liquid jet, such as a stream of water, will disintegrate and form droplets if the length-to-radius ratio exceeds a critical value. This occurs due to propagating surface instabilities, a phenomenon known classically as the Rayleigh instability. At the nanoscale, thermal fluctuations affect the breakup dynamics, which may enter a stochastic regime [1]. Placing an elongated nanoscale liquid drop with a high aspect ratio on top of a highly compliant surface, the breakup process is affected by additional noise from thermally excited flexural phonons [2] as well as effects whereby the wetting causes the underlying surface to deform. We use large scale molecular dynamics (MD) simulations to examine the dynamics of the Rayleigh instability in the presence of elastocapillary effects at ambient temperatures. Specifically, we study the interactions between water and suspended graphene, where wetting induced deformations may occur for nanoscale droplets [3]. We focus on characterising the breakup and instability wavelength and isolate the effects of introducing graphene through a comparison of these results to simulations of only water. We also identify the correlation between out-of-plane fluctuations of the graphene and the concentration of water.

[1] J. Eggers, Phys. Rev. Lett. 89, 084502 (2002).
[2] M. Ma et al., Nature Mater. 15, 66 (2016).
[3] M. Kateb et al, Langmuir 39, 12610 (2023).

CPP 10.2 Mon 15:15 ZEU/0118

Air layers and wetting under drops impacting on pre-wetted surfaces — •Kirsten Harth and Shiva Moradimehr — Fachbereich Technik, Technische Hochschule Brandenburg, Germany

Drop impact at low Weber numbers causes the formation of a (temporary) air cushion between the drop liquid and the substrate. On hard, dry substrates, its qualitative thickness profile and the location of the thinnest point are strongly governed by the Weber number. For impact on bulk, soft surfaces, like PDMS gels, it was found that impacts on softer substrates entrap more air [1]. Are there similar effects of thin liquid films?

We address the air layer shapes, entrapped air volume and wetting underneath droplets impacting on a hard substrate pre-wetted by microscopic oil layers. We control the Weber number, the oil layer thickness (in the range of micrometers), the oil viscosity, and in that way the *softness* of the substrate. Despite the thinness of the film, we observe clear effects of the oil layer on the volume and drainage of the air entrapment, its profile shapes, and the wetting behavior.

[1] K.R. Langley et al., Soft Matter 16, 5702 (2020)

We acknowledge funding by DFG within SPP2171 (HA8467/2-1, 2-2).

CPP 10.3 Mon 15:30 ZEU/0118

Memory Effects in Contact Line Friction — •Niklas Wolf and Nico van der Vegt — TU Darmstadt, Darmstadt, Germany

When a drop of liquid comes into contact with a solid surface, it relaxes towards an equilibrium configuration, either wetting the surface or remaining in a droplet-like shape with a finite contact angle. The speed of this relaxation strongly depends on a friction force opposing the movement of the three-phase contact line. In analogy to the treatment of hydrodynamic friction we present an exact method, based on the Mori-Zwanzig formalism, to extract this friction from equilibrium data. Within the linear response regime, we obtain the frequency-dependent dissipative and elastic response of the contact line to an external perturbation, including a frequency-dependent friction coefficient. We find that the contact line exhibits long-lasting memory with a power-law decay due to coupling to the systems hydrodynamic modes. As a result the microscopic contact line dynamics are neither Markovian nor determined by the movement of a few molecules in the vicinity of the contact line.

CPP 10.4 Mon 15:45 ZEU/0118

Reaction-Mediated Arrest and Gradient-Driven Droplet Transport — •Stefan Köstler[1,2], Yicheng Qiang[1], Malcolm Steen[1,2], Guido Kusters[1], and David Zwicker[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany — [2]University of Göttingen, Institute for the Dynamics of Complex Systems, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Controlling droplet size and position is central to many biological and engineering processes. Chemical reactions can arrest coarsening and sustain spatial concentration gradients, while hydrodynamic flows generally accelerate coarsening and drive droplets along chemical gradients. Using continuum theory, we show that the competition between reactions, diffusion, and hydrodynamic advection yields rich behavior even in binary systems: Advection dominates the coalescence of small droplets, diffusion leads to Ostwald ripening for intermediate sizes, and reactions finally suppress coarsening. Interestingly, a range of droplet sizes is stable, depending on initial conditions and the strength of advection. Crucially, chemical gradients can actively steer droplets and couple to size-control. Our results demonstrate practical routes to control both the size distribution and spatial organization of droplets by tuning chemical activity and gradient-driven flows.

CPP 10.5 Mon 16:00 ZEU/0118

From bipedal to chaotic motion of chemically fueled partially wetting liquid drops — •Florian Voss[1] and Uwe Thiele[1,2] — [1]Institute of Theoretical Physics, University of Münster — [2]Center for Data Science and Complexity (CDSC), University of Münster

Chemomechanical coupling is essential to various phenomena in soft matter systems that are kept permanently out of thermodynamic equilibrium, e.g., in reactive complex liquids. Based on a thermodynamically consistent continuum model, we demonstrate that partially wetting liquid drops covered by chemically reacting surfactants display a variety of biomimetic motility modes like shuttling, bipedal, rotational and quasi-random motion when supplied with chemical fuel from an ambient bath. The dynamics originates from chemomechanical feedback between the reaction network on the drop and the Marangoni effect [1] and becomes increasingly complex as a result of competing length scales. Due to the generic underlying thermodynamic structure, we expect that our results are also relevant for other chemically active mixtures and soft matter systems.

[1] F. Voss and U. Thiele, Phys. Rev. Fluids 10, 94005 (2025).

CPP 10.6 Mon 16:15 ZEU/0118

Odd Droplets — •Thomas Appleford — University of Amsterdam, Amsterdam, Netherlands

In chiral systems such as active spinning colloidal matter, time-reversal symmetry-breaking interactions often give rise to a macroscopic continuum description in which the stress tensor contains off-diagonal terms. In fluids, these off-diagonal components lead to so-called "odd-viscous" deformations, in which energy is not dissipated. Odd viscous fluids have been shown to exhibit a rich variety of phenomena, including symmetry-broken flow around translating droplets and asymmetric droplet spreading on superhydrophobic surfaces. Our work investigates the behaviour of droplets in suspension. In particular, we present an analytical solution to the droplet-in-shear problem within the framework of two-dimensional odd Stokes flow, followed by the derivation of a formula for the apparent viscosity of a dilute emulsion. We then explore how chirality can be parametrically varied to tune the bulk rheological properties and control the system's overall energy dissipation.

CPP 10.7 Mon 16:30 ZEU/0118

Stretching and Sliding Capillary Bridges — •Lennard Holschuh and Lars Pastewka — University of Freiburg, Department of Microsystems Engineering

Capillary forces play a critical role in the adhesion between two contacting bodies. However, existing theories of macroscopic adhesion on rough surfaces often assume dry conditions, attributing adhesive interactions solely to dispersion forces and overlooking the effects of capillary bridge formation. This study em-

ploys molecular dynamics simulations to directly examine the interactions of nanoscale probes with nominally flat surfaces in the presence of liquid bridges, which form due to condensation in humid environments. The objective is to link the thermodynamic understanding of capillary bridges with molecular simulations and atomic-force microscopy experiments. These calculations focus on investigating energy dissipation during adhesion (normal separation of the probe from the surface) and friction (lateral motion of the probe). By quantifying the interplay between relative humidity, adhesion, and friction, this work aims to improve the understanding of macroscopic adhesion in humid conditions and guide the development of materials with tailored properties for high-precision applications, such as microelectronic manufacturing.

15 min. break

CPP 10.8 Mon 17:00 ZEU/0118

Hyperuniformity in Ternary Fluid Mixtures: The Role of Wetting and Hydrodynamics — •Nadia Bihari Padhan and Axel Voigt — Institute of Scientific Computing, TU Dresden, 01069 Dresden, Germany

Phase separation in multicomponent fluids underlies the organization of complex materials and biological structures, including biomolecular condensates. The Cahn-Hilliard-Navier-Stokes (CHNS) framework provides a natural description of such systems by coupling diffusive and hydrodynamic processes. In this talk, I will present our study of hyperuniformity–suppressed large-scale density fluctuations–in ternary CHNS mixtures. We show that hydrodynamics systematically drives the system toward less hyperuniform states and generates a rich set of morphologies, such as interconnected droplets and double emulsions reminiscent of biological phase separation. In partial-wetting regimes, all three components display comparable hyperuniformity, whereas in complete-wetting regimes the preferred wetting component exhibits a marked loss of hyperuniformity. These results identify wetting asymmetry as a key control parameter for spatial order in multiphase fluids and offer a pathway for tuning large-scale organization in soft-matter and biological systems.

References [1] Boyer, F. and Lapuerta, C., Study of a three component Cahn-Hilliard flow model, ESAIM: Mathematical Modelling and Numerical Analysis, 40, 653-687 (2006). [2] Padhan, Nadia Bihari and Voigt, Axel, Hyperuniformity in ternary fluid mixtures: the role of wetting and hydrodynamics, arXiv:2506.22647, (2025).

CPP 10.9 Mon 17:15 ZEU/0118

Effect of Flow Coupling on Defect Binding and Unbinding in Nematic Fluids — •Jayeeta Chattopadhyay, Simon Guldager Andersen, Kristian Thijssen, and Amin Doostmohammadi — Niels Bohr Institute, University of Copenhagen, Blegdamsvej 17, Copenhagen, Denmark.

Topological defects play a central role in the ordering and dynamics of nematic fluids. We investigate how coupling to fluid flow modifies defect-mediated phase transitions in two-dimensional nematics using fluctuating nematohydrodynamic simulations. The system is driven by tuning the fluctuation strength, with increasing and decreasing fluctuations defining forward and backward protocols. Without flow coupling, the system undergoes a Berezinskii–Kosterlitz–Thouless (BKT)–like transition via the reversible binding and unbinding of $\pm 1/2$ defect pairs. When hydrodynamics is included, the transition depends on the flow–alignment parameter: non-aligning nematics ($\lambda = 0$) retain BKT-like behavior, whereas strain-rate–aligning nematics ($\lambda \neq 0$) form bend–splay walls, lowering the defect-creation threshold and preventing recombination, leaving defects unbound across all fluctuation strengths. In active nematics, defects remain unbound for all λ, showing that self-generated flows also inhibit bound-pair formation. These results demonstrate that coupling to fluid flow fundamentally alters topological phase behavior, suppressing the equilibrium BKT binding mechanism.

CPP 10.10 Mon 17:30 ZEU/0118

Electrophoresis in charged chiral active fluids with odd viscosity — •Reinier van Buel, Bogdan Cichocki, and Jeffrey Everts — Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland

Understanding the motion of colloidal particles dissolved in fluids that exhibit odd viscosity – a specific component of the viscous stress tensor found in e.g. chiral active fluids – is of particular interest for realising nontrivial particle transport and characterising out-of-equilibrium thermodynamic properties. Although three-dimensional odd viscosity has not yet been experimentally observed, charge stabilisation is expected to be vital in enabling such measurements. Therefore, we introduce the notion of a charged chiral active fluid and we investigate some of its non-trivial electrokinetic properties. In particular, we focus on electrophoresis of a charged sphere suspended in such an odd viscous fluid. Here, the peculiar nature of odd viscosity breaks the spherical symmetry of the system, and through coupling with the electric double layer and its screening properties, alters the electrophoretic mobility. Using the Lorentz reciprocal theorem, we derive expressions for the electrophoretic mobility of a spherical particle based on the analytical solution for the uncharged flow. Furthermore, we highlight how the Hückel and Smoluchowski limits of the electrophoretic mobility are affected by odd viscosity. Our results demonstrate that odd viscosity leads to directional asymmetries in the electrophoretic mobility tensor, suggesting mechanisms for active control of charged colloidal motion in systems where odd viscosity is prevalent.

CPP 10.11 Mon 17:45 ZEU/0118

Experimentally probing microscale torsional memory in a viscoelastic fluid — •Niloyendu Roy[1], Rupayan Saha[2], Debankur Das[2], Matthias Krüger[2], and Clemens Bechinger[1] — [1]Fachbereich Physik, Universität Konstanz, Konstanz, Germany — [2]Institut für Theoretische Physik, Universität Göttingen, Göttingen, Germany

Motion of a colloid inside viscoelastic fluids follows non-Markovian dynamics, meaning its trajectory is influenced by past motion. Such memory effects are typically attributed to intrinsic material timescales arising from relaxation of the fluid microstructure and are usually probed using translationally driven colloids. Here we show experimentally that rotational driving of a colloid by a controlled torque elicits a far richer form of memory: the relaxation of the resulting torsional stresses spans a broad distribution of timescales, even though the fluid itself possesses a single dominant relaxation time. This behaviour allows time-dependent torsional driving histories to be encoded and subsequently read out through characteristic non-monotonic recoil responses. By mapping the flow field and the spatial distribution of torsional stresses, we demonstrate that the geometry of rotation generates an orthogonality between the propagation of angular momentum and the storage of torsional stresses, producing a spatio-temporal memory field not accessible through translational forcing. These results establish torsional driving as a powerful route to generate, store, and retrieve memory in viscoelastic fluids, opening new possibilities for soft-matter information storage and torque-responsive microdevices.

CPP 10.12 Mon 18:00 ZEU/0118

3D Optofluidic Control Using Reconfigurable Thermal Barriers — •Falko Schmidt[1,2], Carlos David Gonzalez[3], Marc Sulliger[1], Emilio Ruiz-Rena[4], Raul A. Rica[3,5], Jaime Ortega-Arroyo[1], and Romain Quidant[1] — [1]Department of Mechanical and Process Engineering, ETH Zurich, Zurich 8092, Switzerland — [2]Peter Debye Insitute for Soft Matter Physics, Leipzig University, 04103 Leipzig, Germany — [3]Universidad de Granada, Department of Applied Physics, Granada 18071, Spain — [4]Department of Applied Physics II, University of Malaga, Malaga 29071, Spain — [5]Universidad de Granada, Research Unit Modeling Nature (MNAT), Granada 18071, Spain

Optothermal manipulation enables precise control of small particles via optical and thermal forces, leveraging thermo-osmotic and convective flows for short- and long-range motion. We present a reconfigurable optofluidic method enabling diverse manipulations such as guiding, sorting, trapping, and separating particles. Using light absorption on plasmonic surfaces of gold nanorods, localized hot spots are generated, creating temperature-driven flows. A near-infrared laser spatially modulates temperature landscapes, monitored by 3D holographic microscopy and optical diffraction tomography. Single and double heat sources produce three-dimensional flow control. This creates an optofluidic barrier that redirects particles within a microfluidic chamber. This approach offers a versatile foundation for advancing microfluidic technologies, enabling applications in sorting, trapping, and adaptive system design.

CPP 10.13 Mon 18:15 ZEU/0118

Dynamics and Ordering of Microdroplets in Marangoni Flow Field — •Akshay Kallikkunnath and Frank Cichos — Molecular Nanophotonics, Peter Debye Institute for Soft Matter Physics, Faculty of Physics and Earth System Sciences, Leipzig University, Linnéstraße 5, 04103 Leipzig, Germany

Collective organization and internal dynamics are intimately linked and emerge across biological scales, with ordered structures providing a framework within which individual constituents remain dynamically active. Here, we study a system of water-in-oil microdroplets containing heat-releasing particles that organize under thermally induced flows. A sub-kelvin temperature increase from the heated particle at the air-oil interface generates Marangoni circulation that advects the droplets. Interactions through the flow field lead to robust ordering, while internal particle dynamics reflect coupling between local thermal gradients and microscale hydrodynamics. This provides a controllable platform to probe self-organization and emergent order by generating flows driven by weak, localized thermal fields in a fully fluid-in-fluid environment.

CPP 11: Active Matter II (joint session DY/BP/CPP)

Time: Monday 15:00–18:30 Location: ZEU/0160

CPP 11.1 Mon 15:00 ZEU/0160

Field-controlled self-organization in an active spin system — Mintu Karmakar[1,2,3], •Matthieu Mangeat[4], Swarnajit Chatterjee[5,4], Heiko Rieger[4], and Raja Paul[3] — [1]WIUCAS, Beijing, China — [2]Universitat de Barcelona, Barcelona, Spain — [3]IACS, Kolkata, India — [4]Saarland University, Saarbrücken, Germany — [5]CY Cergy Paris Université, Cergy-Pontoise, France

We investigate the collective response of active Potts particles to an external magnetic field and uncover three striking nonequilibrium phenomena. We first examine how the flocking transition is reshaped for a homogeneous and unidirectional field: the coexistence regime between an apolar gas and a polar liquid is replaced by a phase separation between two polar-ordered phases, a low-density, weakly polarized background and a high-density, strongly polarized band, both moving along the field. Second, when the particles self-organize into a high-density longitudinal lane whose long axis is perpendicular to the field, the lane slowly treadmills against the field direction, driven by the weakly polarized background. Finally, we identify a field-induced interface pinning regime that arises when the domain is divided into two regions with opposite field directions, causing particles to accumulate and perform a back-and-forth motion at the interface. This pinning phenomenon also leads to the emergence of a disordered state in the presence of a random field orientation. A coarse-grained hydrodynamic theory supports and confirms the phenomena observed in our microscopic simulations.

CPP 11.2 Mon 15:15 ZEU/0160

Nucleation kinetics in two-dimensional polar active fluids — •Yuta Kuroda and Thomas Speck — Institute for Theoretical Physics IV, University of Stuttgart, Germany

Polar active fluids constitute one of the most important classes of active matter. These systems possess alignment interactions that cause the local polarization to align with that of neighboring particles, leading to a flocking transition in which global polar order emerges. Extensive numerical and analytical studies have established that the flocking transition is discontinuous, and consequently, the phase diagram possesses a coexistence region in which propagating polar bands appear. Despite intensive studies on flocking transitions, the nucleation mechanism responsible for the formation of these bands remains poorly understood. In this work, we numerically investigate the nucleation kinetics of polar bands using a particle model, namely active Brownian particles with a Kuramoto-type alignment interaction, and we report the behavior of the nucleation rate over a wide range of parameters.

CPP 11.3 Mon 15:30 ZEU/0160

Collision dynamics of active Brownian hard disks — •Jonas Buba — Soft Matter Theory Group, Theoretical Physics: Lab for Emergent Phenomena, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Active matter systems, composed of self-driven agents, display emergent behaviors such as collective motion, clustering, and motility-induced phase separation (MIPS). To better understand the microscopic origin of MIPS, we study collisions of active Brownian hard disks within the framework of dynamical density functional theory (DDFT). The particle interactions are modeled using fundamental measure theory (FMT). Each particle is represented by a Gaussian density peak, which allows us to quantify the mean delay from collisions for different configurations. The post-collision density resulting from the simulation can be described by a convolution of the pre-collision density, enabeling the analysis of different contributions to the delay.

CPP 11.4 Mon 15:45 ZEU/0160

Active Ornstein-Uhlenbeck Particles: A Stochastic Path Integral Approach — •Carsten Littek, Mike Brandt, and Falko Ziebert — Institut für Theoretische Physik, Universität Heidelberg, Germany

In a recent publication (arXiv:2509.26296) we have developed a path integral formulation of the stochastic dynamics of a single active Brownian particle (ABP), with or without a constant torque, confined by a harmonic trap. This approach is based on the particle's microscopic degrees of freedom and we have derived exact analytic time-dependent expressions for key observable quantities such as the mean position and mean square displacement without the necessity of solving the Fokker-Planck equation. Here we present the application of this approach to the dynamics of active Ornstein-Uhlenbeck particles (AOUP). In particular, we generalize our formulation to systems of many AOUPs interacting via a suitable two-particle potential and derive the statistical quantities relevant in the context of collective phenomena, such as motility-induced phase separation (MIPS).

CPP 11.5 Mon 16:00 ZEU/0160

Self-alignment and chirality in dense active matter: from flocking to circling crystals — •Marco Musacchio[1], Alexander Antonov[1], Hartmut Löwen[1], and Lorenzo Caprini[2] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf, Germany — [2]Physics Department, University of Rome La Sapienza, P.le Aldo Moro 5, IT-00185 Rome, Italy

Several experimental systems in active matter are characterized, at the single-particle level, by an effective torque that aligns particle orientation with their instantaneous velocity. This mechanism, known as self-alignment, appears in both biological and granular active systems. In dense active systems, a sufficiently strong self-alignment can suppress mips and drive the system from a clusterized flocking state to an homogeneous one, where all particles move collectively, with aligned velocities. This flocking transition is approached for a broad range of densities, even close to maximal packing, where the system is in a crystalline configuration. Specifically, in the crystal case, the flocking transition can be predicted analytically since the dynamics can be mapped onto a velocity-dependent Landau*Ginzburg free energy, revealing that this disorder*order transition is second order. The onset of chirality drives the system from collective flocking to a circling crystal phase, characterized by coherent circular motion of all the system. Further increasing chirality suppresses the global rotation, leading to a vortex-like structure in the velocity field. These findings are experimentally testable in systems governed by self-alignment and chirality.

CPP 11.6 Mon 16:15 ZEU/0160

Number fluctuations distinguish different self-propelling dynamics — •Tristan Cerdin[1,2], Sophie Marbach[2], and Carine Douarche[1] — [1]Université Paris-Saclay, CNRS, FAST, 91405, Orsay, France — [2]CNRS, Sorbonne Université, Physicochimie des Electrolytes et Nanosystèmes Interfaciaux, F-75005 Paris, France

In nonequilibrium suspensions, static number fluctuations N in virtual observation boxes reveal remarkable structural properties, but the dynamic potential of $N(t)$ signals remains unexplored. Here, we develop a theory to learn the dynamical parameters of self-propelled particle models from $N(t)$ statistics.

Theoretical plots of the mean-squared number difference $\langle \Delta N^2(t) \rangle$ exhibit 3 scaling regimes in time corresponding to the 3 regimes of self-propelled particles: diffusive, advective and effectively diffusive again at long times. By expanding the theory in each of these regimes, we recover limiting laws for the number fluctuations, which can be used in practice to quantify self-propulsion properties.

Additionally, unlike traditional trajectory analysis, $N(t)$ statistics distinguish between models, by sensing subtle differences in reorientation dynamics that govern re-entrance events in boxes. This paves the way for quantifying advanced dynamic features in dense, out-of-equilibrium suspensions.

CPP 11.7 Mon 16:30 ZEU/0160

Flocking transitions in dense mixtures of active self-aligning and passive particles — •Weizhen Tang[1], Amir Shee[2], Zhangang Han[1], Pawel Romanczuk[3,4], Yating Zheng[3,4], and Cristián Huepe[1,5,6] — [1]School of Systems Science, Beijing Normal University, Beijing, China — [2]Department of Physics, University of Vermont, USA — [3]Department of Biology, Humboldt Universität zu Berlin, Unter den Linden 6, Berlin, Germany — [4]Research Cluster of Excellence 'Science of Intelligence', Berlin, Germany — [5]Northwestern Institute on Complex Systems and ESAM, Northwestern University, Evanston, USA — [6]CHuepe Labs, 2713 West Augusta Blvd #1, Chicago, USA

We investigate the passivity-driven flocking transition in a dense mixture of self-aligning active particles and passive particles, using a minimal model of active polar disks. We show that anisotropic damping leads to a discontinuous flocking transition as a function of the fraction of passive components, whereas isotropic damping produces a smooth transition where the final ordered state can display sustained oscillations and remain trapped in a metastable state, depending on the exact spatial arrangement of the passive particles. We also explore in detail the emergence of metastable oscillatory ordered states and their relation to the spatial distribution of passive particles and interstitial voids. Our findings demonstrate that heterogeneous activity and mobility anisotropy can result in a rich variety of self-organized states in various biological systems, synthetic active materials, and robotic swarms.

15 min. break

Invited Talk CPP 11.8 Mon 17:00 ZEU/0160

Topological transition in filamentous cyanobacteria: from motion to structure — •Marco Mazza — Loughborough University, Loughborough, UK

Many active systems are capable of forming intriguing patterns at scales significantly larger than the size of their individual constituents. Cyanobacteria are

one of the most ancient and important phyla of organisms that has allowed the evolution of more complex life forms. Despite its importance, the role of motility on the pattern formation of their colonies is not understood. Here, we investigate the large- scale collective effects and rich dynamics of gliding filamentous cyanobacteria colonies, while still retaining information about the individual constituents' dynamics and their interactions. We investigate both the colony's transient and steady-state dynamics and find good agreement with experiments. We furthermore show that the Péclet number and aligning interaction strength govern the system's topological transition from an isotropic distribution to a state of large-scale reticulate patterns. Although the system is topologically nontrivial, the parallel and perpendicular pair correlation functions provide structural information about the colony, and thus can be used to extract information about the early stages of biofilm formation. Finally, we find that the effects of the filaments' length cannot be reduced to a system of interacting points. Our model proves to reproduce both cyanobacteria colonies and systems of biofilaments where curvature is transported by motility.

CPP 11.9 Mon 17:30 ZEU/0160

Novel Phase Coexistence in a Multi-Species Vicsek Model — •Eloise Lardet[1], Letien Chen[1,2], and Thibault Bertrand[1] — [1]Imperial College London, UK — [2]University of Edinburgh, UK

A hallmark in natural systems, self-organization often stems from very simple interaction rules between individual agents. While single-species self-propelled particle (SPP) systems are well understood, the behavior of mixtures of self-propelled particles with general alignment interactions remains largely unexplored with a few scattered results hinting at the existence of a rich emergent phase behavior. Here, we first present a generalization of the two-species Vicsek model with reciprocal intra- and interspecies (anti-)alignment couplings, uncovering a rich phenomenology of emergent states. Notably, we show that rather than destroying polar order, anti-aligning interactions can promote phase separation and the emergence of global polar order. Secondly, we derive a kinetic theory for the system, finding good agreement between theoretical predictions and particle simulations. This includes a novel mechanism for microphase separation, as predicted by a Turing instability. We finally show that these coexistence patterns can be generalized to multi-species systems with cyclic alignment interactions.

CPP 11.10 Mon 17:45 ZEU/0160

Flocking in weakly nonreciprocal mixtures — •Charlotte Myin — Max Planck Institute for Dynamics and Self-Organization (MPI-DS), 37077 Goettingen, Germany

We show that weakly nonreciprocal alignment leads to large-scale structure formation in flocking mixtures. By combining numerical simulations of a binary Vicsek model and the analysis of coarse-grained continuum equations, we demonstrate that nonreciprocity destabilizes the ordered phase formed by mutually aligning or anti-aligning species in a large part of the phase diagram. For aligning populations, this instability results in one species condensing in a single band that travels within a homogeneous liquid of the other species. When interactions are anti-aligning, both species self-assemble into polar clusters with large-scale chaotic dynamics. In both cases, the emergence of structures is accompanied by the demixing of the two species, despite the absence of repulsive interactions. Our theoretical analysis allows us to elucidate the origin of the instability, and show that it is generic to nonreciprocal flocks.

CPP 11.11 Mon 18:00 ZEU/0160

Collective behavior in nonreciprocal multi-species Vicsek model with permutation symmetry — •Jae Dong Noh[1], Chul-Ung Woo[2], and Heiko Rieger[2] — [1]Department of Physics, University of Seoul, Seoul 02504, Korea — [2]Department of Theoretical Physics and Center for Biophysics, Saarland University, Saarbrücken, Germany

Nonreciprocal systems are typically built upon asymmetric roles among interacting agents, such as a pursuer-evader relationship. We propose a multi-species nonreciprocal active matter model that is invariant under permutations of the particle species. The nonreciprocal, yet symmetric, interactions emerge from a constant phase shift in the velocity alignment interactions, rather from an asymmetric coupling matrix. This system displays rich collective behaviors, including a species-mixed chiral phase with quasi-long-range polar order and a species-separated vortex cell phase. We present numerical evidence for these phases using particle-based Monte Carlo simulations and analytic evidence using continuum Boltzmann and hydrodynamic equations. Our work demonstrates that multi-species chiral fluids can be realized by a nonreciprocal but symmetric alignment interaction, where the rich collective behavior is a consequence of the interplay between nonreciprocity and permutation symmetry.

CPP 11.12 Mon 18:15 ZEU/0160

Flocking with random non-reciprocal interactions — •Jiwon Choi[1], Jae Dong Noh[2], and Heiko Rieger[1] — [1]Department of Physics & Center for Biophysics, Saarland University, Campus E2 6, 66123 Saarbrücken, Germany — [2]Department of Physics, University of Seoul, Seoul, 02504, Korea

Flocking is ubiquitous in nature and emerges from alignment interactions among self-propelled agents. Two species that anti-align or interact non-reciprocally exhibit complex collective phenomena, ranging from parallel and anti-parallel flocking and run-and-chase behavior to chiral phases. Whether such behavior survives in the presence of many species with random non-reciprocal interactions has remained unclear. As a first step, we study a continuous-time Vicsek-like model with fully random non-reciprocal interactions between particles. For infinite-range interactions, flocking emerges once the alignment bias becomes comparable to the non-reciprocal interactions, and deep inside this phase random non-reciprocity can still support slow global chiral and oscillating states. For short-range interactions, even without alignment bias, self-organized cliques form, where medium-sized clusters with predominantly aligning interactions remain stable over long times. We further investigate the robustness of clique formation and the coexistence phase under angular noise using a discrete-time Vicsek model with random non-reciprocal interactions. These results provide a basis for studying multi-species flocking with complex non-reciprocal interactions.

CPP 12: French-German Session: 2D Materials, Thin Films and Interfaces I

Time: Monday 15:00–17:00 Location: ZEU/0255

Invited Talk CPP 12.1 Mon 15:00 ZEU/0255

Multifunctional films by tailoring chemistry and morphology of polymer brushes at the nanoscale — •Petra Uhlmann and Alexander S. Münch — Leibniz-Institut für Polymerforschung Dresden, Hohe Strasse 6, 01069 Dresden

Functional polymer thin films, like stimuli-responsive polymer brushes or crosslinked polymer networks, are a group of smart surface coatings which are beneficial for the design of intelligent interfaces. One emphasis of our work is the synthesis of polymer brushes as a toolbox for the creation of specific surface functions and stimuli-responsive layers using a bottom-up approach. For many technical applications control and switching of wettability is a key property. In this contribution it will be shown how tailored co-polymers containing zwitterionic phosphorylcholine groups (MPC) and benzophenone (BPO) as anchoring and UV cross-linking units can be used to create multifunctional films with easy-to-clean, anti-fog, anti-fouling and anti-icing properties. For the achievement of the desired surface functions the control of not only the wettability, but also other thin film properties like thickness and degree of swelling, are crucial and require the respective optimization of the chemical polymer composition and the degree of crosslinking. For verification and adjustment of the interfacial and thin film properties atomic force microscopy (AFM), infrared spectroscopy (ATR-FTIR), contact angle measurements, and in-situ spectroscopic ellipsometry were used and correlated with respective coatings performance and sustainability tests.

CPP 12.2 Mon 15:30 ZEU/0255

Increase in elastic modulus of thin elastic films and membranes containing rigid inclusions - revisiting Einstein's relation in two dimensions — •Konstantin Zisiadis and Andreas Menzel — Otto-von-Guericke-Universität Magdeburg

Elastic matrices with well-separated inclusions can be described by effective elastic moduli obtained via homogenization methods. Probably the most basic relation for dilute systems is the Einstein equation $\eta_{\text{eff}} = \eta(1 + 2.5\phi)$. We consider the two-dimensional geometry of an elastic matrix in two dimensions with two-dimensional elastic moduli as counterparts to the three-dimensional case. Both plane-stress and plane-strain geometries are treated. We employ a generalized stresslet formalism. Our derived formulae for the effective moduli of the two-dimensional geometry are expressed using the two-dimensional elastic moduli for an arbitrarily compressible matrix. We find that the plane-stress and plane-strain equations for the effective moduli have the same form, while the associated two-dimensional moduli differ. Our results are consistent with previous research based on different approaches. For an incompressible matrix, we recover the known effective shear modulus $\mu_{\text{eff}} = \mu(1 + 2\phi)$.

We acknowledge support by the German Research Foundation (DFG) through Research Unit FOR 5599 on structured magnetic elastomers.

CPP 12.3 Mon 15:45 ZEU/0255

Structure and optical properties of donor-HATCN blends — •Gianfranco Melis, Dmitry Lapkin, Ainur Abukaev, Alexander Hinderhofer, and Frank Schreiber — Universität Tübingen, Tübingen, Germany

Organic thin films made of molecular semiconductors have the potential to advance the range of functional materials for technological progress. In this regard, electron donor-acceptor complexes (DAC) show unique physical properties at specific ratios due to their non-linear structure-property-composition dependence. A systematic study across the full mixing range is therefore essential to understand how structure and optical response evolve with composition.

Compositional-gradient thin films were prepared in a custom-built organic molecular beam deposition chamber by co-depositing donor materials—diindenoperylene (DIP), pentacene (PEN), coronene (COR), picene (PIC), α-sexithiophene (α-6T), zinc phthalocyanine (ZnPc), and perylenetetracarboxylic acid bis(propylimide) (PTCDI-C_3)—with the prospective non-fullerene acceptor hexaazatriphenylenehexacarbonitrile (HATCN). Grazing-incidence wide-angle X-ray scattering (GIWAXS), atomic force microscope (AFM), and UV-Vis absorption spectroscopy were applied to study and correlate structural and optical properties with the donor-acceptor stoichiometry. New absorption bands appear below the optical bands of pure materials at specific stoichiometric compositions, together with different surface morphologies and the formation of new mixed structural phases.

CPP 12.4 Mon 16:00 ZEU/0255

Optimized Phenyl-Modified g-C3N4/ZnO Hybrid Thin Films: Structural and Optical Insights — •Sahar Aghapour Ghourichay[1,2], Morgan Le Du[2], David P. Kosbahn[2], Guangjiu Pan[2], Hagen Uebele[2], Thomas Baier[2], Jinsheng Zhang[2], Lyuyang Cheng[2], Pier Carlo Ricci[1], and Peter Müller-Buschbaum[2] — [1]Department of Physics, University of Cagliari, Cittadella Universitaria, Monserrato, Italy — [2]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany

Phenyl-modified graphitic carbon nitride (PhCN)/ZnO hybrid thin films were fabricated with different PhCN loadings to investigate the influence of interface engineering on their structural and optical properties. UV-vis reflectance results show that the film containing 1 mL PhCN exhibits the lowest reflectance and the strongest absorption in the visible region. Photoluminescence analysis confirms that this optimized film has significantly reduced emission intensity, indicating more effective charge separation. XRD, AFM, and GIWAXS measurements reveal improved crystallinity and enhanced nanoscale ordering of ZnO in the presence of moderate PhCN content. SEM/EDS mapping verifies uniform hybrid formation, and XPS provides evidence of interfacial chemical interaction. Overall, controlled PhCN incorporation effectively tunes the optical response and nanoscale structure of PhCN/ZnO thin films, offering useful insights for photocatalytic and optoelectronic applications.

CPP 12.5 Mon 16:15 ZEU/0255

Machine Learning for Grazing-Incidence Diffraction (GID): from Raw Data to Crystalline Structure — •Dmitry Lapkin, Ainur Abukaev, Ekaterina Kneschaurek, Mikhail Romodin, Constantin Völter, Vladimir Starostin, Alexander Hinderhofer, and Frank Schreiber — Universität Tübingen

The optimization of novel materials in the form of thin films for specific applications requires the appropriate structural characterization methods. X-ray and neutron scattering techniques, such as grazing incidence small- and wide-angle X-ray/neutron scattering (GISAXS/GIWAXS/GISANS) or grazing-incidence diffraction (GID), offer the ultimate spatial resolution and high surface sensitivity, making them indispensable tools for thin film studies. At the same time, advancements in X-ray and neutron sources, in conjunction with developments in area detector technologies, enable the recording of several terabytes of raw two-dimensional detector data within a single experiment. Conventional methods of analyzing the GID data are severely under-paced compared to the data generation rates, representing a significant bottleneck and leaving much of the measured data unanalyzed. To make the thin film studies more efficient and increase the amount of analysed and published GID data that can be reused, we are developing a comprehensive machine learning based data analysis pipeline that goes from raw detector patterns to the corresponding crystalline structures. This pipeline comprises several stages, including data preprocessing and reduction, Bragg peak identification and refinement, and crystal structure determination.

Invited Talk CPP 12.6 Mon 16:30 ZEU/0255

Thin-film and interface properties in energy conversion devices unveiled by X-rays — •Marcus Bär — Department Interface Design, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH (HZB), Berlin, Germany — Energy Materials In-Situ Laboratory Berlin, HZB, Berlin, Germany — Department of Chemistry and Pharmacy, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — Department of X-ray Spectroscopy at Interfaces of Thin Films, Helmholtz-Institute Erlangen-Nürnberg for Renewable Energy, Berlin, Germany

This invited talk will present recent advances in the characterization of the chemical and electronic structure of interfaces and thin films that are central to modern energy-conversion technologies. A combination of X-ray spectroscopies enables non-destructive, depth-resolved insight into composition, chemical structure as well as bonding and energy-level landscapes across complex and often (deeply) buried interfaces. Interfacial intermixing, interlayer formation, oxidation processes, and energy-level alignment govern charge transport and recombination in energy conversion materials and devices. Illustrative case studies will be used to demonstrate how changes (e.g., in the thin-film deposition process) affect interfacial chemistry and electronic structure, highlighting the importance of the ability to probe interface properties as a prerequisite for deliberate interface design. In addition, the talk will outline recent progress in establishing dedicated sample environments allowing for in-situ and operando studies opening new pathways for understanding dynamic interface phenomena.

CPP 13: Charged Soft Matter, Polyelectrolytes and Ionic Liquids

Time: Monday 15:00–17:00 Location: ZEU/0260

Invited Talk CPP 13.1 Mon 15:00 ZEU/0260

Modelling and simulation of pH-sensitive polyelectrolyte microgels — •Stefanie Schneider — Institute of Physical Chemistry, RWTH Aachen University, Aachen, Germany

For weak polyelectrolytes (PE) as well as for weak polyampholytes (PA), not only the pH-pKA value but also the local electrostatic environment of the ionisable group determines the degree of ionisation and structural properties of the polymer. The proximity of already ionised groups, which is enforced by the interconnectivity of the polymer chain, influences the probability of additional groups to become ionised. Therefore, the degree of ionisation for polymers with different architectures differs from the ideal value, obtained for monomers at low concentrations.

Polyelectrolyte and polyampholyte microgels of different topologies have been investigated using constant pH-Monte Carlo simulations. Ionisation, swelling as well as the uptake and release of guest molecules were studied. [1-5]

Especially, the interaction with guest molecules is an important aspect for the use of microgels for drug delivery.

[1] C. Hofzumahaus, P. Hebbeker, S. Schneider, Soft Matter, 2018, 14, 4087.
[2] C. Hofzumahaus, C. Strauch, S. Schneider, Soft Matter, 2021, 17, 6029.
[3] C. Strauch, S. Schneider, Soft Matter, 2023, 19, 938.
[4] C. Strauch, S. Schneider, Soft Matter, 2024, 20, 1263.
[5] C. Strauch, L. Roß, S. Schneider, Soft Matter, 2024, 20, 9664.

CPP 13.2 Mon 15:30 ZEU/0260

Beyond electrostatic screening: Effect of ion pairing on acid-base equilibria in complex electrolyte solutions — •Varun Mandalaparthy[1], Johannes Hunger[2], Mischa Bonn[2], and Nico van der Vegt[1] — [1]Technical University, Darmstadt — [2]Max Planck Institute for Polymer Research, Mainz

The modulation of acid-base equilibria by salts is central to solution chemistry, yet the molecular origins of these effects in multi-component electrolyte mixtures remain incompletely understood. Building on evidence that individual salts induce ion-specific shifts in the pKa values of weak acids, we combine experiments with constant-pH molecular dynamics simulations to examine how ion pairing and specific ion interactions regulate the pKa of acetic acid in single and mixed sodium salt solutions. Across anions of differing charge density (sulfate, chloride, iodide), we show that cation-anion association-rather than electrostatic screening alone-governs the observed pKa changes. In solutions containing mixtures of sodium chloride and sodium sulfate, the impact on acetic acid pKa deviates from simple additivity because of complex ion-ion interactions. We present an ion-pairing-enhanced Debye-Hückel model that quantitatively reproduces these behaviors, offering a predictive framework for pH regulation in multi-salt environments. This work provides a mechanistic foundation for interpreting and forecasting pH-dependent behavior in complex systems relevant to biochemistry and soft matter.

Mandalaparthy et al. ChemRxiv. 2025; doi:10.26434/chemrxiv-2025-p2chl (under review at J. Phys. Chem. Lett.)

CPP 13.3 Mon 15:45 ZEU/0260

How polymer chain flexibility influences orientation and entanglements in polyelectrolyte solutions — Sascha Bartosch and •Ulrich Scheler — Leibniz-Institut für Polymerforschung Dresden e.V.

Entanglements in long-chain polymers are important for their mechanical properties and strongly impact the processability. In solutions the formation of entanglements depends on chain length, concentration and the chain flexibility. The flexibility of polyelectrolyte chains is influenced by the ionic strength of the solution that may screen the repulsive electrostatic interaction along the chain. That is reflected in the variation of the hydrodynamic radius of the polyelectrolytes measured by diffusion NMR. Upon shear polymers can orient or polymer chains maybe pulled out of entanglements. The NMR transverse relaxation time T2 is a good measure for the slow polymer-chain dynamics affected by polymer entanglements. Aligning polymer chains results in a shortened T2 while the loss of entanglements yielding longer chain segments between entanglements results in a longer T2. Short-chain polyelectrolytes under shear in a Searle cell show chain orientation. Long-chain polyelectrolytes at low ionic strength orient as well, while at higher ionic strength a loss of entanglements is observed. The transition from stiff to flexible entangled polymer is triggered solely by the electrostatic interaction modulated by the ionic strength under experimental control.

CPP 13.4 Mon 16:00 ZEU/0260

Molecular Mechanisms Underlying LCST and UCST Transitions in Thermoresponsive Ionic Liquids — •Hussen Oumer Mohammed[1,2], Abel De Cozar[1,2], and Ronen Zangi[1,2] — [1]Donostia International Physics Center (DIPC), Donostia, Spain — [2]University of the Basque Country UPV/EHU, Donostia, Spain

We investigate liquid-liquid phase separation (LLPS) of ionic liquid (IL)-water mixtures through atomistic MD simulations. Two model systems are studied: [P_{4444}] [TMBS], which exhibits a lower critical solution temperature (LCST) phase separation, and [Hbet][Tf_2N], which displays an upper critical solution temperature (UCST) behavior.

Aiming to elucidate the driving forces governing the two types of phase separation, we performed a detailed analysis of energy decompositions, HB networks, and microstructural organizations. We find that for [P_{4444}][TMBS]/water phase demixing, increasing temperature weakens IL-water HB, augments the enthalpic penalty of hydration, and favors ion pairing and mesoscale segregation. Conversely, for [Hbet][Tf_2N]/water demixing, cooling enhances water self-networking and suppresses ion hydration, promoting like-like association, while heating disrupts the water network and re-establishes miscibility through stronger ion-water HB.

By shedding light on these molecular-level mechanisms underlying those behaviors in distinct ILs, this study offers a predictive simulation-based framework for the rational design of thermoresponsive draw solutes in FO desalination, enabling tunable and energy-efficient regeneration cycles.

CPP 13.5 Mon 16:15 ZEU/0260

Machine-Learning Prediction of Ionic Conductivity from Short-Time Structural Data in Ionic Liquids — •David Bienek — Helmholtz-Institut Münster, Münster, Germany

Molecular dynamics (MD) simulations are a powerful tool for studying electrolyte materials, but the reliable calculation of ionic conductivities and transference numbers requires long trajectories. In this project, we explore whether machine-learning (ML) models can predict dynamic properties of ionic liquids (ILs) from structural information obtained in much shorter simulations. ILs are chosen as model systems because prior work has demonstrated links between structure and hydrodynamic behaviour. Their simple cation-anion composition also allows systematic generation of simulated systems. As structural descriptors, we employ radial distribution functions (RDFs), which are physically interpretable.

We test linear regression, random forests, and neural networks for predicting ionic conductivity. After feature engineering we find substantial improvements in accuracy. A peak-based representation proves particularly helpful for identifying structure-dynamics relations. Feature-importance analyses consistently indicate that the dominant information originates from the first coordination shell. Moreover, simpler models (random forest, linear regression) outperform neural networks, highlighting the necessity to use appropriate model complexity. Overall, our results show that ML can support the identification of structure-dynamics correlations in electrolytes and may help estimate transport properties from short MD trajectories.

CPP 13.6 Mon 16:30 ZEU/0260

Dissociation of weak polyacid systems in solution and brush coatings determined by IR titration — •Martin Müller[1,2], Luise Wirth[1,2], Birgit Urban[1], Leo Dagand[1,2], Alexander Münch[1], and Petra Uhlmann[1] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, Dresden D-01069, Germany — [2]Technische Universität Dresden, Dresden D-01062, Germany

The dissociation degrees a of poly(acrylic acid) (PAA) and propionic acid (PA) solutions were determined by infrared (IR) titration and potentiometric (POT) titration concept. Stepwise increasing pH value from 2 to 12 by adding NaOH portions, IR spectra of PAA and PA show decrease of n(C=O) band due to carboxyl (COOH) and increase of n(COO-) band due to carboxylate (COO-) groups. From the respective normalized band integrals A, dissociation degree was calculated according to a=A(COO-)/(A(COOH)+A(COO-)). Plotting pH versus a and fitting by modified Henderson-Hasselbalch equation according to pH=pKa+B*log(a/(1-a)) the parameters pKa and B were determined. The slight pKa deviation found for IR and POT titration, the respective deviation between monomeric PA and polymeric PAA and the PAA molecular weight trend (PAA-2K, PAA-50K, PAA-450K) are discussed considering the two-phase model of polyelectrolyte solutions and Gibbs-Donnan theory. Furthermore, a and pKa of thin PAA brush coatings under aqueous ambient and the influence of metal ion type (Na+, Ca++, Ce+++) and concentration were determined by FTIR titration revealing higher pKa values compared to solution state and significant effects of ion valency on a.

CPP 13.7 Mon 16:45 ZEU/0260

Unconventional Layer-by-Layer Assembly of Films with PEDOT: Write, Read, and Delete — •Muhammad Khurram, Martin Hunger, and Christiane A. Helm — muhammad.khurram@uni-greifswald.de

PEDOT:PSS films are widely used because they offer high conductivity & tunable electro-optical properties. We present an unconventional layer-by-layer (U-LbL) method for PEDOT:PSS/PDADMA multilayers. Masking was used to create either homogeneous coatings or narrow conductive strips. Each bilayer is only 7-9 nm thick, indicating that films form by adsorption of PSS-linked PEDOT, with unbound nanoparticles removed during rinsing. Flow-cell produces higher conductive films (260 kS/m) than dip coating. The U-LbL process also provides a natural framework for repeated Write/Read/Delete modulation, including PEDOT addition, partial & controlled PEDOT removal, forming molecular cavities that rebind PEDOT & restore percolative pathways.

CPP 14: French-German Session: Simulation Methods and Modeling of Soft Matter II

Time: Monday 17:15–19:00 Location: ZEU/LICH

CPP 14.1 Mon 17:15 ZEU/LICH

Lateral interactions in Bisphenol A adsorption on Carbon Nanotubes — •Oliver Cunningham and David Wilkins — Queen's University Belfast, Belfast, Northern Ireland

Endocrine disrupting chemicals (EDCs) such as Bisphenol A (BPA) are being found in water supplies with increasing frequency and our methods of water treatment need to improve alongside this ever increasing problem to mitigate the risks they pose to human health. Molecular Dynamics paired with enhanced sampling methods such as Metadynamics have proven to be very effective at studying the free energy profiles for processes like adsorption. To this end we present the effects lateral interactions between BPA molecules have on their adsorption onto a single walled carbon nanotube (SW-CNT) and how this depends on the number of BPA. The free energy of adsorption is studied as it gives insight into how well a SW-CNT adsorbs BPA and therefore how effective it is at removing it from water. Studying the free energy of adsorption for systems with varying numbers of BPA, we find that the free energy of adsorption increases with the number of BPA. This shows that lateral interactions between BPA molecules have a noticeable effect on how well they adsorb on the surface. We find two free energy minima corresponding to different conformations of the BPA, and the energy barrier between these minima decreases with the number of BPA. We also show that Parallel Bias Metadynamics provides an efficient way to bias all of the BPA in a system, providing better statistics than individually biased runs, while still achieving free energy's adsorption in agreement with the individual runs.

CPP 14.2 Mon 17:30 ZEU/LICH

Multiscale Modeling of Grain Boundary Effects on Charge Transport in Pentacene — •Sonali Garg, Farhad Ghalami, and Marcus Elstner — Karlsruhe Institute of Technology, Karlsruhe, Germany

Organic semiconductors have emerged as crucial materials in the development of electronic and optoelectronic devices due to their exceptional mechanical flexibility, lightweight nature, and cost-effectiveness. However, the presence of grain

boundaries (GBs) can significantly impede device performance by introducing structural defects that affect charge-carrier movement and reduce mobility. In this study, we developed a model to investigate the influence of GB characteristics, including misorientation angles and GB width, on charge carrier mobility, and compare the results with intrinsic mobility. Non-Adiabatic Molecular Dynamics (NAMD) simulations, employing the Fewest Switches Surface Hopping (FSSH) approach[1,2,3] were used to model charge transport dynamics. The charge transfer Hamiltonian was constructed using a fragment orbital approach, with its elements computed via the Density Functional Tight Binding (DFTB) method[4,5]. These insights provide a deeper understanding of the effects of GBs on charge-carrier mobility in organic semiconductors.

[1]Spencer. J et al. J. Chem. Phys. (2016) [2]Roosta. S J. Chem.Theory Comput. (2022) [3]Xie. W et al. J. Chem Theory Comput.(2020) [4]Elstner. M et al. Phys. Rev. B (1998) [5]Kubař. T et al. J.Phys. Chem. B (2010)

CPP 14.3 Mon 17:45 ZEU/LICH

A classical model to describe the electric potential-dependent water structure at metal interfaces — •Damien Toquer[1], Henrik Stooss[1], Philipp Stärk[1,2,3], and Alexander Schlaich[1] — [1]Institute for Physics of Functional Materials, Hamburg University of Technology, 21073 Hamburg, Germany — [2]Institute for Computational Physics, University of Stuttgart, 70569 Stuttgart, Germany — [3]SC Simtech, University of Stuttgart, 70569 Stuttgart, Germany

Nano- and microfabrication enable the development of functional materials tunable across length scales. While atomistic simulations are a powerful tool for studying and designing such materials bridging atomic-to-macroscopic properties remains challenging. The electrode/water interface exemplifies this challenge, explicit electronic treatment limits simulation scalability. Various schemes have been proposed that aim to incorporate metallic electronic response into classical molecular dynamics. Recently, the constant potential method has shown promise, where charges are attached to the metal atoms to maintain a fixed electrode potential. Our goal is to develop an efficient classical model that reproduces interfacial water structure across various electrode potentials, using gold surfaces as a prototype. Gold charges are adjusted to capture long-range continuum electrostatic interactions, while short-range interactions are tuned to match ab initio energy calculations. We anticipate this model will reliably predict interface-dependent thermodynamic properties both at equilibrium and under applied electrode potential, and plan to use it to study electrowetting in parallel with experimental work.

CPP 14.4 Mon 18:00 ZEU/LICH

Acoustic Effects in Electrolytes with Interfaces: Mechanistic Insights from MD Simulations — •Katharina Kintrup[1], Youssef Mabrouk[1,2], Diddo Diddens[1,3], and Andreas Heuer[1] — [1]Universität Münster, Institut für Physikalische Chemie, Deutschland — [2]Friedrich-Schiller-Universität Jena, Institut für Physikalische Chemie, Deutschland — [3]Helmholtz-Institut Münster, Deutschland

Interfaces such as electrodes strongly affect transport and dynamics in electrolytes. However, Molecular Dynamics (MD) simulations often assume periodic boundary conditions (pbc), thereby neglecting interfacial effects. This enforces a fixed center-of-mass frame in simulations, whereas electrophoretic NMR (eNMR) experiments [1,2] have shown that, in laboratory electrolytes, the center of mass drifts and local volume conservation is the appropriate assumption.

To mimic laboratory conditions, we introduce explicit interfaces in MD simulations and employ external fields for comparison with eNMR. As expected, we also observe a drift of the center of mass, but we do not find ideal local-volume conservation. Instead, we obtain oscillatory signals that reveal a strong dominance of acoustic effects over the intrinsic ionic dynamics. For binary electrolytes, we formulate a theoretical description that accurately incorporates the finite compressibility of the fluid. Overall, our work provides spatial and temporal insights into electrolyte dynamics in the presence of interfaces and highlights the importance of the chosen reference frame. [1] J. Phys. Chem. Lett. 2022, 13, 37, 8761-8767; [2] ACS Appl. Polym. Mater. 2025, 7, 13, 8432-8444

CPP 14.5 Mon 18:15 ZEU/LICH

Understanding electrode/electrolyte interfaces for electrocatalysis using constant potential DFT simulations — •Henrik Stooss[1], Philipp Stärk[2], and Alexander Schlaich[1] — [1]Institute for Physics of Functional Materials, Hamburg University of Technology, 21071 Hamburg — [2]Institute for Computational Physics, Universität Stuttgart, 70569 Stuttgart

This study explores the complex dynamics at electrode/electrolyte interfaces under constant potential, which is crucial for advancing electrocatalysis and designing efficient energy systems. We combine advanced computational techniques to gain insights into the mechanisms at these interfaces. Specifically, we perform Density Functional Theory (DFT) simulations of interfacial systems while maintaining a constant electrode potential. Despite the associated challenges and computational costs, these simulations provide valuable insights into the electronic structure and behavior of electrode surfaces. We calculate IR spectra of water in front of a gold electrode at different applied potentials and compare the results with experimental ATR-SEIRAS data, thereby strengthening the connection between first-principles calculations and experimental observations for material design.

CPP 14.6 Mon 18:30 ZEU/LICH

Atomistic modeling of azopolymers: light-induced deformation — •Dmitry Ryndyk[1,2], Olga Guskova[1], and Marina Saphiannikova[1,2] — [1]Leibnitz Institute of Polymer Research Dresden, Germany — [2]Technische Universität Dresden, Germany

In our recent study [1], we employ, for the first time, a fully atomistic force-field approach to model light-induced deformations in side-chain azopolymers. To mimic sample illumination, we introduce an orientation potential that reorients the azo chromophores perpendicular to the light polarization direction. This strategy enables us to capture both the microscopic details of chromophore behavior and the collective, anisotropic response of the polymer matrix. The atomistic simulations show a clear correlation between chromophore reorientation and sample contraction, as well as between backbone alignment and sample elongation. The separation of time scales between these two processes is controlled by the relative distance to the glass-transition temperature. Furthermore, the simulations elucidate a role of the flexible spacer in transferring the light-induced torque to the polymer backbone.

[1] D.A. Ryndyk, O. Guskova, M. Saphiannikova, Light-induced deformation of side-chain azo-polymer: Insights from atomistic modeling, arXiv:2511.19787 (2025)

CPP 14.7 Mon 18:45 ZEU/LICH

Self-Assembly of Porphyrin-Based Monomers into Supramolecular Polymers — •Mira Mors[1], Hanna Rieger[2], Oliver Stach[2], Thomas Speck[1], and Pol Besenius[2] — [1]Institute for Theoretical Physics IV, University of Stuttgart, Germany — [2]Department of Chemistry, Johannes Gutenberg-University Mainz, Germany

Through a combination of computational modeling and experiments, we investigate the assembly pathways of water-soluble supramolecular porphyrin-peptide amphiphiles. Our computational approach employs a coarse-grained, nine-bead planar model that captures the essential molecular interactions. Simulations show that stronger interactions promote polymerization, whereas increased monomer flexibility hinders it, consistent with experiments in which an additional glycine is introduced into the peptide arms. The observed power-law dependence of the polymerization half-time suggests a nucleation-elongation-aggregation pathway; however, experiments show no concentration-dependent aggregation. To probe oligomer stability, we apply a simplified free energy model and enhance sampling by generating a grand canonical system to map free energies across cluster sizes. Aggregation kinetics are additionally studied by solving the rate equations explicitly and using moment-based approaches. These analyses reproduce the dynamics from low to high interaction strengths, highlighting the vital role of recombination in the polymerization regime. Overall, our results provide a framework for a better understanding of supramolecular polymerization under varying conditions.

CPP 15: Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods II

Time: Monday 17:15–19:00 Location: ZEU/0255

CPP 15.1 Mon 17:15 ZEU/0255

Deep Learning-Driven Grazing Incidence Small-Angle X-ray Scattering Data Processing for Nanostructure Characterization — •Yufeng Zhai[1], Jungui Zhou[1], Shachar Dan[1], Julian Heger[2], Benedikt Sochor[1,3], Arno Jeromin[4], Wenbo Wang[5], Wolfgang Parak[5], Sarathlal Koyiloth Vayalil[1,6], Thomas Keller[4,5], Andreas Sitierle[4,5], Alexander Hexemer[3], Peter Müller-Buschbaum[2], and Stephan V. Roth[1,7] — [1]DESY, Hamburg, Germany — [2]TUM, Garching, Germany — [3]ALS/LBNL, California, United States — [4]CXNS, Hamburg, Germany — [5]UHH, Hamburg, Germany — [6]UPES, Dehradun, India — [7]KTH Stockholm, Sweden

Nanostructured thin films formed via nanoparticle deposition or self-assembly exhibit diverse morphologies that are crucial for their functional properties. Grazing-incidence small-angle X-ray scattering (GISAXS) provides detailed structural information on such systems, but conventional model-based fitting remains limited by simplified assumptions and convergence difficulties. We employ the distorted wave Born approximation (DWBA) to simulate a wide range of two-dimensional GISAXS patterns, which are used to train convolutional neural networks (CNNs) for predicting nanoparticle size distributions. The trained models demonstrate robust performance on both simulated and experimental data, providing a faster and more flexible alternative to traditional fitting. In ad-

dition, we have developed a graphical user interface (GUI) that integrates conventional fitting routines with our deep learning framework, providing a user-friendly platform for rapid GISAXS analysis.

CPP 15.2 Mon 17:30 ZEU/0255

Chirp-DMA for expanded frequency and reduced aging — •Juan Pablo Segovia Gutiérrez[1], José Alberto Rodríguez Agudo[2], Jan Haeberle[2], Dominic Oppen[2], Jörg Läuger[2], and Natalie Germann[1] — [1]University of Stuttgart, Stuttgart, Germany — [2]Anton Paar Germany GmbH, Ostfildern, Germany

Optimal Fourier Rheometry (OFR), or Chirp rheometry, is an advanced technique that uses a continuous, sine wave-shaped stress/strain signal characterized by an exponential frequency increase. This approach is important for measuring rapidly time-evolving soft materials, where conventional frequency sweeps are impractical; their slow, sequential data acquisition often fails to capture fast structural changes before the material itself mutates. A key advantage of Chirp is its ability to drastically reduce measurement time, making it highly effective at low and very low frequencies. This speed is essential to circumvent undesirable material aging, for instance in the dehydration observed in hydrogels, which modifies properties during long acquisition times. Conventionally, Chirp has been implemented using standard plate-plate geometries. The novelty of this study is the implementation of Chirp within a Dynamic Mechanical Analysis (DMA) setup utilizing extension and torsion modes. This permits the characterization of soft, fragile materials outside the typical rheometer configuration. By combining this novel Chirp-DMA approach with conventional sweeps on gellan gum/alginate hydrogels, we extend the practical frequency range and prove that Chirp recovers true viscoelastic moduli, thereby eliminating dehydration-induced effects.

CPP 15.3 Mon 17:45 ZEU/0255

PIERS-Based Mechanistic Insights into PVC Micro- and Nanoplastics Degradation on Ag Nanoflake-TiO2 Platform — •Olugbenga Ayeni[1], Josiah Ngenev Shondo[2], Tim Tjardts[3], Sinan Şen[4], Franz Faupel[3], Salih Veziroglu[3], Oral Cenk Aktas[3,4], and Tayebeh Ameri[1] — [1]Chair for Composite Materials, Department of Materials Science, Kiel University, Germany. — [2]Department of Energy Conversion and Storage, Technical University of Denmark, Denmark. — [3]Chair for Multicomponent Materials, Department of Materials Science, Kiel University, Germany. — [4]Department of Orthodontics, University Hospital of Schleswig-Holstein (UKSH), Kiel, Germany.

Conventional characterization techniques such as FTIR and SERS have been applied to Polyvinyl chloride (PVC) micro- and nanoplastics (MNPs) degradation, but they lack the combined real-time sensitivity and photocatalytic functionality needed to probe early-stage PVC-MNPs degradation. In this work, we report the use of Photo-induced enhanced Raman spectroscopy (PIERS) technique under continuous UV illumination to monitor the degradation of PVC-MNPs in real time on a highly active photocatalytic platform based on Ag nanoflakes (Ag NFs) grown on TiO2 thin films. Our PIERS-based approach reveals the chemical transformations and structural disorder occurring in the PVC-MNPs backbone within 10 min of UV irradiation. Our results establish PIERS as a promising mechanistic probe for tracking real-time PVC degradation pathways at the nanoscale. This study advances the mechanistic understanding of plastic degradation at the nanoscale.

CPP 15.4 Mon 18:00 ZEU/0255

Exploring Colloidal Kinetics Using DLS — •Mohit Agarwal and Jiaxing Sun — Swabian Instruments GmbH, Stuttgart, Germany

The kinetic behavior of colloidal and soft matter systems arises from particle diffusion, aggregation, and structural rearrangement, which collectively determine how microstructures evolve over time. Accurate characterization of these dynamics is crucial for understanding nonequilibrium phenomena such as gelation, crystallization, and phase separation in complex fluids. Conventional experimental techniques often lack the temporal and angular resolution needed to resolve these fast and heterogeneous processes in their native state, especially when multiple relaxation mechanisms coexist. We present a time-resolved, multi-angle Dynamic Light Scattering (DLS) technique that records individual photon arrival events in real-time across multiple scattering angles. This configuration enables angle-dependent temporal correlation analysis with improved sensitivity to both short-time diffusive motions and long-time relaxation processes that reflect evolving particle interactions. By employing complete photon statistics rather than time-averaged intensity correlations, the method captures transient fluctuations and kinetic transitions in colloidal suspensions. Measurements on well-defined colloidal dispersions reveal subtle temporal variations in particle dynamics and aggregation behavior that remain inaccessible with conventional single- or multi-angle goniometer-based DLS. The technique establishes a robust framework for real-time, multi-scale investigation of kinetic processes in colloidal and soft matter systems.

CPP 15.5 Mon 18:15 ZEU/0255

The Power of One Oxygen: How a Single Atom Alters the Field Evaporation of Liquid Crystals — •Kuan Meng, Sebastian Eich, and Guido Schmitz — University of Stuttgart, Institute for Materials Science, Heisenbergstr. 3, 70569 Stuttgart, Germany

In this study, we established a cryo-atom probe tomography (cryo-APT) workflow to investigate how the presence of a single oxygen atom alters the field evaporation behavior of two structurally similar liquid crystals: 8CB and 8OCB. Both compounds exhibited over 70% intact molecular retention and comparable fragmentation patterns.

Mass spectra revealed that the oxygen in 8OCB hinders the formation of extended cyanobiphenyl fragments across the linkage and promotes full cleavage of the alkyl chain. In contrast, 8CB allows the formation of longer backbone fragments. Spatially, 8CB evaporated mainly as intact molecules across both crystalline and smectic domains. 8OCB, however, evaporated predominantly as small fragments in low volume-density domains while as larger fragments or intact molecules in the high volume-density regions, which are suspected to crystalline and smectic phases, respectively. Further structural validation is required.

This work illustrates how cryo-APT enables the characterization of the molecular structure of organic liquid systems and demonstrates that even a single oxygen atom can fundamentally alter their field evaporation pathways. It further proposes a tunable fragmentation strategy to investigate molecular orientation in soft matter at an unprecedented resolution.

CPP 15.6 Mon 18:30 ZEU/0255

Depth-resolved cathodoluminescence for mapping exciton diffusion in rubrene thin film polymorphs — •Heiner Thiersch[1,2], Jonas Schröder[1], Anna-Lena Hofmann[1], Wooik Jang[1], Nora Engelmann[1], Fritz Henke[1], Maximilian F. X. Dorfner[3], Shu-Jen Wang[4], Frank Ortmann[3], Johannes Benduhn[1,2], Ellen Hieckmann[1], and Karl Leo[1] — [1]IAPP, TU Dresden, Germany — [2]DZA Görlitz, Germany — [3]Dep. of. Chem., TU München, Germany — [4]Dep. of. Phys., HKBU, China

The exciton diffusion length (L_D) is a key parameter in opto-electronic devices, as it governs the transport and recombination of photo-generated excitons. However, accurately measuring L_D remains challenging due to the limited penetration depth and lateral resolution of conventional techniques such as photoluminescence quenching and transient absorption spectroscopy. Here, we will introduce a novel approach for L_D determination based on quenching processes observed by depth-resolved cathodoluminescence (CL) measurements with highly localized excitation. The method combines CL experiments with kinetic Monte Carlo simulations and a diffusion model derived from Fick's second law. Applied to the organic semiconductor rubrene- renowned for its high hole mobility in single crystals- the technique yields L_D values ranging from 50 to 100 nm across different thin-film polymorphs. The results provide new insights into the exciton dynamics of rubrene and present a new methodological tool for accurate L_D characterization in semiconductors.

CPP 15.7 Mon 18:45 ZEU/0255

Towards Theoretical UV/Vis Spectra with Experimental Accuracy - Functional Errors and Thermal Broadening — •Robert Strothmann[1], Johannes T. Margraf[2], and Karsten Reuter[1] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]University of Bayreuth, Bayreuth, Germany

First principles methods like time-dependent density-functional theory (TD-DFT) can be used to predict molecular UV/Vis spectra relying on a number of approximations such as the choice of functionals, the description of solvation, as well as the treatment of thermal broadening. For the latter, simple (smeared) line spectra or structural ensembles obtained within the harmonic approximation are the most common choices. With the rise of machine learning interatomic potentials (MLIP) prohibitively costly *ab initio* molecular dynamics (MD) simulations can be replaced with similarly accurate MLIP MDs. This allows a detailed comparison of these approaches for a large number of systems for the first time.

In this talk, we benchmark predicted UV/Vis spectra against experimental references. To this end, the agreement with a curated set of literature reported spectra for diverse organic molecules in various solvents is assessed in terms of full spectral overlap, beyond a "peak to peak" comparison. We emphasize the influence of functional choice and thermal sampling approaches (e.g. harmonic vs. anharmonic), as well as the role of different conformers. How important each of these effects is and how it affects computational cost will be studied with the goal of providing best practise guidelines.

CPP 16: Energy Storage Materials and Devices II

Time: Monday 17:15–19:00 Location: ZEU/0260

Invited Talk CPP 16.1 Mon 17:15 ZEU/0260

Understanding the Passivation Properties of Solid Electrolyte Interphases (SEIs) in Batteries: Generator-Collector Experiments combined with a Transport and Reaction Model — •Bernhard Roling, Falk Krauss, Annalena Duncker, and Isabel Pantenburg — Department of Chemistry, University of Marburg, Germany

The solid electrolyte interphase (SEI) is a passivation layer in lithium-ion batteries, which has a strong impact on the battery lifetime. The SEI is formed by reductive decomposition of the electrolyte at the graphite particles of the anode during the first charging of the battery. The passivation of the SEI is not perfect, which leads to battery aging and to a reduced battery lifetime. The transport and reaction mechanism in the SEI governing the passivation properties are not well understood. Here, we elucidate transport and reaction processes during the formation of model-type SEIs by combining generator-collector experiments with a transport and reaction model. In the generator-collector experiments, we use a four-electrode-based setup to compare the electrolyte reduction current with a redox molecule reduction current at the SEI-covered electrode. We find that the current ratio depends on the SEI formation potential as well as on the formation time. The experimental results are compared to a transport and reaction model predicting four distinct transport and reaction regimes depending on the rate constant for the molecule-electron reaction. Using this combined approach, we obtain good estimates for the transport coefficients of both electrons and molecules inside the SEI.

CPP 16.2 Mon 17:45 ZEU/0260

Insight into SEI formation and dendrite growth in all-solid-state lithium metal batteries by Operando nWAXS — •Yingying Yan[1], Liangzhen Liu[2], Yuxin Liang[1], Lyuyang Cheng[1], Fabian A.C. Apfelbeck[1], Guangjiu Pan[1], Anton Davydok[3], Christina Krywka[3], Roland A. Fischer[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]TUM School of Natural Sciences, Chair of Inorganic and Metal-Organic Chemistry, Garching, Germany — [3]Helmholtz-Zentrum Hereon, Max-Planck-Str. 1, Geesthacht, Germany

Composite solid polymer electrolytes (CSPEs) have emerged as promising candidates for next-generation all-solid-state lithium batteries (ASSLBs). However, the limited ionic conductivity and poor interphase stability have seriously hindered their practical application. Herein, the anion-trapping layered double hydroxide (LDH) was introduced to enhance ionic conductivity and interfacial compatibility in poly(ethylene oxide) (PEO)-based CSPEs for stabilizing lithium metal anodes. Importantly, operando nano-focus Wide-angle X-ray scattering (nWAXS) was employed to spatially map the distribution of both the solid electrolyte interphase (SEI) layer and lithium dendrites across micron-scale lateral and vertical dimensions. Therefore, this study provides a novel strategy for designing high-performance CSPEs with stabilized interfaces and establishes an innovative approach for real-time visualization of SEI evaluation and dendrite growth in ASSLBs.

CPP 16.3 Mon 18:00 ZEU/0260

Temperature effects on the electrochemical behavior of graphite cathodes for aluminium-polymer batteries — •Mohammad Mostafizar Rahman, Mohammad Jony Rana, Shuvrodev Biswas, Amir Mohammad, Hartmut Stöcker, and Dirk C. Meyer — Institute of Experimental Physics, TU Bergakademie Freiberg, Leipziger Str. 23, Freiberg, 09599, Germany

This study assesses the performance of Aluminium-polymer batteries at variable temperatures between −20 °C and 80 °C. Pouch cells were constructed utilizing a solid polymer electrolyte (SPE) coupled with two different types of graphite cathode: mesocarbon microbeads (MCMB) and spherical graphite (SpG). Cyclic voltammetry and galvanostatic cycling with potential limitation measurements were conducted at different temperatures combined with variable current densities (25...100 mA/g). The results reveal that the resistance degradation below 0 °C is reversible, with performance being recovered when returning to positive temperatures. However, at moderately high temperatures above 60 °C, the degradation becomes permanent. MCMB cells operate effectively between −10 °C and 40 °C, while SpG cells function from 0 °C to 60 °C. The capacity of MCMB cells peaks at 20 °C at all current densities and then drops significantly at 60 °C. In contrast, SpG cells exhibit their highest capacities at 40 °C or 60 °C, followed by a rapid decline. Together with the good Coulombic efficiencies > 95 % both types of cells are proven suitable for varying environmental conditions.

CPP 16.4 Mon 18:15 ZEU/0260

X-Ray Absorption Near-Edge and Photoemission Spectroscopy of Deintercalation and Redox Reactions in Alluaudite-Type Na-Ion Cathodes — •Neama Imam[1], Karsten Henkel[1], Stephan Werner[2], Christoph Pratsch[2], Anna Milewska[3], Janina Molenda[3], Jan Ingo Flege[1], and Ehrenfried Zschech[1] — [1]Brandenburg University of Technology Cottbus - Senftenberg, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, BESSY II, Germany — [3]AGH University of Science and Technology, Krakow, Poland

We have investigated alluaudite-type $Na_{2.5-x}Fe_{1.75}(SO_4)_3$ cathodes that exhibit a three-dimensional open-channel framework with multiple Na sites. Using spatially resolved X-ray absorption near-edge spectroscopy (XANES), performed within a transmission X-ray microscope (TXM), and lab-based X-ray photoelectron spectroscopy (XPS), we have examined Na^+ deintercalation and Fe^{2+}/Fe^{3+} charge compensation at different selected charging states. This combination of bulk- and surface-sensitive methods allows correlating Na^+ depletion with Fe^{3+} formation, potentially identifying nanoscale redox heterogeneities and tracking changes in the local Na chemical environment. Our study builds on a broader investigation [1] that includes theoretical calculations as well as structural and electrochemical analyses.

[1] J. Molenda *et al.*, *Acta Mater.* **301**, 121582 (2025).

CPP 16.5 Mon 18:30 ZEU/0260

Understanding the Impedance Spectra of Composite Materials using a 3D Electrical Network Model — •Felix Schug[1,2], Sascha Kremer[2,3], Christian Heiliger[1,2], and Janis K. Eckhardt[1,2,3] — [1]Institute for Theoretical Physics, Justus-Liebig-University Giessen, Germany — [2]Center for Materials Research (ZfM), Justus-Liebig-University Giessen, Germany — [3]Institute of Physical Chemistry, Justus-Liebig-University Giessen, Germany

All-solid-state batteries (ASSBs) are promising candidates for next-generation energy storage systems, offering enhanced energy density and safety compared to conventional lithium-ion batteries. Electrochemical Impedance Spectroscopy (EIS) is a powerful method for determining charge transport characteristics in these systems. However, the presence of multiple phases, each with distinct transport processes, as well as complex microstructures result in complex impedance spectra that are challenging to interpret.

To address this challenge, we use a microstructure-resolved 3D electrical network model to simulate charge transport on microscopic length scales. This approach enables us to disentangle the contributions of different transport processes and microstructural features to the impedance response. Our model offers insights into the local potential and current distributions influenced by material heterogeneities, directly connecting them to impedance signals. We provide insights into the impedance of composite materials, identifying the key factors that dominate the impedance signal.

CPP 16.6 Mon 18:45 ZEU/0260

Dual-Ion $AlCl_4^-$ / $AlCl_2^+$ Charge Storage Mechanism in Composite Cathode for Aluminum-Polymer Batteries — •Shuvrodev Biswas, Thomas Köhler, Amir Mohammad, Hartmut Stöcker, and Dirk C. Meyer — Institute of Experimental Physics, TU Bergakademie Freiberg, Leipziger Str. 23 09599 Freiberg, Germany

Rechargeable aluminum batteries have emerged as a promising post-lithium-ion technology. Graphite, the most widely used cathode that relies on $AlCl_4^-$ intercalation, offers limited capacity, whereas organic cathodes, such as phenanthrenequinone (PQ), coordinate with $AlCl_2^+$ but suffer from limited cycling stability. Here, we design a composite (SPGPQ) consisting of spherical graphite (SPG) and PQ through melt diffusion, enabling dual-ion charge storage by coupling $AlCl_4^-$ intercalation with $AlCl_2^+$ coordination. FTIR, XPS, *in situ* XRD, and cyclic voltammetry using polyamide-6 (PA6) electrolytes (SPE) provide clear evidence of this synergistic mechanism. Whereas the PA6-SPE limits capacity due to low ionic conductivity, the higher-conductivity polyacrylonitrile (PAN)-based SPE delivers improved capacity but shows limited cycling stability. To enhance stability, we further developed an ACPQ+SPG composite through solvent-assisted impregnation using activated carbon (AC). This composite features an identical mechanism to SPGPQ, while offering significantly enhanced capacity and stable long-term cycling.

CPP 17: Poster I

Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates; Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics; Energy Storage Materials and Devices; French-German Session: 2D Materials, Thin Films and Interfaces; Wetting, Fluidics and Liquids at Interfaces and Surfaces

Time: Monday 19:00–21:00 Location: P5

CPP 17.1 Mon 19:00 P5

How do interfaces shape molecular conformations in condensates? — •Nora-Elen Giesinger[1] and Arash Nikoubashman[1,2] — [1]Leibnitz-Institut für Polymerforschung, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany

The interface between biomolecular condensates and their surrounding environment plays an important role for, e.g., regulating the condensate's stability and interactions with other cellular components. These interfacial properties are primarily dictated by the density and conformation of the constituent biomolecules, but it remains experientially challenging to resolve interfacial properties on the molecular level. Further, the conformations of the constituent biomolecules are influenced by many intertwined factors like sequence patterning, electrostatics, and chain-length diversity. To understand how polymer conformations evolve from the dense condensate interior through the interfacial region into the surrounding dilute phase, we use a minimal model of fully flexible homopolymers. To disentangle effects arising from chain ends, we examine condensates formed from both linear and ring polymers. Molecular dynamics simulation show that polymers gradually collapse as they transition from the bulk-like interior of the condensate to the surrounding dilute aqueous phase. Notably, the condensate interface induces a highly non-monotonic structural crossover between the dense and dilute regions, irrespective of the polymer architecture: the side facing the interface flattens, while the inward-facing side is also compressed. As a result, the monomer cloud loses its spherical symmetry, and chains tend to align tangentially along the interface.

CPP 17.2 Mon 19:00 P5

Effects of Activity on Polymeric Condensates — •Rahul Yadav[1] and Arash Nikoubashman[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, 01069 Dresden, Germany

Biological systems are inherently out of equilibrium as external sources of energy are constantly consumed; for example, microtubules and filamentous actin seemingly move through the cytoplasmic matrix via the continuous addition and removal of subunits. At the same time, equilibrium thermodynamic properties, governed by the interactions and length scales of the (macro)molecular constituents, play a central role in phenomena such as the formation of biomolecular condensates. A central open question is whether such non-equilibrium activity enhances phase separation or, conversely, hinders it. To answer this, we performed molecular dynamics simulations of a bead-spring polymer model, systematically varying both the attrac- tion strength and activity. When the active forces act along the contour of the polymer, the miscibility gap narrows and the critical temperature decreases with increasing activity, indicat- ing that this form of activity opposes phase separation. Based on these observations, we expect that contractile active forces will instead broaden the miscibility gap and increase the critical temperature, and we plan to test this prediction in future work.

CPP 17.3 Mon 19:00 P5

Using the Patchy Particle Model to simulate Biomolecular Condensates — •Mubarrat Mursalin[1,2], Simon Dannenberg[1], and Stefan Klumpp[1,2] — [1]Georg August University Göttingen — [2]Max Planck School of Matter to Life

Biomolecular condensates are formed through liquid-liquid phase separation (LLPS) of proteins, often together with nucleic acids, typically driven by low-affinity interactions. Phase separation allows biological systems to spatially organize molecules for biological functions. Theoretical studies of LLPS are usually based on continuum descriptions of fluids, which allows access to the biologically relevant time and length scales, but neglects all molecular details of the interactions, which implements their genetic programmability and determines the local structure of the condensates. Here, we use the coarse grained patchy particles to simulate LLPS, which provides an intermediate level of description between atomistic MD and continuum descriptions, thus allowing to access systems large enough to describe droplets and still retain a coarse-grained picture of the local structure inside the condensate. We look at the effects of repulsive crowding particles on the critical values, dynamics and structures of biomolecular condensates formed by three patch patchy particles. Using NVT simulations, combined with the direct coexistance method, we study the effects of crowder concentration and size, and recreate the known depletion and excluded volume effects.

CPP 17.4 Mon 19:00 P5

Partial demixing of RNA Polymerase II condensates in transcription regulation — Arya Changiarath[1], Rosa Herrera Rodriguez[1], Jasper Michels[3], Friederike Schmid[1], Jan Padeken[2], and •Lukas Stelzl[1,2] — [1]Johannes Gutenberg University Mainz — [2]Institute of Molecular Biology (IMB) — [3]Max Planck Insitute for Polymer Research

Phase-separated condensates may spatio-temporally regulate RNA polymerase II (Pol II) during the transcription of genes. Distinct condensates may underpin the two key stages of transcription, initiation and elongation. However, it remains unclear whether these condensates mix or maintain distinct chemical environments. To investigate this, we combined multi-scale molecular dynamics simulations with experiments in C. elegans. We identified a lower critical solution temperature (LCST) behavior for Pol II, where higher temperatures promote condensation. This behavior correlates with an incremental transcriptional response to temperature but is largely uncoupled from the classical heat stress response. Our simulations demonstrate that the phosphorylation state of the disordered CTD controls the demixing of CTD and pCTD, resulting in full or partial engulfment depending on composition. Remarkably, we observe such partially-demixed of RNA polymerase II condensates by super resolution microscopy of C. elegans embryos. Overall, our results suggest that partially demixed condensates provide distinct chemical environments and binding platforms to facilitate transcription initiation and elongation.

CPP 17.5 Mon 19:00 P5

Optimization of Slot-Die Printed Organic Solar Cells — •Dinusha M. Egalla, Christoph G. Lindenmeir, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany

Organic solar cells (OSCs) are promising candidates for lightweight, flexible, and low-cost photovoltaic technologies due to their solution processability and compatibility with large-area printing. The performance and stability of printed OSCs, however, are highly influenced by the morphology and uniformity of the active layer, which are sensitive to changes in coating and processing conditions. In this work, we investigate the optimization of printed donor-acceptor active layers by systematically varying key fabrication parameters, including coating temperature, printing speed, and solution preparation. The resulting thin films are characterized using UV-Vis spectroscopy to evaluate optical absorption, and microscopy to investigate the film homogeneity, while X-ray reflectivity (XRR) is used to determine film thickness and roughness. Full devices are built and assessed through current-voltage (J-V) measurements under standard illumination to establish how different printing conditions affect active-layer morphology and overall photovoltaic performance.

CPP 17.6 Mon 19:00 P5

Tuning Two-Photon Absorption Cross Sections in Azaacene Diradicals — •Gabriel Sauter[1], Antonia Papapostolou[2], Julia Weyandt[1], Pascal Merten[3], Kerstin Brödner[3], Uwe H. F. Bunz[3], Andreas Dreuw[2], and Petra Tegeder[1] — [1]Physikalisch-Chemisches Institut — [2]Interdisziplinäres Zentrum für Wissenschaftliches Rechnen — [3]Organisch-Chemisches Institut, Universität Heidelberg

Diradical bithiophene azaacenes have been shown as an outstanding class of nonlinear optical (NLO) materials with potential applications in bioimaging, photodynamic therapy, and 3D nanoprinting, while exhibiting exceptionally high two-photon absorption (2PA) cross sections exceeding 53000 GM [1]. Using a combined approach of experimental z-scan measurements and theoretical modeling, we analyzed the structure-property relationships governing NLO efficiency and tuning. Here especially the influence of diradical character, molecular extension, and sulfur substitution on the 2PA response was investigated. The results reveal fundamental insights into the synergy between molecular symmetry and electronic structure for optimizing the NLO responses. This enables a more targeted design of near-infrared active materials for photonic applications.

[1] G. Sauter, A. Papapostolou et al., *Angew. Chem. Int. Ed.* 2025, 64, e2503073.

CPP 17.7 Mon 19:00 P5

Long Chain, Strong Gain: How SubPC side chains control the pseudoferroelectric bulk photovoltaic effect — •Kaspar Haas[1], Sophia Klubertz[1], Victor Rodriguez[2], David González-Rodríguez[3], Miguel García Iglesias[2], and Martijn Kemerink[1] — [1]Universität Heidelberg, Heidelberg — [2]Universidad de Cantabria, Santander — [3]Universidad Autónoma de Madrid, Madrid

While most studies of the bulk photovoltaic effect (BPE) in recent years have focused on inorganic materials, this fascinating effect should also be observable in organics. In contrast to the conventional photovoltaic effect, the BPE voids the need for doping by utilizing an intrinsic symmetry breaking and could allow for wider absorption spectra while theoretically overcoming the Shockley-Queisser limit. Going organic holds the additional promise of lightweight, low-fabrication- and low-energy-cost devices, and, particularly, of a much greater tunability of the active material.

Here, we investigate organic molecules of the semiconducting π-conjugated SubPC-F family with the purpose of finding and quantifying a bulk photovoltaic effect. Combining electrical measurements with polarization optical microscopy (POM), XRD and AFM, we investigate the dipole alignment in these liquid crystalline materials, before assessing their photovoltaic performance under irradiation. We further build our own liquid crystal cells for measuring in out-of-plane structures to draw a connection between device thickness and performance. We also aim to quantify the influence of different side chain lengths on material properties like open-circuit voltage and photocurrent.

CPP 17.8 Mon 19:00 P5

Thin Films of Substituted Imidazoquinolines as Emitters for Blue OLED Devices — •Lasse Freitag[1], Pascal Schweitzer[1], Carina Rössiger[2], Thomas Oel[2], Richard Göttlich[2], and Derck Schlettwein[1] — [1]Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen — [2]Justus-Liebig-Universität Gießen, Institut für Organische Chemie, Heinrich-Buff-Ring 17, D-35392 Gießen

Organic semiconductors are routinely applied in microelectronics. Still challenging is the field of organic blue light emitting diodes (OLED), due to degradation of the emitters. We study the application of imidazoquinolines such as 4EstPhPh(iso)IC as emitters. Different substitutional patterns allow for tuning of their opto-electronic properties. We achieved thin films of 4EstPhPh(iso)IC via physical vapor deposition (PVD). Promising blue photo- and electroluminescence was found in solid state. Film formation at interfaces with contact materials was studied by in-situ Kelvin-probe force microscopy (KPFM). On the p-conducting poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) we found a Stranski-Krastanov (SK) growth of the emitter. X-ray diffraction (GI-XRD) confirmed a crystalline structure in these films, in line with single crystal data. Further, the growth of n-conducting bathocuproine (BCP) on the emitter layer was monitored by KPFM, revealing SK growth followed by formation of 3D crystalline islands. As a fundamental prerequisite, morphological stability at air was confirmed by microscopy. Therefore, we built OLED with varying thickness to find the best-performing layer stack.

CPP 17.9 Mon 19:00 P5

The aggregation of DPND dyes in the solid state studied by nuclear magnetic resonance spectroscopy — •Sascha Bartosch[1], Mohamed Bouajhine[2], Łukasz Kielesiński[3], Marieta Levichkova[4], Eva Bittrich[1], Petra Uhlmann[1], Patrick Brocorens[2], Martin Pfeiffer[4], Daniel T. Gryko[3], David Beljonne[2], and Ulrich Scheler[1] — [1]Leibniz-Institut für Polymerforschung Dresden e. V. - Dresden, Germany — [2]Laboratory for Chemistry of Novel Materials, University of Mons - Mons, Belgium — [3]The Institute of Organic Chemistry of the Polish Academy of Sciences - Warsaw, Poland — [4]Heliatek GmbH - Dresden, Germany

Dipyrrolonaphthyridinediones (DNPDs) have recently been introduced as a novel class of cross-conjugated dyes. Their promising photophysical properties make them a potential candidate for various applications. Although the packing type is expected to have an influence on the performance, their aggregation remains to be studied.

Solid-state NMR 1H-1H double-quantum-single-quantum correlation experiments are suitable to probe the spatial proximity of functional groups since it is based on short-range dipolar interactions between the spins. The proximity information is used for the understanding of the packing of molecules. Signals have been assigned by comparison of the experimental to simulated chemical shifts. Strong up-field shifts of aromatic protons induced by packing effects like pi-pi-interactions were observed, consistent with predicted crystal structures. Intermolecular homo couplings were used to identify different aggregation patterns.

CPP 17.10 Mon 19:00 P5

Influence of antisolvents and interfacial layers on charge carrier dynamics of hybrid perovskite films — •Leon Weintz[1], Patrick Dörflinger[1], Volodymyr Vasylkovskyi[1], Junmo Park[2], Hobeom Kim[2], and Vladimir Dyakonov[1] — [1]Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany — [2]Department of Materials Science and Engineering, Gwangju Institute of Science and Technology, 61005, Gwang-ju, Republic of Korea

Charge carrier behavior in perovskite thin films is crucial to their optoelectronic performance; yet, the impact of antisolvents and self-assembled monolayers (SAMs) on their basic charge carrier transport properties remains not fully understood. In this work, $FAPbI_3$ and $FAMACsPbBr_3$ perovskite systems are investigated to gain a more comprehensive understanding of how processing additives influence charge generation, transport, and recombination. The mobility and lifetime of photogenerated charge carriers in perovskite layers are determined in a non-contact way using Time-Resolved Microwave conductivity (TRMC), where the interaction of an applied electro-magnetic field with the charge carriers results in a time-dependent change in conductance. Complementary time-resolved photoluminescence (trPL) measurements support the interpretation of TRMC-derived carrier dynamics. Together, TRMC and trPL provide insight into how processing additives influence charge-carrier dynamics in perovskite materials.

CPP 17.11 Mon 19:00 P5

Comparative Analysis of Excited-State Dynamics in Thiophene based D-A-Polymers — Tobias Reiker[1], Marek K Charyton[2], Liu Zitong[3], Deqing Zhang[3], Nicolas D. Boscher[2], and •Helmut Zacharias[1] — [1]Center for Soft Nanoscience, University of Münster, Germany — [2]Materials Research and Technology Department, Luxembourg Institute of Science and Technology, Esch-sur-Alzette, Luxembourg — [3]Institute of Chemistry, Chinese Academy of Science, Beijing, China

We investigate the excited state dynamics of conjugated thiophen based polymers using several kinetic models commonly discussed in the literature. These models describe scenarios in which a short lived excited state acts as a precursor for one or more long lived states and are formulated through coupled rate equations. Four representative models were fitted to the dynamics of DPP4T-1 and subsequently applied to pDPP4T, DPP DTT, pF8T2 and pTDPP to identify trends linked to structural variations within the polymer series. This analysis provides a coherent framework for comparing relaxation pathways and for assessing how precursor states influence the formation of long lived excited state populations.

CPP 17.12 Mon 19:00 P5

Tuning the switching response of purely organic photonic devices by polymer blending — •Jinghan Lin, Sebastian Schellhammer, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics, Technische Universität Dresden, Dresden, Germany

Programmable luminescent tags (PLTs) provide a promising photonic technology for UV sensing by utilizing the oxygen-sensitivity of room-temperature phosphorescence (RTP) from purely organic emitters [1]. In the emissive layer, the emitter molecules are diluted at low concentration in a rigid polymer host, like Polystyrene (PS) or Poly(methyl methacrylate (PMMA), to reduce photonic loss mechanisms, e.g. triplet-triplet annihilation and non-radiative relaxation. Here, we tailor the microenvironment of RTP emitters and, thus, the photophysical characteristics of the emissive layer by blending different polymers. While the blending of PMMA550k with PS350k led to inhomogeneous films with insufficient photophysical properties, mixing of PS350k with PS40k allows the finetuning of the UV dose required to activate the RTP emission in the PLTs. By combining polymers with different physical characteristics, the local matrix rigidity, oxygen permeability, and intermolecular interactions can be varied in a controlled manner. The study demonstrates how polymer-host engineering provides a systematic route to modulate the characteristics of PLTs while maintaining their key characteristics.

[1] Gmelch et al., Science Advances 2019. aau7310

CPP 17.13 Mon 19:00 P5

Unraveling biodegradable phosphorescent emitters by combining quantum chemical simulations with photophysical spectroscopy — •Philipp Wieland, Iuliia Malakhova, Sebastian Reineke, and Sebastian Schellhammer — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics, Technische Universität Dresden

Naturally derived organic emitters are required for the design of efficient biodegradable photonic devices. For instance, quinoline alkaloids exhibit sufficient emission via room-temperature phosphorescence (RTP), enabling their successful application in programmable luminescent tags for sustainable information storage [1]. Despite minimal structural differences between specific emitters of this quinoline alkaloid material family, they result in very different device performances.

In this work we present a combined experimental and computational characterization of RTP-active quinoline alkaloids, aiming to improve the understanding of their structure-property relationship. Photoluminescence analysis of quinine and cinchonine shows that phosphorescence dominates as the radiation process in cinchonine, whereas fluorescence is much more pronounced in quinine. To understand the origin of these differences, Density Functional Theory simulations are conducted. Conventional modelling approaches typically rely on static descriptions, which, while efficient, fail to capture the behavior of highly dynamic molecules. To overcome this limitation, we explicitly incorporate Molecular Dynamics into the screening of excited state properties. [1] Thomas et al. Adv. Mater. 2024, 36, 2310674.

CPP 17.14 Mon 19:00 P5

Stabilization via Confinement of Halide Perovskites — •Marius Kaiser[1], Osama Alsheika[2], Helen Grüninger[2], and Eva M. Herzig[1] — [1]Dynamik- und Strukturbildung - Herzig Group, University of Bayreuth, Germany — [2]Bavarian Center for Battery Technology (BayBatt) and Inorganic Chemistry, University of Bayreuth

The practical use of halide perovskites (HPs) for optoelectronic applications is severely limited by degradation caused by intense light exposure, heat, and unintended ion transport under external electric fields [1]. Key challenges in this field include understanding the underlying mechanisms, stabilizing the semiconductor, and achieving controlled electron and ion transport.

Methylammonium lead bromide (MAPbBr3) is used as a model system, and its lattice parameters are systematically investigated in both bulk form and when confined within SBA-15 silica nanopores (average diameter ~8.4 nm), across a range of temperatures and pore loadings.

Furthermore, we examine thermal expansion behaviour of the materials and evaluate the effect of surface functionalization.

These results provide valuable insights for the development of more stable HP-based optoelectronic devices with directionally controlled charge transport.

[1] Greve, C. et al. To Stop or to Shuttle Halides? The Role of an Ionic Liquid in Thermal Halide Mixing of Hybrid Perovskites. ACS Energy Lett. 8 (2023).

CPP 17.15 Mon 19:00 P5

Early-Stage Growth and Morphological Evolution of Ag Electrodes during Sputter Deposition on PDINN — •Doan Duy Ky Le[1], Kristian Reck[2], Benedikt Sochor[3], Thomas Strunskus[2], Jungui Zhou[3], Anuragk Keloth[3], Lyuyang Cheng[1], Sarathal Koyiloth Vayalil[3], Stephan V. Roth[3], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]CAU, Kiel, Germany — [3]DESY, Hamburg, Germany

The integration of sputtered metal electrodes with organic interlayers remains a key challenge for the scalable fabrication of organic solar cells (OSCs). PDINN is an efficient cathode interlayer, yet its behavior under sputter deposition is not well understood. Here, we use *in situ* GISAXS to resolve the nanoscale morphological evolution of Ag during direct-current magnetron sputtering (DCMS) onto PDINN thin films. Time-resolved scattering reveals distinct early-stage growth regimes, including the nucleation of small Ag clusters, their coalescence into medium-sized species, and the formation of laterally connected domains. Compared to thermally evaporated Ag, sputtered Ag achieves continuous coverage at significantly reduced thickness. These findings confirm the feasibility of sputter-deposited Ag/PDINN interfaces and establish a foundation for scalable electrode fabrication in next-generation OSCs.

CPP 17.16 Mon 19:00 P5

Spin-Sensitive Spectroscopy of TADF OLEDs — •Andreas Kohrmann, Ahmed Mohamed, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

The performance of the blue emitter *ν*-DABNA in thermally activated delayed fluorescence (TADF) organic light-emitting diodes (OLEDs) is closely related to the dynamics of triplet excitons. In optically excited host-guest thin films, triplet states are generated and evolve through the intricate interplay of triplet diffusion, triplet recombination, and triplet-triplet annihilation (TTA). Thereby TTA and triplet diffusion are inherently host-dependent. Consequently, the host environment exerts a pivotal influence on exciton loss and delayed emission pathways. We used spin-sensitive optical spectroscopy, specifically photoluminescence-detected magnetic resonance (PLDMR) to examine the spin nature of the singlet-triplet interaction in optically excited host-guest thin films. Correlating these with exciton kinetics from transient photoluminescence (trPL) yields insights on the luminescence as well as the formation, diffusion, and annihilation of triplet excitons. The findings of this study offer a more profound understanding of the triplet harvesting mechanisms in TADF emitters. Additionally, they offer guidance for host selection strategies that are intended to enhance the efficiency and stability of the devices.

CPP 17.17 Mon 19:00 P5

Excimers in carbazole-substituted 4NICz TADF emitters: from frozen solution to films. — •Anatolii Kuimov[1], Oliver Lee[2], Eli Zysman-Colman[2], and Anna Köhler[1] — [1]Soft Matter Optoelectronics, University of Bayreuth, 95440 Bayreuth, Germany. — [2]Organic Semiconductor Centre, EaStCHEM School of Chemistry, University of St Andrews, St Andrews, UK, KY16 9ST

To obtain high brightnesses in OLEDs, emitters need to be packed sufficiently densely for good charge transport. However, too close a proximity between chromophores can lead to the formation of excimers. We investigate under which conditions such excimers are formed in carbazole-substituted 4NICz blue emitters and how this formation can be controlled. In dilute solution at room temperature, we see only emission from non-interacting molecules, whereas in frozen glass a weak red-shifted emission band appears that grows with laser intensity. A similar increase is observed in films. We attribute excimer formation in the glass and in films to structural reorganization after local heating that results from the absorption of the laser pulses.

CPP 17.18 Mon 19:00 P5

Bulk-Heterojunction Morphology Engineering in D18:Y6 Solar Cells — •Dennis Straub, Lixing Li, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

Organic solar cells based on non-fullerene acceptors have attracted considerable interest due to their favourable optoelectronic properties and compatibility with low-temperature solution processing. In this work, the D18 polymer donor and the non-fullerene acceptor Y6 (BTP-4F) are used as the active layer materials. The study investigates how variations in fabrication parameters influence the evolution of the bulk-heterojunction morphology and the resulting photovoltaic behaviour. Key factors examined include solvent choice, wet-film formation, drying kinetics, and thermal treatment, which govern phase separation, domain purity, and molecular ordering within the active layer.

To further explore morphology control, selected additives are introduced that may affect miscibility, aggregation, and domain formation. Their influence on the structural organisation of the D18:Y6 blend is analysed to determine how additive-induced morphological changes impact charge generation, transport pathways, and recombination processes. By correlating structural characteristics with device performance, this work aims to clarify how processing and material modification shape the efficiency and reproducibility of D18:Y6 organic solar cells and to provide guidance for future optimisation.

CPP 17.19 Mon 19:00 P5

Spray Engineering for High-Efficiency Organic Solar Cells — •Xinyu Jiang[1], Kang An[2], Nadja Koelpin[1], Ning Li[2], and Stephan V. Roth[1,3] — [1]Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg — [2]Institute of PolymerOptoelectronic Materials and Devices, State Key Laboratory of Luminescent Materials and Devices, South China University of Technology (SCUT), Guangzhou, Guangdong 510641, China — [3]Department of Fibre and Polymer Technology, KTH Royal Institute of Technology,Teknikringen 56-58, SE-100 44 Stockholm, Sweden

Spray coating has emerged as a powerful and scalable technique for fabricating high-performance organic solar cells (OSCs), offering precise control over ink deposition and rapid compatibility with large-area manufacturing. Compared with conventional solution-processing methods, spray deposition enables fine tuning of droplet dynamics, solvent evaporation, and wet-film thickness, which are critical for achieving optimal phase separation and molecular ordering in the active layer. In this work, we demonstrate that rational engineering of spray parameters such as atomization rate, nozzle substrate distance, carrier-gas flow, and solvent volatility significantly improves film uniformity and reduces morphological defects, leading to enhanced charge transport and suppressed recombination losses. By integrating these optimized spray processes, the resulting OSCs exhibit markedly improved device efficiency and excellent reproducibility across enlarged areas. These results highlight spray coating as a highly efficient and industry-ready pathway for the scalable integration of organic solar cells.

CPP 17.20 Mon 19:00 P5

Narrowband organic Photodetectors with J-Aggregate materials — •Angelina Stoer[1], Jakob Wolansky[1], Matthias Stolte[2], Frank Würthner[2], Karl Leo[1], and Johannes Benduhn[1] — [1]Institut für Angewandte Physik und Photonik, TU Dresden — [2]Institut für Organische Chemie, Universität Würzburg

With the development of organic photodetectors, new opportunities for narrowband photodetection have emerged. Instead of relying on costly and unwieldy optical filters, the molecular structure of organic materials can be chemically tailored to tune their absorption range. Recently, the material class of merocyanine dyes has been investigated as a promising candidate for this purpose, exhibiting favorable absorption properties. By post-annealing these dyes, the molecules can rearrange and form J-aggregated thin films, resulting in a narrowband absorption spectrum due to the intermolecular interactions.

In this work, the merocyanine dye 1(Hex) is used in fully vapor-deposited organic photodetectors. Narrowband detection with a FWHM as low as 15 nm could be realized at a center wavelength of 755 nm. Through careful optimization of the heating conditions and device structure, a notable external quantum efficiency was achieved, accompanied by very low noise at zero voltage. Based on this, the resulting specific detectivity exceeds 10^{12} Jones. The comprehensive photodetector characterization is complemented by an in-depth analysis of changes in the thin film's morphology and energetics induced by the J-aggregation formation process.

CPP 17.21 Mon 19:00 P5

Nanoscale Structural and Electronic Characterization of the DTDCPB:C70 donor-acceptor system for vacuum-deposited organic solar cells — •Milena Merkel[1,2], Jan ter Glane[1,2], and Harry Mönig[1,2] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]Center for Nanotechnology (CeNTech), Münster, Germany

The active layer of organic solar cells is produced either by solution-processing or vacuum thermal evaporation. While solution-processed cells have achieved

higher efficiencies to date, vacuum-deposited cells exhibit higher morphological stability and thus a longer durability. For a future commercialization of organic solar cells, where both efficiency and durability are crucial, understanding the current limitations of vacuum-deposited cells is thus of major interest.

Cells based on an active layer made of the DTDCPB:C70 donor-acceptor system have so far achieved one of the highest efficiencies in the group of vacuum-deposited organic solar cells, while also exhibiting high durability [1,2]. We used a combined approach of high-resolution scanning tunneling microscopy and spectroscopy to investigate the structural and electronic properties of assemblies of these donor and acceptor molecules deposited on single-crystalline substrates, as well as of their lateral and vertical interfaces.

[1] Griffith et al., Phys. Rev. B 92, 085404 (2015)
[2] Zou et al., J. Mater. Chem. A 2, 12397 (2014)

CPP 17.22 Mon 19:00 P5

Interfacial modification of transport layers for enhancing the performance and stability of organic solar cells — •Saib Jahan Qazi[1,2], Md. Moidul Islam[1,2], Md. Zobaer Ahmed Rahat[1,2], Md. Farhatul Hassan[1,2], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC Jena), Friedrich Schiller- University Jena, Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich-Schiller-University Jena, Jena, Germany

Organic solar cells are emerging as promising prospects in the field of solar energy technology due to their low-cost, lightweight and simple roll to roll fabrication properties. A record power conversion efficiency above 19% has already been reported. However, long-term stability is still the main obstacle for commercialization due to inherent instability particularly at the interfaces. In this study, we demonstrate solution processed interfacial modification of zinc oxide (ZnO). ZnO is widely used in organic solar cells for electron extraction, but it brings performance and lifetime limitations due to surface defects and photochemical reactions under UV exposure, which generates radicals resulting into accelerated degradation of the photoactive layer in the device. Here we compare approaches using organic acids with polysilazane, for successful ZnO passivation.

CPP 17.23 Mon 19:00 P5

Simulation of Pump-Probe Spectra Including Linear Vibronic Coupling – A Study on Naphthalene Diimide — •Matthias Knechtges, Maximilian F. X. Dorfner, and Frank Ortmann — Department of Chemistry, TUM School of Natural Sciences, and Atomistic Modeling Center, Munich Data Science Institute, Technical University of Munich, München, Germany

Non-linear optical techniques such as pump-probe spectroscopy provide insight into the dynamical processes governing excited-state evolution, which are often influenced by electron-vibrational interactions.

The theoretical computation of pump-probe spectra remains an open research field [1] due to the complicated treatment of coupled electronic and nuclear dynamics, which require feasible but accurate approximations [2]. In particular, including the full quantum nature of the nuclei remains a major challenge.

In this contribution, we present a framework for calculating pump-probe spectra of molecules based on an analytic linear electron-vibrational coupling model. Evaluating the third-order response function in the Franck-Condon approximation and including vibrational transitions enables us to predict the pump-probe signal in the infrared region as well. We apply this to the Naphthalene Diimide molecule, a building block for a prospective solar cell material.

[1] Gelin, M., et al., Comp. Mol. Sc. (2025); [2] Park, J. W., et al., J. Chem. Theory Comput. (2017)

CPP 17.24 Mon 19:00 P5

QD-based hybrid organic photo detectors for narrowband IR sensing — •Johann Demel[1], Louis Conrad Winkler[1,3], Andrey Iodchik[2], Moritz Flemming[1], Tobias Antrack[1], Karl Leo[1], and Johannes Benduhn[1,3] — [1]IAP, TU Dresden — [2]Chemistry, TU Dresden — [3]German Center for Astrophysics

The ability to detect infrared radiation is relevant across a multitude of fields. Autonomous driving and deep space exploration utilize its ability to propagate long distances with little absorption losses. While, e.g., medical diagnostics can profit from its penetration depth into biological tissue. Organic materials have proven to be a viable platform for photo detection, with advantages such as low-cost fabrication, flexible devices, and tunable absorption; however, their IR absorption capabilities are limited.

This work presents a hybrid structure combining organic transport layers and PbS nanoparticles into optical microcavities. Based on transfer-matrix simulations, the resonance wavelength of the stack can be precisely predicted and tuned by adjusting the thickness of the organic transport layers. By combining precise thermal evaporation of the organic layers with interface assembly to incorporate nanoparticle layers into the stack, wavelength-selective devices are achieved whose resonance feature can be tuned from 750 nm up to 1800 nm. This expands the advantageous properties of the organic device framework by the wavelength-tunable IR absorption capabilities of semiconductor nanoparticles, leading to devices with specific detectivity values D^* of $10^{11}\ cm \cdot \sqrt{Hz} \cdot W^{-1}$ (based on noise measurements).

CPP 17.25 Mon 19:00 P5

Heat induced morphological changes in P3HT:PCBM solar cells — •Jose Prince Madalaimuthu[1,2], Edward Wijaya[1,2,3], Ulrich S Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC Jena), Friedrich-Schiller-Universität Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich-Schiller-Universität Jena, Germany — [3]Department of Chemical Engineering, Swiss German University, 15143 Tangerang, Indonesia

Organic solar cells are becoming an important technology for next-generation energy applications since they can be made into flexible and lightweight devices. However, attaining thermal stability remains a significant challenge for its actual deployment. Heat-induced morphological alterations within the photoactive layer typically led to considerable performance reductions. It's interesting to note that this effect may be reversed in some circumstances. Our investigations on P3HT:PCBM solar cells show that devices subjected to high-temperature exposure (up to 250°C) demonstrated substantial performance recovery upon cooling. Thermally driven and reversible morphological change in the active layer was demonstrated by photoluminescence analysis.

CPP 17.26 Mon 19:00 P5

Trace Intrinsically Microporous Polymer Additives Induce LiF-Rich SEI for Enhanced Performance of Silicon-Based Lithium-Ion Batteries — •Ming Yang[1], Ruoxuan Qi[1], Ya-Jun Cheng[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]College of Renewable Energy, Hohai University, Changzhou, Jiangsu Province, P. R. China

Silicon-carbon (Si/C) composite anodes are promising candidates for high-energy-density lithium-ion batteries due to the high theoretical capacity of silicon. However, their practical application is hindered by severe volume expansion and unstable solid electrolyte interphase (SEI) formation during cycling. Fluoroethylene carbonate (FEC) is commonly used to improve interfacial stability, but its effectiveness is limited by concentration sensitivity and uncontrollable side reactions. This study introduced carboxyl-functionalised intrinsically microporous polymer (PIM-COOH) as a functional additive, achieving dual regulation of electrode structural evolution and interfacial chemistry. Only 0.5wt% PIM-COOH is required to achieve these effects. The Si/C@PIM||Li half-cell retains 90% of its capacity after 300 cycles at 1.0 C, demonstrating excellent long-term stability. The utilisation of 1Ah NCM811-Si/C pouch cells demonstrates its commercial potential. These results demonstrate a scalable and effective strategy for stabilizing silicon-based anodes, offering valuable insight into the design of next-generation lithium-ion batteries with both high energy density and long cycle life.

CPP 17.27 Mon 19:00 P5

In-situ WAXS observation of 3D porous electrodeposition Cu in lithium-metal batteries — •Lyuyang Cheng[1], Zhuijun Xu[1], Yingying Yan[1], Fabian Apfelbeck[1], Yuxin Liang[1], Anton Davydok[3], Christina Krywka[3], Yajun Cheng[2], and Peter Müller-buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany — [2]Hohai University, 213022 Changzhou, China — [3]Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany

Lithium (Li) metal is the ultimate anode for rechargeable batteries. Its high specific capacity (3860 mAh/kg) and low voltage warrant optimal cell energy density. However, these anodes rely on repeated plating and stripping of Li, which leads to consumption of Li and the growth of dendrites that can lead to self-discharge and safety issues. To address these issues and problems, a number of different porous conductive scaffolds have been reported to create high surface area electrodes on which Li can be plated reliably. While impressive results have been reported in literature, current processes typically rely on either expensive or poorly scalable techniques. Herein, we report a scalable fabrication method to create porous Cu anodes using a one-step electrodeposition process. The areal loading, pore structure, and electrode thickness can be tuned by changing the electrodeposition parameters, and we illustrate the in-situ nano WAXS images with lithium growth, which can help to explain the mechanism. We also provide a feasible method to fabricate the porous Cu cathodes with different electrodeposition solution concentrations.

CPP 17.28 Mon 19:00 P5

Ionic-Liquid-Regulated PVC-Based Solid Polymer Electrolyte for High-Performance Lithium Metal Batteries — •Jiaqi Ding and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany

Lithium metal batteries (LMBs) are regarded as one of the most promising next-generation energy-storage systems owing to their ultrahigh theoretical capacity. However, the safety issues associated with conventional liquid electrolytes, including dendrite-induced short circuits and interfacial instability, severely hin-

der their practical application. Solid polymer electrolytes (SPEs) offer a potential pathway to address these challenges. In this work, we develop a poly(vinyl carbonate) (PVC)-based solid polymer electrolyte incorporating the ionic liquid [EMI][TFSI] to enhance both ion transport and mechanical integrity. Structural and electrochemical characterizations show that the ionic liquid effectively regulates ion transport within the polymer matrix, enabling the formation of continuous Li ion conduction pathways and improving the compatibility of the electrolyte with lithium metal. This tailored ion-transport behavior leads to enhanced ionic conductivity, mitigated interfacial degradation, and significantly extended cycling stability in LMBs. The results highlight the critical role of ionic-liquid modification in tuning transport properties of polymer electrolytes and provide a viable materials strategy for high-performance lithium metal batteries.

CPP 17.29 Mon 19:00 P5

Investigation of the Effects of LiDFOB Salt Concentration on the Fast-Charging Performance of LiCoO2 Cathodes — •Yifeng Liu, Ming Yang, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany

Fast-charging lithium-ion batteries have drawn increasing interest, yet lithium cobalt oxide ($LiCoO_2$) paired with commercial electrolytes generally suffers from severe capacity fading and limited cycle life at high charging rates. This study aims to explore strategies for improving capacity retention of $LiCoO_2$-based lithium-ion batteries under fast-charging conditions. We employ boron-containing lithium salt LiDFOB as an electrolyte additive and systematically investigate its concentration-dependent effects on the capacity retention of LCO cells under fast-charging operation. Interfacial stability and charge-transfer kinetics associated with different LiDFOB levels are evaluated through cyclic voltammetry (CV), linear sweep voltammetry (LSV), Tafel analysis, and chronoamperometry (CA). The results show that the concentration of LiDFOB has a pronounced influence on the cycling performance. In particular, the optimized LiDFOB concentration enables the LCO cells to stably cycle for over 1000 cycles at 1C and 3C, benefiting from the improved interfacial stability and enhanced Li^+ transference number. Morphological and material characterizations further reveal that different LiDFOB concentrations generate SEI films with distinct compositions and structures, which account for the disparities in fast-charging capacity retention.

CPP 17.30 Mon 19:00 P5

High-Power Continuous Laser-Guided Synthesis of Bimetallic Metal-Organic Framework (NiCoMOF) Structures and Their Composites: Photophysical, Photochemical, and Electrical Characterization — •Saliha MUTLU[1,2], Bülend ORTAÇ[2], Ali KARATUTLU[2,3], Nergis ARSU[4], and Sevil SAVAŞKAN YILMAZ[1,2] — [1]Karadeniz Technical University Chemistry Department, Trabzon, Türkiye — [2]Bilkent University, Institute of Materials Science Nanotechnology and National Nanotechnology Research Center (UNAM), Ankara, 06800 Turkey — [3]Sivas University of Science and Technology, Department of Engineering Basic Sciences, Sivas, 58100 Turkey — [4]Department of Chemistry, Yildiz Technical University, Davutpasa Campus, Istanbul 34210, Turkey;

Metal-organic frameworks (MOFs) are among the most innovative breakthroughs in chemistry and materials science. In this study, the first bimetallic synthesis of MOFs was achieved using the high-power laser-induced rapid synthesis (LIRS) method via two different ligand and metal salt combinations with different π-conjugated linkers. The synthesis of NiCo-MOF structures (in 1:2 and 2:1 ratios) was completed in just 70 minutes using the LIRS method. Furthermore, the synthesis of MOF composites (rGO/MOF) containing reduced graphene oxide (rGO) was also achieved for the first time. On top of these, the electrical properties of the epoxy acrylate-based MOF and rGO@MOF composites prepared by in situ photopolymerization were investigated in detail. This study was supported by TÜBITAK-BIDEB 2211-A National PhD Scholarship Programs.

CPP 17.31 Mon 19:00 P5

A gel polymer electrolyte interface layer-amphiphilic polymer/salt composite nanoarray for lithium metal batteries — •Thomas Bullinger, Ming Yang, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany

Research on lithium-ion batteries has been focused on improving energy density, which is mainly limited by conventional graphite anodes. Therefore, lithium metal has emerged as a desirable anode material due to its high energy density. However, it easily reacts during cycling, thus forming lithium dendrites, which can lead to short-circuiting of the battery. As liquid electrolytes cannot solve this problem, solid-state polymer electrolytes have shown promise as an alternative, but their ionic conductivity at room temperature limits their practical use, leading to the compromise of gel polymer electrolytes. In this project the block copolymer P2VP-b-PEO together with the lithium salt lithium nitrate, both dissolved in tetrahydrofuran (THF), surprisingly lead to the solvent phase changing to a gel polymer, which was then used as the electrolyte in coin cells. For the cycling and rate performance tests, Li||LFP batteries were investigated. Further experiments include cycling voltammetry (CV), linear sweep voltammetry (LSV), Tafel curves and impedance spectroscopy.

CPP 17.32 Mon 19:00 P5

In-situ interface film forming on the high-voltage LiCoO2 cathode by a tiny amount of nanoporous polymer additives — •Ruoxuan Qi[1], Ming Yang[1], Tianle Zheng[1], Xingchen Liu[2], Yonggao Xia[2], Ya-Jun Cheng[2,3], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]NIMTE, CAS, Zhejiang Province, P. R. China — [3]College of Renewable Energy, Hohai University, Jiangsu Province, P. R. China

The LiCoO2 (LCO) cathode has been foreseen for extensive commercial applications owing to its high specific capacity and stability. Therefore, there has been considerable interest in further enhancing its specific capacity by increasing the charging voltage. However, single-crystal LCO suffers from a significant capacity degradation when charged to 4.5 V due to the irreversible phase transition and unstable structure. Herein, an ultra-small amount (0.5 wt% in the electrode) of multi-functional PIM-1 (a polymer with intrinsic microporosity) additive is utilized to prepare a kind of binder-free electrode. PIM-1 modulates the solvation structure of LiPF6 due to its unique structure, which helps to form a stable, robust, and inorganic-rich CEI layer on the surface of LCO at a high voltage of 4.5 V. This reduces the irreversible phase transition of LCO, thereby enhancing the cyclic stability and improving the rate performance, providing new perspectives for the electrodes fabrication and improving LCO-based high-energy-density cathodes.

CPP 17.33 Mon 19:00 P5

Effects of differently sized and shaped active and passive Filler for PVDF-HFP CPEs in All Solid-State Lithium-Ion Batteries — •Daniel Karlinger, Yuxin Liang, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, Graching, Germany

All-solid-state lithium-ion batteries are regarded as highly promising due to their enhanced safety and potentially higher energy density compared to conventional cells with liquid electrolytes. In this project, solid polymer electrolytes based on PVDF-HFP are investigated with the aim of improving ionic conductivity and overall electrochemical performance. The approach is to incorporate combinations of ac tive and passive fillers to tailor the material properties. Conductivity and mechanical stability will be systematically examined with cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS), X ray diffraction (XRD) and other methods, in order to identify opti mized compositions for solid-state battery applications.

CPP 17.34 Mon 19:00 P5

Tracing the Path from Solvation to Transport in Lithium and Sodium Electrolytes — •Chinwendu Nancy Anabaraonye[1,2], Diddo Diddens[3], and Andreas Heuer[1,2] — [1]Institute of Physical Chemistry, University of Münster, Corrensstraße 28/30, 48149 Münster, Germany — [2]International Graduate School for Battery Chemistry, Characterization, Analysis, Recycling and Application (BACCARA), University of Münster, Corrensstr. 40, 48149 Münster, Germany — [3]Forschungszentrum Jülich GmbH, Helmholtz-Institute Münster (IMD-4), Corrensstraße 48, 48149 Münster, Germany

Advancing technology continues to increase demands on energy storage devices and their performance requirements. Over the years, lithium-ion batteries have consistently remained the market leader. However, their long-term sustainability remains questionable due to the limited lithium reserves. Therefore, there is need for increased research toward alternative battery chemistries, among which are sodium-ion batteries. The present work is a comparative study of the transport properties of lithium hexafluorophosphate (LiPF6) and sodium hexafluorophosphate (NaPF6) in carbonate electrolytes consisting of ethylene carbonate (EC) and ethyl methyl carbonate (EMC). Based on molecular dynamics simulations, we analyse the influence of EC ratio and salt concentrations on the solvation structure with particular focus on the formation of contact ion pairs (CIP), solvent-seperated ion pairs (SSIP) and ion aggregates and how this correlates with the ionic transports within the systems.

CPP 17.35 Mon 19:00 P5

Modeling Electron Transfer at Electrode-Electrolyte Interfaces — •Joshua Krieger[1,2,3], Johannes Tölle[4,5,3], Diddo Diddens[2,6], and Andreas Heuer[2,6] — [1]International Graduate School BACCARA, University of Münster, 48149 Münster, Germany — [2]Institute for Physical Chemistry, University of Münster, Münster, Germany, 48149 Münster, Germany — [3]Center for Multiscale Theory and Computation (CMTC), University of Münster, 48149 Münster, Germany — [4]Department of Chemistry, University of Hamburg, 22761 Hamburg, Germany — [5]The Hamburg Centre for Ultrafast Imaging (CUI), 22761 Hamburg, Germany — [6]Helmholtz Institute Münster - Forschungszentrum Jülich GmbH (IEK 12), 48149 Münster, Germany

The solid electrolyte interphase (SEI) is an important component in rechargeable battery performance and lifetime, but the complex mechanisms behind its for-

mation are still not yet fully understood. Accurate electron-transfer (ET) rates are important for simulating SEI growth, e.g. using reactive molecular dynamics simulations that require electrolyte reduction rates. To obtain the ET rates, we investigate a simplified Anderson impurity-type model designed to describe non-equilibrium electron transfer between an electrode and the redox-active species under an applied potential. This framework enables systematic exploration of how molecular distance, electronic coupling, as well as solvent interactions and reorganization effects influence electron-transfer dynamics. The resulting insights provide a foundation for constructing more reliable, physics-based rate expressions that can be integrated into large-scale SEI formation simulations.

CPP 17.36 Mon 19:00 P5

Toward Improved Lithium Batteries: Performance of Magnetron-Sputtered Silicon Anodes — •Thomas Köhler[1], Christian Ludt[1], Tina Weigel[1], Marc Ferch[2], Robert Hahn[2], Annekatrin Delan[3], Charaf Cherkouk[4], Hartmut Stöcker[1], and Dirk C. Meyer[1] — [1]TU Bergakademie Freiberg, 09599 Freiberg, Germany — [2]Fraunhofer IZM, 13355 Berlin, Germany — [3]Fraunhofer IZM-ASSID, 01468 Moritzburg, Germany — [4]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Silicon is considered one of the most promising anode materials for lithium-ion batteries due to its high theoretical specific capacity of 3590 mAh/g in the $Li_{3.73}Si$ phase at room temperature and its broad availability. However, its practical application remains limited because i) significant volume changes occur during cycling, ii) its intrinsic electronic conductivity is low, and iii) the stability of the solid-electrolyte interphase is insufficient.

In this work, silicon thin-film anodes were fabricated by magnetron sputtering onto copper foil. The electrodes were thoroughly characterized regarding their chemical composition and surface morphology. Scanning electron microscopy was used to evaluate the structural stability of the silicon layers in contact with a polymer-based solid electrolyte and to compare their degradation behavior with that in conventional liquid electrolyte. Electrochemical testing with the polymer electrolyte shows promising cycling performance; the reduced surface degradation observed in SEM correlates with improved long-term stability of the cell system.

CPP 17.37 Mon 19:00 P5

Structural and Ionic Transport Properties of Li3-3xDy1+xCl6 Solid Electrolytes — •Francesco Falsina[1,2], Peter Müller-Buschbaum[1], and Anatoliy Senyshyn[2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]MLZ, TUM, Garching, Germany

Ternary lithium lanthanide chlorides, Li_3RCl_6 (R = rare earth), have recently emerged as promising solid electrolytes. Although initially thought to exhibit low ionic conductivity, later studies showed that ball milling synthesis, by leading to microstructure modification, can raise conductivity to $\sim 10^{-3}$ S·cm^{-1}. In this work we studied the $Li_{3-3x}Dy_{1+x}Cl_6$ system (x = −0.1 to 0.1). For $x = 0$, we assessed how annealing conditions affect structure and conductivity. Ionic transport was measured using isostatically pressed, gold-sputtered pellets and broadband impedance spectroscopy. XRD, DSC, and EIS analyses of as-milled, annealed, and melt-synthesized samples show that conductivity decreases by nearly an order of magnitude after annealing, while over-lithiated compositions consistently display higher conductivity, highlighting the impact of lithium retention. DSC and XRD also reveal an orthorhombic-to-trigonal transition with increasing lithium content. Overall, these results clarify how composition and disorder govern ionic transport in the Li_3MCl_6 electrolyte family.

CPP 17.38 Mon 19:00 P5

Investigating the Interfacial Impedance Characteristics of Composite Materials — •Janne Mattis König[1,2], Felix Schug[1,2], Christian Heiliger[1,2], and Janis K. Eckhardt[1,2,3] — [1]Institute of Theoretical Physics, Justus-Liebig-University Giessen, 35392 Giessen, Germany — [2]Center of Material Research (ZfM), Justus-Liebig-University Giessen, 35392 Giessen, Germany — [3]Institute of Physical Chemistry, Justus-Liebig-University Giessen, 35392 Giessen, Germany

All-solid-state batteries (ASSBs) are a promising alternative to conventional lithium-ion batteries, offering high energy and power densities, long-term stability, and fast-charging capability. Consequently, significant effort is focused on identifying suitable materials. Electrochemical impedance spectroscopy (EIS) is a key characterization technique, but interpreting spectra from realistic composite systems remains challenging. In this work, we investigate interfacial impedance in simplified composite microstructures using a 3D electrical network model. The simulations reveal that high charge-transfer resistances lead to geometric constriction effects, producing an impedance signature that closely resembles a migration process or a charge-transfer reaction. This constriction impedance is strongly influenced by the composite microstructure. Furthermore, increased conductivity along the interface introduces a characteristic deformation in the impedance spectrum shape. Overall, these findings clarify the origin of interfacial impedance features in composite materials and support more informed interpretation of EIS measurements in ASSB research.

CPP 17.39 Mon 19:00 P5

Aluminium-Polymer Batteries as a viable Post-Lithium Technology — •Oliver Schmidt[1,2], Amir Mohammad[1,2], Shuvrodev Biswas[1,2], Mostafizar Rahman[1,2], Nathan Leubner[1,2], Thomas Köhler[1,2], Hartmut Stöcker[1,2], and Dirk C. Meyer[1,2] — [1]TU Bergakademie Freiberg, Institute of Experimental Physics, Leipziger Str. 23, 09599 Freiberg — [2]Zentrum für effiziente Hochtemperatur-Stoffwandlung, Winklerstr. 5, 09599 Freiberg

One of the key challenges of the energy transition is the rising demand for lithium. In the future, there will be a supply gap, even taking into account recycling and the development of new mining areas. In addition to the limited availability, safety risks such as fire hazards make lithium-ion batteries less suitable for the long-term requirements of the energy transition.

Here, we present the aluminium-polymer battery as a novel technology adressing these issues. Aluminium is the most abundant metal in the Earth's crust and therefore inexpensive. It is available in Europe and is highly recyclable. The battery cells are free of toxic or critical raw materials and eliminate the risk of fire.

Pouch cells consisting of a simple 3-layer setup have been developed: aluminium anode, polymer electrolyte (consisting of $AlCl_3$, Et_3NHCl and PAN) and graphite cathode. Capacity, safety and recycling tests show promising results. Remaining challenges are tackling the self-discharge and scaling up the cell fabrication. The future goal is making large-scale storage systems cost-effective, efficient and safe.

CPP 17.40 Mon 19:00 P5

Microstructure-Resolved Impedance Modeling of Cathode Composite Electrodes for Solid-State Batteries — •Matthias Braun[1,2], Felix Schug[1,2], Christian Heiliger[1,2], and Janis K. Eckhardt[1,2,3] — [1]Institute for Theoretical Physics, Justus-Liebig-University Giessen, Germany — [2]Center for Materials Research (ZfM), Justus-Liebig-University Giessen, Germany — [3]Institute of Physical Chemistry, Justus-Liebig-University Giessen, Germany

Solid-state batteries (SSBs) rely on composite cathodes whose complex microstructures critically influence ionic and electronic transport. Electrochemical impedance spectroscopy (EIS) is widely used to probe these transport processes. The impedance behavior of mixed ionic electronic conductors is commonly interpreted using transmission-line models (TLMs). However, the extent to which composite microstructure governs impedance features and the validity of TLM-based interpretations remains insufficiently understood. In this work, we employ microstructure-resolved impedance simulations to investigate how key structural characteristics of cathode composites shape their impedance response. We demonstrate that interface morphology and porosity significantly modulate the spectra, giving rise to microstructure-specific features that conventional TLMs fail to capture. In particular, geometric current-constriction effects at the cathode active material/solid-electrolyte interface emerge as dominant contributors to impedance behavior. These findings provide a deeper mechanistic understanding of microstructure-induced impedance signatures and offer practical guidance for interpreting EIS data in composite electrodes for SSBs.

CPP 17.41 Mon 19:00 P5

Optimization in Fabrication Process and Understanding the Impact of Crystal Size and Growth in RbCsMAFA Perovskite Solar Cells — •Bashudev Bhandari[1,2,3], Sai Durga Prasad Sudana[1,2], Chikezie Williams Ugokwe[1,2], Ulrich S Schubert[1,2], and Harald Hoppe[1,2] — [1]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich-Schiller-University Jena, Germany — [2]Laboratory of Organic and Macromolecular Chemistry (IOMC Jena), Friedrich-Schiller- University Jena, Germany — [3]Faculty of Physics and Astronomy, Friedrich-Schiller- University Jena, Germany

Perovskite solar cells (PSCs) emerged as remarkable and promising cutting-edge clean and green energy sources. Recent breakthroughs in their performance attract researcher's interest. Despite its promising performance, degradation issues and defects are critical obstacles to overcome. Our work explores different mechanisms to suppress defects and improve stability via improved crystallization. We have systematically optimized different processing parameters such as annealing time, antisolvent dropping time, hot casting, etc., and introduced additives like different phosphonium salts and PEAI for passivation and seeding for perovskite growth. Different Characterization and imaging techniques illustrate improved crystalline and opto-electronic properties of the perovskite film and solar cells.

CPP 17.42 Mon 19:00 P5

In Situ Investigation of Ag Sputter Deposition on a Zwitterionic Polymer Film — •Georgios Panagiotidis[1], Christoph Lindenmeir[1], Grace Leone[2], Lixing Li[1], Lyuyang Cheng[1], Doan Le[1], Yufeng Zhai[3], Kristian Reck[4], Benedikt Sochor[3], Matthias Schwartzkorpf[3], Anurag Keloth[5], Sarathlal Vayalil[3,5], Todd Emrick[2], Thomas Russell[2,6], Stephan V. Roth[3,7], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]UMass Amherst, Massachusetts, United States — [3]DESY, Hamburg — [4]CAU, Kiel, Germany — [5]UPES, Dehradun, India — [6]LBNL, Berkeley — [7]KTH, Stockholm, Sweden

While organic electronic devices mainly use organic or organic-inorganic hybrid materials, many electrodes still rely on pure metals due to their unparalleled electrical conductivity. Thus, the polymer-metal interface is crucial to device performance. Studies have demonstrated the use of ultrathin metal electrodes for (semi)transparent organic solar cells, and the quality of the interface influences the formation of structural defects, which can increase resistance and the likelihood of a short circuit. These metal contacts are typically deposited through lab-scale methods such as thermal evaporation, while industrial manufacturing prefers large-scale sputter deposition. Moreover, zwitterionic polymers can reduce the work function of metals and serve as interlayers in inverted organic solar cells. Therefore, understanding the growth behavior of sputtered silver on zwitterionic polymer surfaces is critical.

CPP 17.43 Mon 19:00 P5

Probing the Distribution of Residual Stresses in Thin Polymer Films Using Mechanochromic Molecular Springs — •Meirui Fu[1], Raphael Hertel[2], Bence Dajka[3], Michael Walter[3], Michael Sommer[2], and Günter Reiter[1] — [1]Institute of Physics, University of Freiburg, Germany — [2]Institute for Chemistry, Chemnitz University of Technology, Germany — [3]FIT Freiburg, University of Freiburg, Germany

Polymer thin films prepared rapidly from solution by spin coating often retain residual stresses originating on a molecular level. However, typically these stresses are probed on a macroscopic level, yielding spatially averaged responses, but do not resolve forces acting on individual chains. Here, we employed mechanochromophores, covalently integrated along the backbone of a glassy polymer, as optical reporters whose emission response varies continuously with the applied force. By combining optical microscopy and spectroscopy, we were able to measure the sum of the forces acting on individual chains with high spatial resolution. In particular, we investigated the distribution of forces acting on non-equilibrated polymer chains. Samples prepared under different spin coating conditions exhibited systematic variations in the emission spectra, which reflect differences in the distribution of the sum of forces acting on individual chains. We distinguish contributions from polymers experiencing low and high forces, respectively, which exhibited opposite trends with preparation conditions. We tentatively relate the heterogeneity of the acting forces to differences in conformation of the non-equilibrated polymer chains.

CPP 17.44 Mon 19:00 P5

Real Time Spectroscopy of Plasmonic Core-Shell Microgels during Compression at Air/Water Interfaces — •Matthias Karg and Déborah Feller — Martin Luther University Halle-Wittenberg, Halle, Germany

Plasmon resonance coupling is strongly distance-dependent. In contrast to near-field coupling of plasmonic nanoparticles in close proximity, periodic superstructures support plasmonic-diffractive coupling. The resulting surface lattice resonances are interesting for their narrow linewidth and sensitivity to refractive index environment and lattice periodicity. Typically studied periodic arrays are (solid) substrate-supported and thus structurally fixed unless elastic substrates are used. Seeking an alternative approach, we demonstrate the large dynamic control of periodic plasmonic lattices using soft and deformable core-shell microgels self-assembled at air/water interfaces. Using microgels with gold cores and sufficiently thick microgel shells, we realized periodic monolayers where the periodicity can be controlled by compression using a Langmuir trough. The implementation of an extinction spectrometer setup was used to probe the optical response of the monolayer in situ during continuous reduction of the available area, in real time. We monitor plasmon resonance coupling with a never before reported stepsize in interparticle spacing by following peak position, width and intensity. The observed spectral changes support recent findings that confined microgel monolayers at fluid interfaces show a continuous reduction in spacing when uniaxially compressed opposed to the cluster formation that is observed after drying on solid substrates.

CPP 17.45 Mon 19:00 P5

In-situ FTIR spectroscopy on organic semiconductor electric double-layer transistors — •Marvin Schmidt[1], Pushi Wang[2], Jun Takeya[2,3], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Graduate School of Frontier Sciences, The University of Tokyo, Kashiwa, Japan — [3]Research Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba, Japan

The field of organic electronics is ever-growing due to the enormous range of unique properties and possible applications exhibited by organic molecules. Electric double-layer transistors (EDLTs) consisting of the organic semiconductor 3,11-dinonyldiaphtho[2,3-*d*:2′,3′-*d*′]benzo[1,2-*b*:4,5-*b*′]dithiophene (C_9-DNBDT-NW) have recently attracted attention because they are highly processable and, thus, allow for the fabrication of large-scale single-crystal transistors with excellent crystallinity and high mobility. Furthermore, Hall effect measurements indicate the emergence of a metallic phase with strong correlations upon doping.

Here, we performed, for the first time, in-situ Fourier-transform infrared spectroscopy on EDLTs composed of C_9-DNBDT-NW single crystals for different sheet conductivities and temperatures down to 6K in the mid and far infrared regions. Our results give insights into how thermal fluctuations are suppressed with decreasing temperature and increasing electrostatic doping concentration, which manifests itself in the behavior of the displaced Drude peak.

CPP 17.46 Mon 19:00 P5

Measurement of photon antibunching of organic molecules by substrate scanning — •Janne Oskar Becker, Robert Schmidt, Steffen Michaelis de Vasconcellos, and Rudolf Bratschitsch — Institute of Physics, University of Münster

Single-molecule photoluminescence spectroscopy is often performed in solution, with molecules drifting in and out of a stationary focus. To immobilize single molecules, they are typically diluted in a solvent and spin-coated on a substrate. However, bleaching processes lead to decreasing photoluminescence count rates when illuminating isolated single-molecules over time, making photon antibunching measurements extremely challenging. To circumvent this, we measure multiple molecules sequentially by spatially scanning the spin-coated surface and accumulating photons of multiple single-molecules. In that way, we are able to measure photon antibunching Si/SiO_2 substrate.

CPP 17.47 Mon 19:00 P5

Large-Area Semiconducting 2D Imine-COF Polymer Films on Dielectric Glass for Electronic Applications — •Diksha Srivastava[1], Vipin Mishra[2], Showkat H. Mir[3], Jyotirban Dey[1], Jayant K. Singh[1], Manabendra Chandra[1], and Thiruvancheril G. Gopakumar[1] — [1]Indian Institute of Technology Kanpur, Kanpur 208016, India — [2]Vellore Institute of Technology, Vellore, Tamil Nadu 632014, India — [3]University of Kashmir, Hazratbal, Srinagar 190006, Jammu and Kashmir, India

Two-dimensional imine-based covalent organic frameworks (2D COFs) are a growing class of crystalline π-conjugated organic polymers with strong potential in thin-film electronics and optoelectronics. We present a scalable and reproducible strategy for producing 2D imine-COF-based polymer thin films through a quasi-equilibrium Schiff-base reaction between p-phenylenediamine (PDA) and benzene-1,3,5-tricarboxaldehyde (TCA). This method enables the growth of large-area polymer films (up to 2 cm) on dielectric substrates with controlled thickness. SEM, TEM, and AFM confirmed the layered and crystalline morphology of the films. Optical absorption and scattering measurements revealed a semiconducting band gap consistent with the DFT-calculated band structures, indicating the presence of delocalized states suitable for charge transport. To probe intrinsic electrical behaviour, COF polymer films were integrated into Ag/COF/Glass devices. The I-V curves revealed semiconducting behaviour with low current density and field-assisted conduction limited by electrode-COF injection barriers.

CPP 17.48 Mon 19:00 P5

Designing functional polymer surfaces by initiated chemical vapor deposition — •Stefan Schröder, Lynn Schwäke, Tobias Giez, Thomas Strunskus, Franz Faupel, and Tayebeh Ameri — Kiel University, Kiel, Germany

Polymer thin films and organic surfaces have attracted significant interest across diverse application areas, ranging from wearable electronics to biomedicine and encapsulation. The demand for new functional surfaces, combined with ongoing device miniaturization, requires defect-free nanoscale polymer films with precise control over thickness and chemistry. Chemical vapor deposition (CVD) of polymer surfaces addresses these challenges by eliminating the dewetting and surface tension effects commonly encountered in conventional solution-based thin film fabrication. In particular, initiated chemical vapor deposition (iCVD) enables the fabrication of conformal polymer coatings with nanoscale precision on large-area substrates as well as on complex geometries. Moreover, iCVD allows for room-temperature deposition on delicate substrates, including flexible organic materials, copy paper, and biomedical patches. This contribution presents the fundamentals of the iCVD process and highlights selected application examples.

CPP 17.49 Mon 19:00 P5

Controlling Surface Wetting through Light- and Electric-Fields — •Billura Shakhayeva[1], Bas ter Beest[2], Frieder Mugele[2], and Björn Braunschweig[1] — [1]University of Münster, Institute of Physical Chemistry, Germany — [2]University of Twente, Physics of Complex Fluids

Electro-dewetting (EDeW) enables reversible control of surface wettability using ionic surfactants. Using dodecyl tetraethyl ammonium bromide (DTAB) as a cationic surfactant, previous studies achieved a change in the apparent contact angle (CA) of up to 30°. We used vibrational sum-frequency generation (SFG) spectroscopy and ellipsometry to probe the molecular structure close to the three-phase contact line under initial and EDeW conditions. Using 0.15 mM DTAB we observed the largest changes in contact angle and observed spreading of surfactant even at larger distances from the contact line. Further, we extended this approach from DTAB to photoswitchable arylazopyrazole triethylammonium bromide (AAP-TB) surfactants. AAP-TB can undergo E/Z photoisomerization and allows to change the surface activity through the choice of the configurational isomer with the Z being less surface active compared to the E. We demonstrate that EDeW with AAP-TB surfactants is possible similar to DTAB,

but with a smaller maximum change in contact of about 13° once a potential of +3 V is applied. In addition, photo-isomerization of AAP-TB allows to further finetune the CA reversibly by about 4°.

CPP 17.50 Mon 19:00 P5

Dynamic wetting of mixed rod-sphere suspensions and its relation to the suspension rheology — •Reza Azizmalayeri and Günter Auernhammer — Leibniz-Institut für Polymerforschung Dresden e. V.

In this study, we examine dynamic wetting of mixed rod-sphere suspensions near the advancing contact line. We compare pure spherical suspensions with 98:2 sphere-rod mixtures. Using a pinned droplet and moving substrate geometry on an inverted microscope, we achieve a locally stable contact line. Astigmatism Particle Tracking Velocimetry (APTV) measures the trajectories of tracer particles within the refractive index-matched suspension. Pinch-off experiments conducted via the Dripping-onto-Substrate (DoS) method provide Protorheology insights into shear and extensional viscosities. We analyse rod dynamics and orientation as they approach the advancing contact line, interact with the substrate, and re-enter the bulk suspension. In purely spherical suspensions, tracer trajectories near the advancing contact line deviate significantly from hydrodynamic model predictions. Conversely, mixed rod-sphere suspensions exhibit minimal deviations. Rod inclusion reduces effective viscosity during pinch-off, promoting deformation and thread thinning. This effect is amplified by rod-induced polydispersity and the disruption of spherical contact structures, weakening resistance to flow and altering rheology. Visualizations reveal that rods align parallel to the contact line, then rotate 90 degrees to align with the substrate.

CPP 17.51 Mon 19:00 P5

Statics and dynamics of drops on liquid infused surfaces — Hossein Abdolnezhad[1], •Martin Brinkmann[2], Ralf Seemann[2], and Ciro Semprebon[1] — [1]Department of Mathematics, Physics and Electrical Engineering, Northumbria University, Newcastle, UK — [2]Zentrum für Biophysik, Universität des Saarlandes, Saarbrücken, Germany

Slippery liquid-infused porous surfaces (SLIPS), inspired by the slippery properties of the Nepenthes pitcher plant, have been introduced to increase the mobility of wetting drops by minimizing the liquid-solid contact. Preparation of these surfaces involves infusing a lubricating liquid into a porous or textured surface, creating a thin liquid layer on top of the surface resulting in high drop mobility as well as unique properties such as anti-corrosion, self-cleaning, heat transfer enhancing, anti-fouling and anti-icing, water harvesting properties with a broad potential for application in industry.

The complex relationship between lubricant properties and retention mechanisms in liquid-infused surface, particularly the role of the lubrication ridge forming around the drop causing depletion of the lubricant over time brings up the questions of whether the lubricant ridge can be effectively controlled as well as whether there is an optimal size in relation to the volume of the drop sliding over liquid-infused surface. Recent experiments elucidate the role of the lubricant ridge in the dynamics of drops on liquid-infused surfaces, and led to the development of a theoretical understanding of the experimental observations combining finite-element and analytical modeling approaches.

CPP 18: Active Matter III (joint session BP/CPP/DY)

Time: Tuesday 9:30–12:45 Location: BAR/SCHÖ

CPP 18.1 Tue 9:30 BAR/SCHÖ

inertia-driven re-entrant coil-Globule transition of active ring polymers — •Sunil P Singh[1], Roland G Winkler[2], Rakesh Palariya[1], and Arindam Panda[1] — [1]Indian Institute of Science Education and Research Bhopal, India — [2]Theoretical Physics of Living Matter, Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Germany

The role of inertia in the collective dynamics of active systems has been a subject of increasing interest in recent studies. The present study investigates the inertial effects on active agents. We present the conformational and dynamical characteristics of an active Brownian ring polymer using Langevin dynamics simulations. We show that a long active ring polymer shrinks into globular-like structures even in the absence of attractive interactions. This transition becomes sharper and the structures more compressed as the reduced moment of inertia of the monomers increases, particularly in the intermediate range of activity. We demonstrate that the ring polymer undergoes a coil-globule-coil transition, which is modulated by both activity and rotational inertia. The coil-to-globule transition is mapped in the inertial parameter space (J-M) using the radius of gyration. Additional physical quantities, including bond-bond correlations, scaling behavior in the compressed state, monomer contact probability, geometric distances, coordination number, and effective temperature, further elucidate the physical mechanism driving the collapse. Finally, we show that the effective diffusivity of the ring polymer increases with the reduced moment of inertia as $D_p \sim \sqrt{J}$.

CPP 18.2 Tue 9:45 BAR/SCHÖ

Shape selectivity by complex buckling dynamics in poroelastic active gels — •Kinjal Dasbiswas[1], Subhaya Bose[1], Arnab Roy[1], Michael Vennettilli[1], and Anne Bernheim[2] — [1]University of California, Merced, USA — [2]Ben Gurion University, Israel

Shape change in animal cells is prototypically driven by active forces, generated by myosin molecular motors bound to the actin cytoskeleton. Inspired by experiments on disc-shaped extracts of crosslinked actomyosin gels, we aim to show how a family of 3D shapes can arise from buckling caused by non-uniform active stresses. Although synthesized with identical composition of actin, myosin and the crossliker fascin, these gels contract and buckle into different shapes depending on the initial aspect ratio of the disc: thinner gels tend to wrinkle, while thicker gels tend to form domes. By incorporating active stresses, actin alignment, and stress-dependent myosin binding kinetics into a 2D poroelastic gel model, we qualitatively capture trends in gel contraction dynamics observed from quantitative particle image velocimetry (PIV). Next, we carry out numeric simulations of a geometric elastic model for thin sheets to obtain 3D buckled shapes from the strain rates predicted by the poroelastic model. Our results show that the coupling of elasticity to solvent flow, motor binding and fiber alignment play an important role in shape changes in living matter. Our studies have implications for shape changes during tissue morphogenesis and cell migration.

CPP 18.3 Tue 10:00 BAR/SCHÖ

The energy cost to build a spindle — •Dongliang Zhang[1], Xingbo Yang[4], Jan Brugués[2,1,3,4], and Frank Jülicher[1,3,4] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [3]Center for Systems Biology Dresden, Dresden, Germany — [4]Physics of Life, Cluster of Excellence, TU Dresden, Dresden, Germany

Spindle is a structure actively build from microtubules (MTs), and plays an important role for chromosome segregation during cell cycle. It's observed in experiments that the spindle size and shape depends on the cell level metabolic rate. In this work, we developed a minimal model that captures the active, energy-consuming processes such as MT turnover and active stress generation, which shows the energy cost for spindle mass maintenance and spindle-shape formation. We show that a spindle can be self-organized through these active processes. We aim to predict how the size and shape of the spindle depends on the energy input, and explain relative experimental phenomena, e.g. spindle shrinkage when the metabolism level is reduced.

CPP 18.4 Tue 10:15 BAR/SCHÖ

Cytoskeletal oscillations drive large-scale flows and nuclear organization in early embryonic systems. — •Lara Koehler, Elissavet Sandaltzopoulou, and Jan Brugués — Physics Of Life, TU Dresden

Synchronization drives early embryonic development, enabling simultaneous cell divisions and the spatial organization of nuclei within the embryo. In organisms such as Xenopus, Drosophila, and zebrafish, mitotic waves coordinate cell cycles across distances that exceed diffusion limits, guided by a chemical oscillator. At the same time, global cytoplasmic flows in these syncytial tissues contribute to the large-scale self-organization of nuclei, yet the coupling between biochemical signaling and cytoskeletal mechanics that underlies these directed flows remains poorly understood. Here, we relax the geometric constraints of the embryo and investigate nuclear dynamics in Xenopus egg extracts and complementary simulations. We show that the periodic polymerization and depolymerization of microtubule asters are sufficient to generate robust large-scale directed flows, even though the asters are intrinsically isotropic. Furthermore, we demonstrate that cell division stabilizes short-range order in a global synchronized system. Together, these findings reveal a minimal physical mechanism by which cytoskeletal dynamics and biochemical oscillations jointly organize flows and patterns, with implications for understanding the emergent principles that shape early development across species.

CPP 18.5 Tue 10:30 BAR/SCHÖ

Geometric control of cell migration in disordered porous media — •Laeschkir Würthner[1] and Frederik Graw[2] — [1]European Molecular Biology Laboratory, Heidelberg, Germany — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg and Universitätsklinikum Erlangen, Erlangen, Germany

Cell migration is a dynamic process that plays a central role in development, wound healing, and immune responses. Active cell movement is controlled by

several biochemical and mechanical cues, including chemokine gradients and the mechanical properties of the extracellular matrix (ECM). Although the biochemical pathways underlying directed cell motion are increasingly well understood, the influence of the porous structure of the ECM on active cell motion remains largely unexplored. Using a combination of computational modeling and theory, we investigate how active cells move through 3D disordered porous environments. We show that cell migration in disordered porous media can be understood as a generalized random walk among "traps", with the effective diffusivity determined by the geometry of the microenvironment. A key implication of our work is that spatial heterogeneities in porosity effectively direct cell motion, revealing a guidance mechanism that we refer to as porotaxis. Overall, our work connects geometry with cell motility and underscores the microenvironment as a key regulator of cell migration.

CPP 18.6 Tue 10:45 BAR/SCHÖ

Motility-induced mixing transition in exponentially growing multicellular spheroids — •Torben Sunkel[1,2], Lukas Hupe[1,2], and Philip Bittihn[1,2] — [1]MPI for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, University of Göttingen, Germany

Growth drives cellular dynamics in various dense aggregates, but its effects on other relevant activities have only received limited attention. Here, we investigate the interplay of unconstrained growth, steric repulsion and motility in a minimal agent-based model of exponentially growing, three-dimensional spheroids. Our results reveal a diverging mixing time scale at a critical motility threshold, below which mixing of cells is completely suppressed. Above the threshold, large-scale mixing is enabled. Using an effective phenomenological model parameterized from full simulations, we identify two fundamental mechanisms governing this transition: On the cell scale, weak motility-induced active motion is locally suppressed by growth-induced steric repulsion, consistent with an Active Brownian Particle type description of single-cell dynamics. Beyond this, the expanding nature of the system inhibits global mixing purely geometrically by limiting the exploration range of diffusive cell motion. Both mechanisms naturally scale with the growth rate, highlighting the nature of the transition as an interplay between proliferation and motility. The results provide a baseline for identifying additional biological mechanisms in experiments and could be relevant for competition, heterogeneous tumor evolution and other manifestations of motile proliferating active matter.

15 min. break

CPP 18.7 Tue 11:15 BAR/SCHÖ

Fluctuation-Response Theory of Non-Equilibrium Complex Fluids — •Ryota Takaki[1] and Frank Jülicher[1,2,3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Center for Systems Biology Dresden, Dresden, Germany — [3]Cluster of Excellence Physics of Life, TU Dresden, Dresden, Germany

Active soft materials such as cytoplasm and tissues are constantly driven by chemical reactions and often retain long-lived mechanical memory. In this work, we develop a generalized hydrodynamic framework applicable to non-equilibrium fluids with memory at finite wavevectors and frequencies. Our approach is based on exact correlation-function identities, leading to a fluctuation-response relation for steady states, including non-equilibrium. Applying the theory to chemically driven active fluids, we uncover Active Viscoelastic Memory, in which reaction cycles dynamically renormalize the viscous response and can generate negative storage moduli at finite frequency, absent in conventional viscoelastic materials. Our results provide a first-principles basis for modeling memory-dependent dynamics in a broad class of biological and synthetic active systems, and suggest concrete rheological signatures of chemical driving that can be tested experimentally.

CPP 18.8 Tue 11:30 BAR/SCHÖ

Chemically Active Liquid Bridges Generate Repulsive Forces — •Noah Ziethen — DAMTP, University of Cambridge, UK

Intracellular droplets help organize cells by compartmentalizing biomolecules and mediating mechanical interactions. When such droplets bridge two structures, they generate capillary forces that depend on the surface properties and the separation between the structures. While the forces exerted by passive liquid bridges are well understood, the impact of active chemical reactions, ubiquitous in biological condensates, remains unclear.

Here, we investigate a single liquid bridge with continuous chemical turnover, in which the production and degradation of droplet material maintain a non-equilibrium steady state. In this active bridge, the reactions dynamically set the bridge radius, thereby controlling the force-distance relation. In striking contrast to passive systems, we find that activity can generate purely repulsive forces over a broad range of separations. These results show that chemical activity can qualitatively alter capillary forces generated by liquid bridges, suggesting a potential route for cells to actively regulate mechanical coupling via droplets.

CPP 18.9 Tue 11:45 BAR/SCHÖ

Shared Laws of Pattern Formation in Reaction-Diffusion and Phase Separation — •Daniel Zhou[1] and Erwin Frey[1,2] — [1]Arnold Sommerfeld Center for Theoretical Physics — [2]Max Planck School Matter to Life

Many nonlinear field theories generate a strikingly similar repertoire of patterns: arrested coarsening, traveling waves, and spatiotemporal chaos appear both in phase-separating systems and in classical reaction-diffusion models. These descriptions have different physical origins, yet recent studies on Turing mixtures and foams in protein systems [1] and on chemotaxis-driven phase separation in cell populations [2] have already highlighted unexpected connections between these ostensibly different mechanisms, linking foam-like, phase-separating, and reaction-diffusion-type patterns. The present work revisits the relation between kinetic and phase-separating descriptions from a more general viewpoint. A unifying perspective is developed that places different modeling frameworks on comparable footing, identifies the conditions under which they yield effectively equivalent patterns, and suggests how stability criteria and design principles can be translated between them. This points toward a more systematic classification of pattern-forming dynamics that cuts across traditional divides between reaction-diffusion, chemotactic, and phase-separating systems.

[1] H. Weyer et. al, Deciphering the Interface Laws of Turing Mixtures and Foams, arXiv:2409.20070 (2024).

[2] H. Weyer et. al, Chemotaxis-Induced Phase Separation, Physical Review Letters 135, 208402 (2025).

CPP 18.10 Tue 12:00 BAR/SCHÖ

Spatial self-organization of enzymes in complex reaction networks — •Vincent Ouazan-Reboul[1,2], Ramin Golestanian[2,3], and Jaime Agudo-Canalejo[2,4] — [1]LPTMS, CNRS, Université Paris-Sud, 91400, Orsay, France — [2]Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, D-37077, Göttingen, Germany — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, OX1 3PU, Oxford, UK — [4]Department of Physics and Astronomy, University College London, WC1E 6BT, London, UK

Living systems contain intricate biochemical networks whose structure is closely related to their function and allows them to exhibit robust behavior in the presence of external stimuli. Such networks typically involve catalytic enzymes, which can have non-trivial transport properties, in particular chemotaxis-like directed motion along gradients of substrates and products. Here, we find that taking into account enzyme chemotaxis in models of catalyzed reaction networks can lead to their spatial self-organization in a process similar to biomolecular condensate formation. We develop a general theory for arbitrary reaction networks, and systematically study all closed unimolecular reaction networks involving up to six chemicals. Importantly, we find that network-wide propagation of concentration perturbations can be key to enabling self-organization, in a manner which is highly sensitive on the global network structure.

CPP 18.11 Tue 12:15 BAR/SCHÖ

Spatial organisation of the cell's metabolic power plant via phase separation — •Kathrin S. Laxhuber[1,2] and Frank Jülicher[1,2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck School Matter to Life

Cell metabolism is the power plant that fuels the active processes essential to life. Recent experimental results show that glycolytic enzymes, central to sugar metabolism, phase-separate to form foci under energetic stress and can localise to sites of demand. To understand this phenomenon, we build and study a minimal theoretical model. We show that droplet formation can act as a metabolic switch that enables the system to maintain energetic homeostasis at higher output power. Notably, the metabolic droplets that emerge from this switch can self-organise to colocalise with demand. We discuss the non-equilibrium features and spatial energetic profiles in this system.

CPP 18.12 Tue 12:30 BAR/SCHÖ

Emergent interactions lead to collective frustration in robotic matter — •Onurcan Bektas[1,3], Adolfo Alsina[2,3], and Steffen Rulands[1,3] — [1]Arnold-Sommerfeld-Center for Theoretical Physics and Center for NanoSciences, Ludwig-Maximilians-Universität München, Theresienstr. 37, 80333 München, Germany — [2]GISC, Universidad Rey Juan Carlos, Tulipán, 28933, Móstoles, Spain — [3]Max-Planck-Institute for the Physics of Complex Systems, Noethnitzer Str. 38, 01187 Dresden, Germany

Current artificial intelligence systems show near-human-level capabilities when deployed in isolation. Systems with intelligent agents are deployed to perform tasks collectively. This raises the question of whether robotic matter, where many learning and intelligent agents interact, shows emergence of collective behaviour. And if so, what kind of phenomena would such systems exhibit? Here, we study a paradigmatic model for robotic matter: a system composed of a large collection of stochastic interacting particles where each particle is endowed with a deep neural network that optimizes its transitions based on the particles' environments. For a 1D model, robotic matter exhibits complex phenomena arising from emergent interactions, including transitions between long-lived learning regimes, the emergence of particle species, and frustration. We also find an

abrupt, density-dependent change in the behaviour of particles. Using active matter theory, we show that this phenomenon is a reflection of a phase transition with signatures of criticality. Our model captures key phenomena observed in more complex forms of robotic systems.

CPP 19: Focus Session: Water – from Atmosphere to Space I (joint session CPP/DY)

Water plays a vital role in diverse Earth processes across multiple scales, from atmospheric cycles and aerosol chemistry to geological porous media and nanoscale biological functions of hydrated proteins. Despite its fundamental importance and numerous anomalous properties, such as the diverging heat capacity of supercooled water, pure bulk water remains poorly understood. Key phenomena like evaporation and crystallization are relevant not only on Earth but also in extraterrestrial environments. In Germany, molecular water research is flourishing across prestigious centers, exemplified by the new BlueMat cluster at Hamburg University of Technology, the renewed RESOLV cluster at Ruhr-University Bochum, and the Max Planck Society's expanding Liquid Initiative in Mainz. The 2025 inauguration of the Centre for Molecular Water Science (CMWS) at Hamburg's DESY campus further strengthens a Europe-wide interdisciplinary network, uniting 47 founding members from 12 countries to advance water science across disciplines and methods. Within this focus session the state of molecular water research shall be discussed and interactions between the physical sub-fields shall be fostered.

Organized by Alexander Schlaich, Katrin Amann-Winkel, Mischa Bonn.

Time: Tuesday 9:30–11:00 Location: ZEU/LICH

Topical Talk CPP 19.1 Tue 9:30 ZEU/LICH

Surface adsorption and protonation equilibrium of atmospheric organics at the aqueous surface — •Nønne Prisle — Center for Molecular Water Science, Deutsches Elektronen-Synchrotron DESY, Notkestrasse 85, D-22607 Hamburg, Germany — Institute of Inorganic and Applied Chemistry, University of Hamburg, Martin-Luther-King-Platz 6, D-20146 Hamburg, Germany — Center for Atmospheric Research, University of Oulu, P.O. Box 4500, FI-90014, Oulu, Finland

Atmospheric aerosols comprise a significant fraction of organic species which frequently exhibit both surface activity and Brönsted acidity or basicity in aqueous solutions. The high surface area to bulk volume ratios of nano- and microscopic aerosols and droplets further favor surface-specific states, affecting both bulk-phase and heterogeneous chemistry.

We used X-ray Photoelectron Spectroscopy (XPS) in combination with high-brilliance synchrotron radiation to directly observe the protonation state of atmospheric acids and bases at the surfaces of aqueous aerosol and droplet models. We found that for each acid-base pair, the neutral species is enhanced in the surface, consistent with its higher surface activity, compared to the charged conjugate. This introduces a shift in the protonation equilibrium at the aqueous surface corresponding to an apparent change in pKa of 1-2 pH units, depending on the concentration, acidity, and surface activity of the conjugate acidic and basic species.

CPP 19.2 Tue 10:00 ZEU/LICH

The Effect of pH on the Structure of Model Sea Spray Aerosol Surfaces — •Clara M. Saak, Lars Höhner, and Ellen H.G. Backus — Institute of Physical Chemistry, Faculty of Chemistry, University of Vienna, Währinger Straße 42, 1090 Vienna, Austria

Aerosols play a key role in the global climate due to their ability to scatter and reflect solar radiation and to act as cloud condensation nuclei (CCN), exerting a pronounced cooling influence on the global climate. In particular, the surface availability of ions and organic compounds is known to affect the hygroscopicity of the particle and thereby its ability to act as a CCN [1]. While the surface propensity of individual compounds has been studied widely, much less is known about more complex systems. Here we focus on the impact of bulk pH on the architecture of mixed aqueous interfaces. In atmospheric systems the pH has been shown to range from roughly pH 8 to 2 [2]. Using sum-frequency-generation (SFG) spectroscopy in conjunction with surface tension data we study the surface composition and structure of short and long chain organic acids at different protonation stages, obtained by varying the pH. Using this approach, we find pronounced changes in the structuring of the aqueous sub-surface layers depending on the specific composition and pH, and in the Gibbs free energy of adsorption of the studied organics. Our results show that it is feasible for subtle environmental changes to considerably affect structure and composition of the aqueous interface, which is known to play a key role in aerosol hygroscopicity. [1] Zieger, Nat. Commun. 2017, 8, 15883. [2] Angle, PNAS, 2021, 118, 2, e2018397118

CPP 19.3 Tue 10:15 ZEU/LICH

Crystallization behaviour of nanoparticle suspensions — •Isabell Zick[1,2], Eduard Edel[2], and Katrin Amann-Winkel[1,2] — [1]Institut für Physik, Johannes Gutenberg-Universität, Staudinger Weg 7, 55128 Mainz, Germany — [2]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany

Water is one of the most abundant substances in the world and due to this in close contact with many materials including micro- and nanoplastic particles. Those have been detected not only in sea but also in the atmosphere, where the particles can interact with water and act as cloud condensation nuclei or ice-nucleating particles. Emerging evidence suggests that nanoparticles with increased surface roughness or chemical functionalities may promote heterogeneous ice nucleation through different processes like, e.g., contact- and immersion-freezing. Such a behaviour affects cloud properties with significant implications for Earth*s radiative balance and the hydrological cycle.

We investigate atmospherically relevant nanoparticles dispersed in water to investigate their influence on the ice crystallization. Our experiments include calorimetry (DSC) as well as X-ray diffraction measurements (XRD). Our measurements show that the crystallization temperature depends on the particle size, concentration, and the chemical surface of the particles. Using XRD, we investigate the restructuring of the water molecules during supercooling, observed by a shift in the characteristic main diffraction peak of water and the subsequent crystallization process.

CPP 19.4 Tue 10:30 ZEU/LICH

Laser-Excited X-ray Reflectivity of Aqueous SrCl2 at the Air-Water Interface — •Ali Ashtiani Abdi[1,2], Julia Kobus[1,2], Svenja C. Hövelmann[1,2], Philipp Jordt[1,2], Nicolas Hayen[1,2], Prashant Hitaishi[1,2], Ajay Ajay[1,2], Rabia Qamar[1,2], Otto Lippmann[1,2], Chen Shen[3], Florian Bertram[3], and Bridget M. Murphy[1,2] — [1]IEAP, CAU Kiel University, Kiel, Germany — [2]Ruprecht Haensel Laboratory, DESY, Hamburg, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Understanding aqueous interfaces is essential for describing chemical processes in atmospheric, marine, and geochemical environments. While monovalent salts have been widely studied, the interfacial behavior of divalent ions is less understood, despite their relevance in seawater aerosols and reactive brines. SrCl2 is a representative divalent electrolyte whose interfacial structure may show alteration by laser illumination.

We investigate aqueous SrCl2 solutions at different concentrations using X-ray reflectivity (XRR) at the liquid-air interface. Measurements were performed at the LISA setup at beamline P08, PETRA III (DESY), where controlled laser illumination can be applied directly to the X-ray footprint, following the instrumentation concept of Warias and Hovelmann et al. (J. Synchrotron Rad. 2024). Reflectivity curves were recorded with and without laser exposure. The data demonstrate the suitability of SrCl2 surfaces for laser-assisted XRR and the sensitivity of the method to potential changes in interfacial structure, including indications of near-surface layering.

CPP 19.5 Tue 10:45 ZEU/LICH

Monitoring Uptake, Release and Reaction of Gases at the Liquid-Vapor Interface — •Tillmann Buttersack[1], Shirin Gholami[1], Clemens Richter[1], Daniela Torres-Diaz[1], Bernd Winter[1], Pavel Jungwirth[2], Stephen Bradforth[3], Markus Ammann[4], Ruth Signorell[5], Ivan Gladich[6], Remi Dupuy[7], Philip Mason[2], and Hendrik Bluhm[1] — [1]Fritz Haber Institute, Max Planck Society, Berlin, GER — [2]IOCB, Czech Academy of Sciences, Prague, CZ — [3]University of Southern California, Los Angeles, USA — [4]Paul Scherrer Institut, Villigen, CH — [5]EZH Zürich, CH — [6]University of Urbino, Urbino, I — [7]Sorbonne Université, Paris, F

Multiphase reactions are omnipresent in nature, industrial applications. The direct observation of reactions at the liquid-vapor interface requires spectroscopic

techniques that are surface specific and chemically sensitive to detect low concentrations, e.g., photoelectron spectroscopy (XPS). Furthermore, the sample delivery method must allow sufficient time for an interface reaction to proceed. These complex challenges require individual approaches for each system of interest. One example for a multiphase process is the reaction between liquid alkali metal and water vapor, which is extremely fast. We used a slow droplet train of NaK in a wet atmosphere and observed the formation of golden aqueous solutions with metallic properties with XPS. An example with relevance for atmospheric chemistry is the formation and the release of sulfur dioxide (SO2) from aqueous sulfite solutions due to acidification. We demonstrated that dissolved gases can be detected with XPS even though their concentration is only about 1 mM.

CPP 20: Complex Fluids and Soft Matter (joint session DY/CPP)

Time: Tuesday 9:30–12:45 Location: ZEU/0160

CPP 20.1 Tue 9:30 ZEU/0160

Process-Directed Self-Assembly of Copolymer Blends: Micro- and Macrophase Separation — •Jiayu Xie and Marcus Müller — Institute for Theoretical Physics, Georg August University Göttingen, Germany

The equilibrium phase behavior of binary diblock copolymer blends involves a complex interplay between microphase and macrophase separation. We investigate blends of linear diblock copolymers, A_1B_1 (cylinder-forming) and A_2B_2 (cylinder- or lamella-forming), using a combination of self-consistent field theory (SCFT) and single-chain-in-mean-field (SCMF) simulations. When the chain-length asymmetry between the A_1B_1 and A_2B_2 copolymers becomes large, the equilibrium phase diagram exhibits a wide macrophase-separation channel. Strikingly, our simulations reveal a strong pathway dependence within this region: rapid quenching yields a spatially homogeneous structure with narrow cylinder-size distributions and strong hexagonal order, whereas gradual annealing promotes local demixing, resulting in bimodal domain sizes and weaker order. We demonstrate that this process-dependent nonequilibrium behavior can be explained by the distinct evolutions of the system state and free-energy landscape of the blends under quenching or annealing. These findings highlight how different processing conditions can direct nanostructure formation in block copolymer blends, and establish a mechanistic link between processing pathway and the final morphology, thus offering insights into rational design of targeted nanostructured materials.

CPP 20.2 Tue 9:45 ZEU/0160

Topological defect engineering enables size and shape control in self- assembly — Lara Koehler[1,3], Markus Eder[2], Vincent Ouzan-Reboul[3], Christoph Karfusehr[2], Andrey Zelenskiy[3], Pierre Ronceray[4], Friedrich Simmel[2], and •Martin Lenz[3] — [1]MIPPKS, Dresden, Germany — [2]TU Munich, Germany — [3]U. Paris-Saclay, Orsay, France — [4]Aix-Marseille-Université, Marseille, France

Equilibrium self-assembly is a powerful way to build nano- and microscale structures out of interacting subunits. The size and shape of such structures must be controlled in many biological and technological functions, posing significant practical challenges as current strategies require multiple subunit types or the precise control of their shape and mechanics. Here we introduce an alternative approach that circumvents these obstacles. Our method uses subunits whose interactions promote crystals, but also favor crystalline defects. We show theoretically that the magnitude of these interactions, which is well controlled in experiments, governs the self-assembly through topological restrictions on the scope of the defects. Using DNA origami, we demonstrate both size and shape control in two-dimensional disk- and fiber-like assemblies. Our basic concept of defect engineering operates well beyond these examples, and provides a broadly applicable framework to control self-assembly.

CPP 20.3 Tue 10:00 ZEU/0160

Soft colloidal monolayers under drying conditions — •Kai Luca Spanheimer[1], Maret Ickler[2], Julian Ringling[3], Nicolas Vogel[2], Matthias Karg[4], and Hartmut Löwen[1] — [1]Insitut für Theoretische Physik II, Heinrich-Heine-Universität, 40225 Düsseldorf, Germany — [2]Institute of Interfaces and Particle Technology, Friedrich-Alexander University, Erlangen, Germany — [3]Physikalische Chemie I: Kolloide und Nanooptik Heinrich-Heine-Universität, 40225 Düsseldorf, Germany — [4]Institut für Chemie, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle, Germany

Langmuir-Blodgett deposition is a well established technique in research and industry. Even though, there still are effects in this process that are not yet explored from a theoretical standpoint. It is usually assumed that the deposited pattern is identical with the one appearing at the water-air interface. In recent experimental studies, strong reorganization during the drying of soft colloidal monolayers has been observed [1]. Capillary forces during drying are known to change nanoscopic structures, sometimes even leading to their destruction. To model these processes we propose a combination of overdamped particle dynamics coupled to dewetting dynamics of an evaporating liquid film. The patterns produced by this model fit those observed in experiment. This theoretical approach allows exploration of the drying dynamics. Thereby we gain new insights into the drying process and makes experimental results produced with Langmuir-Blodgett deposition more reliable.

[1] K. Kuk, et al: Adv. Sci., 11, 2406977 (2024).

CPP 20.4 Tue 10:15 ZEU/0160

Mechanical assessment of microfluidically-generated poroelastic microgel particles — Aude Sagnimorte[1,2], Anke Lindner[2], and •Joshua McGraw[1] — [1]Gulliver-CNRS, ESPCI-PSL, 10 rue Vaquelin, 75005 Paris — [2]PMMH-CNRS, ESPCI-PSL, 10 rue Vaquelin, 75005 Paris

Soft microgels have numerous applications in diverse fields,such as tissue engineering, drug delivery systems, soft robotics, or as model systems for suspensions or colloids. Among these, photopolymerized hydrogels such as poly(ethylene glycol) diacrylate (PEGDA) are commonly used due to their highly tunable mechanical properties. However, proper characterisation of these properties is challenging, in part due to their small scale, on the order of tens of microns, and in particular the lack of assessment of their time-dependent properties. Here we provide a comprehensive mechanical characterisation of individual photopolymerised microgels particles using atomic force microscopy (AFM) for precise local measurements. In particular, we performed indentation-relaxation tests on PEGDA microdisks immersed in water. By varying indentation depth and probe diameter, we changed the contact area and observed relaxation responses which are indicative of poroelastic behaviour. In particular, larger contact areas resulted in longer relaxation times. Our results also show that increasing the amount of solvent increased the relaxation time. Our collected results are consistent with a simple, Herzian poroelastic model giving good agreement with both the approach and relaxation phases of the experiments.

CPP 20.5 Tue 10:30 ZEU/0160

Nonlinear Viscoelastic Response and Stress Shielding in Driven Bistable Spring Chains — •Sven Pattloch[1,2] and Joachim Dzubiella[1,2] — [1]Applied Theoretical Physics-Computational Physics, Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Germany. — [2]Cluster of Excellence livMatS@FIT-Freiburg Center for Interactive Materials and Bioinspired Technologies, Albert-Ludwigs-Universität Freiburg, Germany

Bistable micromodules are a promising route to design adaptive mechanical metamaterials with tunable viscoelastic response. Here, a driven one-dimensional chain of bistable springs is studied in which both the mechanical deformation and the internal excitation states evolve dynamically under time-dependent forcing. Their coupling produces rich nonlinear viscoelastic behaviour, including frequency-dependent susceptibilities, delayed deformation, and pronounced hysteresis in cyclic loading.

Using analytical linear response theory complemented by numerical simulations, the model quantifies how microscopic parameters and driving protocols control effective stiffness, loss, and phase lags. A key result is a strong attenuation ('shielding') of stress propagation along the chain that is already present for monostable springs but is markedly amplified by excitation switching in bistable modules. These findings provide simple design principles for tailoring nonlinear viscoelasticity, hysteresis, and stress shielding in driven soft matter and mechanical metamaterial systems.

CPP 20.6 Tue 10:45 ZEU/0160

Euler buckling on curved surfaces — •Shiheng Zhao[1,2,3] and Pierre A. Haas[1,2,3] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Max Planck Institute of Molecular Cell Biology and Genetics — [3]Center for Systems Biology Dresden

Nearly three hundred years ago, Euler showed that an inextensible straight elastic line in the plane buckles under compression when the compressive force F reaches a critical value $F_* > 0$. But how does such an elastic line buckle within a general curved surface? Here [1], we reveal that the classical instability changes fundamentally: By weakly nonlinear analysis of the buckling of an asymptotically short elastic line, we show that the critical force for the lowest buckling mode is $F_* = 0$ and discover a new bifurcation structure in which the modes of classical Euler buckling split into pairs. For long elastic lines, we numerically find an additional bifurcation by which the second of these new modes becomes the lowest mode and show that, at sufficiently large F, they undergo discontinuous snap-through to higher end-to-end compression. We explain these bifurcations in terms of the general unfolding of a pitchfork. This constitutes the foundations for a class of mechanical instabilities within curved surfaces from which, for example, biological shape emerges in development.

[1] S. Zhao and P. A. Haas, Phys. Rev. Lett. (in press)

15 min. break

CPP 20.7 Tue 11:15 ZEU/0160

Linking molecular dynamics and experimental FORCs in multicore magnetic nanoparticles — Ekaterina Novak[1], •Malika Khelfallah[2], Andrey Kuznetsov[3], Deniz Mostarac[4], Claire Carvallo[2], Amélie Juhin[2], and Sofia Kantorovich[3] — [1]Ekaterinburg, Russia — [2]Sorbonne Université, Paris, France — [3]University of Vienna, Vienna, Austria — [4]University of Edinburgh, Edinburgh, United Kingdom

Multicore magnetic nanoparticles - clusters of several magnetic grains embedded in a nonmagnetic matrix - exhibit collective behaviour distinct from single-core particles and are promising candidates fro drug targeting and magnetic hyperthermia. Their magnetic cores possess finite anisotropy, and the multicore assemblies range from near-spherical to elongated ellipsoids, features that strongly affect their response to external fields. To study these effects, we use molecular dynamics simulations [1] to model internal structure, anisotropy distribution, and collective switching. As a key diagnostic, we employ First Order Reversal Curves [2], which experimentalists routinely measure for immobilised multicore particles, enabling direct comparison between simulations and experiments. FORC diagrams reveal coercivity distributions and magnetic interactions between grains, offering detailed insight into interaction mechanisms and domain processes.

The work was financially supported by the RSF grant No. 25-22-00762.

[1] R. Weeber et al. (2024), Comprehensive Computational Chemistry, 3, 578-601. [2] C. R. Pike et al., J. Appl. Phys., 1999, 85, 6660

CPP 20.8 Tue 11:30 ZEU/0160

Hydrodynamics substantially affects induced structure formation in magnetic fluids — •Henning Reinken and Andreas M. Menzel — Otto-von-Guericke-Universität Magdeburg, Germany

Magnetorheological fluids consist of micrometer-sized magnetic particles suspended in a carrier liquid [1]. Sufficiently strong external magnetic fields lead to the formation of string-like particle aggregates, which results in complex magnetorheological behavior. This mechanism can further be used in the production of magnetic elastomers during the polymerization process when the carrier medium is still fluid and particulate structure formation still possible [2]. Using numerical simulations that spatially resolve both fluid flows and magnetization, we demonstrate that hydrodynamic interactions play a substantial role during structure formation. Hydrodynamics supports the emergence of string-like aggregates, while magnetic interactions align them. Considering besides this fundamental insight the enormous technical importance and potential of magnetic fluids, our results are substantial also from an application perspective.

We acknowledge support by the German Research Foundation DFG through Research Unit FOR 5599 on structured magnetic elastomers.

[1] S. Odenbach, Arch. Appl. Mech. **86**, 269 (2016).
[2] D. Günther, D. Yu Borin, S. Günther, S. Odenbach, Smart Mater. Struct. **21**, 015005 (2012).

CPP 20.9 Tue 11:45 ZEU/0160

Near-surface colloidal dynamics in jammed and slipping microgel suspensions — •Masoodah Gunny[1], Frédérick Caetano[2], Matilde Bureau[2], Alexandre Vilquin[1], Marie Le Merrer[2], Catherine Barentin[2], and Joshua McGraw[1] — [1]Gulliver - CNRS, ESPCI-PSL 10 Rue Vauquelin 75005 Paris, France — [2]ILM - CNRS, Claude Bernard University, 16 Enrico Fermi 69100 Villeurbanne, France

Jammed suspensions of soft microgel particles exhibit wall slip along smooth boundaries. The direct observation of dynamics within a supposed depletion layer near the wall were difficult to achieve as a result of the layers' supposed sub-micrometric dimensions. We use total internal reflection fluorescence microscopy (TIRFM) to observe colloidal-particle dynamics near the interface between glass and microgel suspensions. Remarkably, microgel suspensions display nanoscale velocity profiles with a slope rupture; particle velocity increases with distance near the wall, and tends to a constant beyond a distance which is characteristic of the ones predicted previously. Beyond velocimetry, we also study the statistical particle altitude distributions near the wall in TIRFM measurements. These distributions are strongly pressure dependent, with nanoparticles more likely found near the solid/liquid interface when the fluid is transported faster near the wall. This high-velocity particle enrichment, not seen for the Newtonian case, is consistent with the development of a depletion layer under such conditions. Taken together, our observations give strong support for the existence of a depletion layer being responsible for wall slip.

CPP 20.10 Tue 12:00 ZEU/0160

Random close packing as a conserved directed percolation transition — •Thomas Axmann and Michael Schmiedeberg — Theoretical Physics: Lab for Emergent Phenomena, Soft Matter Theory Group, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

In studying quenches in soft sphere systems O'Hern et al. related the onset of overlaps to isostaticity [1], and consequently to the random close packing scenario. The conditions that lead to the avoidance of overlaps between spheres can be studied with the random organization model [2], which was initially introduced to investigate self organization in sheared colloids. Modifications of this model, which dynamically reduce interparticle overlaps, were used to characterize the random close packing problem as the critical point of a dynamic absorbing state transition in the $d + 1$ dimensional conserved directed percolation universality [3,4].

We aim to deepen the understanding of this connection by demonstrating that the configuration change at each time step can be chosen with a fully deterministic strategy while retaining the features of the transition. We clarify difficulties in the treatment of percolating clusters and find that the median overlap depth proves to be a more useful order parameter.

[1] O'Hern et al. PRE 68 (2003)
[2] Corté et al. Nat. Phys. 4 (2008)
[3] Milz et al. PRE 88 (2013)
[4] Wilken et al. PRE 128 (2021)

CPP 20.11 Tue 12:15 ZEU/0160

Rescaled mode-coupling scheme for dynamics in binary mixtures of highly charged colloids — •Daniel Weidig and Joachim Wagner — University of Rostock, Rostock, Germany

We investigate dynamic processes in binary mixtures of highly charged colloidal particles by means of Brownian dynamics and multi-component mode-coupling theory (MCT). As input for MCT, thermodynamically consistent, static structure factors from integral equations with Rogers-Young closure are used which are in quantitative agreement to Fourier transforms of static pair correlation functions resulting from simulations.

MCT based on partial structure factors in many-particle systems predicts dynamic properties such as long-time self-diffusion coefficients in qualitative agreement to simulation trajectories. Using instead structure factors from systems with slightly reduced number of effective charges as input, a quantitative agreement of MCT with simulations is achieved. In mixtures of identically charged particles with different short-time mobilities, this rescaled MCT scheme accurately predicts coupling effects in long-time dynamics observed in Brownian dynamics simulations.

CPP 20.12 Tue 12:30 ZEU/0160

Electric double layers - the software package capDFT — Fabienne Dressler and •Andreas Härtel — Institute of Physics, University of Freiburg

Electric Double Layers are used to store electric energy, they can be utilized to harvest energy from waste heat or steps in concentrations, and they stabilize colloidal systems. In all cases, mobile ions arrange themselves to screen surface charges, resulting in sometimes densely packed regions of microscopic particles far from bulk states that dominate the macroscopic physical properties of the system. Modeling these complex systems has theoretical and numerical limitations, but good although expensive solutions exist. We present an open-source software package to treat the described modeling utilizing classical density functional theory [1]. The package has been used successfully in studies of underscreening [2] and allows to go beyond the standard mean-field approximation of primitive models [3]. We will demonstrate the package by discussing an example, where we study capacities of structured electrodes.

[1] https://github.com/andreashaertel/capdft
[2] Anomalous Underscreening in the Restricted Primitive Model. A. Härtel, M. Bültmann, and F. Coupette. Phys. Rev. Lett. 130, 108202 (2023)
[3] The primitive model in classical density functional theory: beyond the standard mean-field approximation. M. Bültmann and A. Härtel. J. Phys. Condens. Matter 34, 235101 (2022)

CPP 21: French-German Session: Simulation Methods and Modeling of Soft Matter III

Time: Tuesday 9:30–11:15 Location: ZEU/0255

Invited Talk CPP 21.1 Tue 9:30 ZEU/0255

Molecular modelling of gas solubility and free volume trends in Si-functionalized ionic liquids — •Kateryna Goloviznina[1,2], Eduards Bakis[3], Inês C. M. Vaz[2,4], Agilio Padua[2], and Margarida Costa Gomes[2] — [1]ICSM, University of Montpellier, CEA, CNRS, ENSCM, 30207 Bagnols-sur-Ceze, France — [2]Laboratoire de Chimie, ENS de Lyon and CNRS, 46 allée d'Italie, 69364 Lyon, France. — [3]Faculty of Chemistry, University of Latvia, Jelgavas 1, Riga, LV-1004, Latvia. — [4]CICECO, Aveiro Institute of Materials,

Department of Chemistry, University of Aveiro, 3810-193 Aveiro, Portugal

Molecular dynamics (MD) simulation is a powerful technique that provides insight into the nanoscale structure and transport properties of liquids in bulk and at interfaces, explaining experimentally observed phenomena and contributing to the rational design. In the present work, we explored Si-functionalized imidazolium-based ionic liquids—low-density, low-viscosity systems—that are promising for gas capture and separation due to their enhanced free volume. [1] Using classical MD simulations with the CL&Pol polarizable force field, [2] we proposed a way to estimate free-volume trends and solubilities of simple gases (e.g., argon) without the need to perform costly experiments. The work was further extended to unsaturated C_2 hydrocarbons, for which we rationalized solubility trends via local structural analysis and estimated the contributions of van der Waals, electrostatic, and polarization terms to the solvation free energy.

[1] E. Bakis et al. Chem. Sci. 2022, 23, 9062.
[2] Goloviznina et al. J. Chem. Theory Comput. 2019, 15, 5858.

CPP 21.2 Tue 10:00 ZEU/0255

Classical DFT compared to AFM measurement of structural forces from confined electrolyte containing charged nanoparticles — •Simone Riva[1], Michael Ludwig[2], Regine von Kltizing[2], and Ofer Manor[1] — [1]Technion, Haifa, Israel — [2]Technische Universität Darmstadt, Darmstadt, Germany

We use classical density functional theory (DFT) to model colloidal-probe atomic force microscopy (AFM) force curves across an aqueous electrolyte containing charged solid nanoparticles. The charged AFM probe and substrate interact through a suspension of silica nanoparticles. The probe experiences oscillatory forces driven by the structuring of the charged nanoparticles, which can enhance the stability of the film. Structural forces are characterized by an alternation of repulsion due to steric and electrostatic nanoparticle interactions, and depletion attraction. We present a self-consistent theory of oscillatory forces in ionic systems. Moreover, we compare different DFT approaches and validate them against AFM measurements, to develop a theory that best fits the rich physics of experiments. We calculate structural and EDL forces by minimizing dedicated functionals. We adopt two types of weighted density functionals, disclosing their applicability in different concentration conditions. We propose a way to include electrostatic interactions between nanoparticles in an effective hard-sphere functional. We further confirm a general scaling law of the oscillation wavelength observed in experiments and connect it to nanoparticle packing structures. The theory agrees well with measurement in the absence of fitting parameters. Riva et al., JCIS 2026, 702, 138901.

CPP 21.3 Tue 10:15 ZEU/0255

Sc-cDFT: A Single-Chain Simulation Framework with Classical Density Functional Theory for Polymers — •Raju Lunkad[1], Alejandro Gallegos[2], Jianzhong Wu[3], and Marcus Müller[1] — [1]Institute for Theoretical Physics, Georg-August University, 37077 Göttingen, Germany — [2]Department of Chemical and Materials Engineering, New Mexico State University, Las Cruces, New Mexico 88001, United State of America — [3]Department of Chemical and Environmental Engineering, University of California, Riverside, CA, United States of America

We present Sc-cDFT, a combination of Single-Chain Simulation with classical Density-Functional Theory (cDFT), for modeling polymer solutions and brushes. In this approach, intramolecular correlations are explicitly treated using Monte-Carlo (MC) simulations, while intermolecular correlations are extracted from cDFT. In this way, we capture structural properties and thermodynamics of multi-chain systems while providing a segment-level description of the dynamic behavior. Importantly, this framework substantially reduces computational cost, enabling the simulation of significantly longer polymer chains that are often inaccessible to fully explicit particle-based simulations. We validate the Sc-cDFT framework for hard-sphere polymer solutions and brushes by comparing polymer configurations and the segmental density profiles with fully explicit particle-based simulations, showing quantitative agreement.

CPP 21.4 Tue 10:30 ZEU/0255

Adsorption Thermodynamics and Kinetics of Complex Fluids: Physical Modeling of Surface Saturation, Reservoir Depletion, Lateral Interactions, and Collective Effects — •Nada Ben Amor[1,2], Daniela Bauer[1], Benjamin Braconnier[1], and Benoit Coasne[2,3] — [1]IFP Energies nouvelles, 92852 Rueil-Malmaison, France — [2]Université Grenoble Alpes, CNRS, LIPhy, F-38000 Grenoble, France — [3]Institut Laue Langevin, F-38042 Grenoble, France

Adsorption at solid surfaces is considered a promising technique to capture and remove emerging pollutants such as PFAS from water. However, a major gap in the literature remains in modeling complex adsorption mechanisms. Three key factors were identified for modeling adsorption thermodynamics and kinetics: surface saturation, reservoir depletion, and lateral interactions. While the first is captured by the celebrated Langmuir model, reservoir depletion, which is crucial for assessing adsorption in batch and dynamic experiments, is often neglected in classical kinetic models. Lateral interactions are also important for pollutants like PFAS as they undergo cooperative adsorption. A 2D lattice gas model with two- and three-body lateral interactions is solved using mean-field and quasi-chemical approximations. The resulting thermodynamics lead to a phase diagram predicting complex adsorption isotherms in agreement with available experiments as well as a first-order dilute to dense phase transition. A mixed-order kinetic model including all three factors is proposed and both thermodynamic and kinetic models are successfully applied to experimental data.

CPP 21.5 Tue 10:45 ZEU/0255

Molecular Dynamics Insights into Thermodynamic and Structural Properties of Water Adsorbed Poly(Heptazine Imide) Zeolites — •Youssef Mabrouk[1], Akshey Suresh[2], Yizak Tzegazab[2], Lingli Ni[2], Martin Oschatz[2], Alexander Croy[1], and Stefanie Gräfe[1] — [1]Friedrich Schiller University of Jena, Insitute of Physical Chemistry, Lessingstraße 4, 07743 Jena, Germany — [2]Friedrich Schiller University of Jena, Institute for Technical Chemistry and Environmental Chemistry, Philosophenweg 7a, 7743 Jena, Germany

The recently reported reversible water adsorption of porous layered carbon nitrogen frameworks suggests their high potential as functional materials for energy storage and conversion applications specifically in view of the controlled crystallinity and polarity and water binding motifs these frameworks offer. Based on molecular dynamics simulations of pressure-controlled solid/gas equilibrium isotherms, the framework structure-dependent adsorption of water in poly(heptazine imides) is here investigated. Using minimal motifs of heptazine sheets in pressure-controlled water vapor environments, the load-dependent transition from monomolecular to condensation-limited adsorption is furthermore investigated. The hydrophilicity characterized by the isotherms agree with physiosorption experiments. The layer planarity and pore geometry-dependent crystallinity characterized by the structure factor and normal modes agree with x-ray diffraction and infrared spectroscopy experiments. Overall, our results contribute to identifying the relevance of each structural motif to adsorption.

CPP 21.6 Tue 11:00 ZEU/0255

Insights into phenylalanine self-assembly and its modulation by nucleotides from molecular dynamics simulations. — •Mattia Borriello — Ruhr-Universität Bochum

Phenylalanine (Phe) can aggregate in water into various fibrillar structures, which is relevant to diseases like phenylketonuria. The precise molecular structure of these aggregates is still unknown, and although they dissolve in the presence of nucleotides such as ATP, the mechanism behind this disassembly remains unclear. We use molecular dynamics simulations to gain new insights on Phe cluster structure, understand which interactions drive this process and how nucleotides can modulate it.

Parallel tempering simulations of Phe in water in zwitterionic form have been performed varying concentration and temperature. Analysis of the trajectories revealed a strong tendency to aggregate in two ordered structures. One is characterized by a tubular shape, while the other by an alternating motif. Cluster stabilization is mainly electrostatic for smaller aggregates, while apolar interactions become significant as the size of the clusters grows.

The same computational approach has been extended to systems containing Phe and NaCl or different nucleotides, such as ATP, ADP and AMP. While NaCl showed a limited influence on aggregation, nucleotides can inhibit cluster formation and disrupt pre-existing aggregates. Our findings provide molecular-level insight into both the structural organization of Phe assemblies and into the mechanisms through which nucleotides modulate their stability.

CPP 22: Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics I

Time: Tuesday 9:30–11:15 Location: ZEU/0260

Invited Talk CPP 22.1 Tue 9:30 ZEU/0260

From Solution to Thin Films: Structure Formation Pathways in Organic Photovoltaic Films — •Eva M. Herzig — Dynamik- und Strukturbildung - Herzig Group, University of Bayreuth, Germany

The performance of organic solar cells is governed by a delicate interplay between molecular packing, phase separation, and mesoscale connectivity in donor-acceptor blends. It is therefore highly desirable to control structure formation; however, this remains a non-trivial task. Several factors contribute simultaneously: the initial aggregation state in solution [1,2], the rapid structure formation during solution processing [2], and subsequent temperature- or solvent-annealing steps [3,4]. In this talk, I will discuss and illustrate with selected examples at which of these stages the final thin-film morphology can be controlled.

Using time-resolved and multimodal characterization methods, including grazing-incidence X-ray scattering and optical spectroscopy, we resolve the evolving structures during and after film deposition. These measurements reveal how subtle variations in processing conditions translate into distinct nanoscale morphologies.

[1] F. Eller & E. M. Herzig, J. Phys. Chem. A 2024, DOI: 10.1021/acs.jpca.4c04902

[2] F. Eller, R. Hildner, R. W. A. Havenith & E. M. Herzig, Small 2023, DOI: 10.1002/smll.202207537

[3] F. Eller, C. R. McNeill & E. M. Herzig, Adv. Energy Mater. 2024, DOI: 10.1002/aenm.202304455

[4] M. Kuhn, X. Huang, M. Gebert, L. Thomsen, C. R. McNeill & E. M. Herzig, Adv. Funct. Mater. 2025, DOI: 10.1002/adfm.202509532

CPP 22.2 Tue 10:00 ZEU/0260

DBTTF:HATCN Cocrystals – experimental details on influence of crystal solvents on crystal structure and on charge transfer — •Andreas Opitz[1], Ana M. Valencia[2], Lisa Schraut-May[3], Marie Siegert[3], Sebastian Hammer[3], Beatrice Cula[4], Alexandra Friedrich[5], Holger Helten[5], Jens Pflaum[3], and Caterina Cochi[6] — [1]Institut für Physik, Humboldt-Universität zu Berlin — [2]Institute of Physics, Carl-von-Ossietzky Universität Oldenburg — [3]Experimental Physics VI, Julius-Maximilians-Universität Würzburg — [4]Department of Chemistry, Humboldt-Universität zu Berlin — [5]Institute of Inorganic Chemistry & Institute for Sustainable Chemistry and Catalysis with Boron, Julius-Maximilians-Universität Würzburg — [6]Institute of Condensed Matter Theory and Optics, Friedrich-Schiller-Universität Jena

Donor-acceptor (D:A) cocrystals offer a promising platform for next-generation optoelectronic applications, but the impact of residual solvent molecules on their properties remains an open question. We investigate six novel D:A cocrystals of dibenzotetrathiafulvalene (DBTTF) and 1,4,5,8,9,11-hexaazatriphenylenehexacarbonitrile (HATCN), prepared via solvent evaporation, yielding 1:1 molar D:A ratios with solvent molecules in the structure, and horizontal vapor deposition, resulting in solvent-free 3:2 cocrystals. Optical properties of these materials are largely unaffected by solvent inclusion. The vibrational energy of the cyano mode depends on the dipole moment of the incorporated solvent molecules, but the degree of charge transfer is consistent across all analyzed cocrystals.

CPP 22.3 Tue 10:15 ZEU/0260

Reassessing Mobility Imbalance in Organic Photodetectors for High-Speed Applications — •Felix Hergenhan, Tianyi Zhang, Karl Leo, and Johannes Benduhn — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics, Technische Universität Dresden

Organic photodetectors (OPDs) are emerging candidates for diverse optoelectronic applications, yet their use in high-speed technologies such as optical communication remains largely believed to be restricted by low effective charge carrier mobilities. To address this challenge, we investigated how the transient behavior of OPDs depends on the mobilities of the respective charge carriers. This relationship is examined through drift-diffusion simulations and experiments across various material systems, under varied bias and illumination conditions. We show, contrary to common assumptions, that obtaining only one fast charge carrier mobility is sufficient to achieve high response speed. Likewise, in systems with pronounced mobility imbalance, the slower carriers do not necessarily govern the maximum operation speed of the device. Leveraging these insights, we demonstrate an OPD tailored for optical communication that achieves data transmission rates up to 170 Mbps, representing one of the highest reported transmission rates for organic-based optical communication systems. These findings establish a refined design framework for ultrafast OPDs, providing guidance on material selection, device design, and operation regimes.

CPP 22.4 Tue 10:30 ZEU/0260

Rational Design of Donor-Acceptor Oligomers for Enhanced Charge Separation — •Jannik Theile[1], Michele Guerrini[2], Surender Kumar[2], and Caterina Cocchi[2] — [1]Physics Department and Center for Nanoscale Dynamics, Carl von Ossietzky Universität Oldenburg, Germany — [2]Physics Department for Solid-State Physics and Optics, Friedrich-Schiller Universität Jena, Germany

Intramolecular charge transfer (ICT) in donor-acceptor (D-A) oligomers is central to organic optoelectronics, yet symmetric D-A-D and A-D-A systems often suffer from delocalized frontier molecular orbitals (FMOs) that hinder efficient photoinduced charge separation. To address this, we present a first-principles study based on (time-dependent) density functional theory of 22 dithieno[3,2-b:2',3'-d]pyrrole oligomers, exploring the interplay between structural asymmetry and site-selective fluorination. Donor fluorination widens the electronic gap, while acceptor fluorination enhances charge imbalance and promotes confinement and spatial segregation of FMOs onto distinct molecular segments. The resulting optical properties reveal asymmetric, acceptor-fluorinated systems as optimal for ICT due to strong charge-transfer excitations with large oscillator strengths in the visible region. This work establishes rational design rules for conjugated D-A oligomers, showing that combining asymmetry with targeted halogenation is key to achieving robust, directional ICT and enabling high-performance organic semiconductors.

CPP 22.5 Tue 10:45 ZEU/0260

Substituted Benzo[*b*]fluorenes as Emitters for OLED With Tunable Electroluminescence in the Full Visible Range — •Pascal Schweitzer[1], Christopher M. Leonhardt[2], Cazibe Arslan[1], Hermann A. Wegner[2], and Derck Schlettwein[1] — [1]Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen — [2]Justus-Liebig-Universität Gießen, Institut für Organische Chemie, Heinrich-Buff-Ring 17, D-35392 Gießen

Organic light emitting diodes (OLED), despite widespread application in displays, still exhibit major challenges. The search for stable and efficient emitting molecules continues, especially in the blue range. Substituted benzo[*b*]fluorenes (BF) show high stability of photoluminescence in solution over months. By exchanging the substitutional pattern, we show that this group of molecules allows for preparation of OLED with tunable emission bands in the full range of the visible spectrum. Thin films of BF can be prepared by solution-based methods or physical vapor deposition, allowing for easy integration into different layer stacks. Photoluminescence spectroscopy of showcase BFs revealed a multi-band emission that is found in line with electroluminescence spectra of the corresponding devices. Contact formation at relevant device interfaces was studied by in-situ Kelvin-probe force microscopy and gave insight into details of film growth and alignment of transport levels. Based on these findings we demonstrate working OLED devices with intense blue or red emission, respectively.

CPP 22.6 Tue 11:00 ZEU/0260

Electrically switchable chiroptical responses in organic ferroelectric thin films — •Lorenz Friedrich Meier[1], Sophia Klubertz[1], Victor Rodriguez[2], Miguel García-Iglesias[2], David González-Rodríguez[3], and Martijn Kemerink[1] — [1]Heidelberg University, Germany — [2]Universidad de Cantabria, Spain — [3]Universidad Autónoma de Madrid, Spain

Organic ferroelectrics potentially allow to introduce switchable polarization into an easily processable material, enabling their integration into next-generation electronic devices. We investigate a liquid-crystalline organic ferroelectric that additionally can exhibit electrically controlled chiroptical responses, relevant for optical data storage, photonic components, and chiroptical sensing. We investigate thin films of trialkylbenzene-1,3,5-tricarboxamide (BTA). These molecules self-assemble into supramolecular columns by forming a triple helix of dipoles connected via hydrogen bonds. By incorporating chirally-biased sidechains, the handedness of the supramolecular helix can be defined. We experimentally show ferroelectric behavior in both in-plane and out-of-plane geometries by double wave and CV measurements. We demonstrate how the unpractically high coercive fields for pure chiral BTA can be reduced by mixing with achiral BTA. Previous simulations show that the energetically preferred mechanism of polarization reversal of a supramolecular column will simultaneously change its chirality. Thus, an electrically switchable chirality is possible. We present an experimental investigation of this mechanism, discussing the challenges including the need for dipole pre-alignment.

CPP 23: Focus Session: Water – from Atmosphere to Space II (joint session CPP/DY)

Time: Tuesday 11:15–12:45 Location: ZEU/LICH

CPP 23.1 Tue 11:15 ZEU/LICH

Microscopic diffusion and reactivity in aqueous solutions: photogenerated nascent halogen atoms, solvated electrons and subsequent dihalide formation — •Zhangatay Nurekeyev[1,2], Hyein Hwang[1,2], Fernando Rodriguez Diaz[1], Mei Bai[3], Michael Thorwart[3], Michaela Schäfer[4], Carmen Herrmann[4], and Christian Bressler[1,2,5] — [1]Institute of Experimental Physics, Universität Hamburg — [2]The Hamburg Centre of Ultrafast Imaging (CUI) — [3]I. Institute of Theoretical Physics, Universität Hamburg — [4]Department of Chemistry, Universität Hamburg — [5]European XFEL, Schenefeld

The solvent plays an important role in the assembly, stability and reactivity of (bio)chemical molecules. Small changes of the caging solvent can alter the reaction outcome, but little is known about the atomic-scale solvation shell dynamics. Our approach utilizes aqueous mono-atomic halide solutes, which are transformed into nascent neutral halogen atoms upon femtosecond optical ex-

citation together with a separated solvated electron. Combining X-ray absorption with transient optical absorption spectroscopies we monitor the subsequent diffusion-driven atom-electron recombination, each focusing on the halogen atom and on the solvated electron, respectively. We also monitor the appearance of dihalides on the tens of picosecond time scale. Using all x-ray and laser observables we deliver a new picture of the ensuing dynamics, for which the existence of the long-lived (X:e) contact pair is not required. Next steps aim to trace more complex guest-host scenarios towards functional proteins in solution.

CPP 23.2 Tue 11:30 ZEU/LICH

Surface Propensity of Halide Ions in Water: New Evidence from LJ-XPS — •Daniela Torres-Díaz[1], Shirin Golami[1], Tillmann Buttersack[1], Qi Zhou[1], Rémi Dupuy[2], Bernd Winter[1], Chistophe Nicolas[3], and Hendrik Bluhm[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Laboratoire de Chimie Physique - Matière et Rayonnement (Sorbonne Université, CNRS), Paris, France — [3]Synchrotron SOLEIL, Saint-Aubin, France

The surface propensity of halide ions in water is still a matter of debate. While the famous Onsager&Samaras model indicates that charged species should avoid the interface, more recent Molecular Dynamics simulations that take into account the polarizability of the ions indicate notably that iodide and bromide prefer the interface while chloride and fluoride avoid it. Different models, however, differ in how strong this effect is, while experimental studies have reported contradictory results. Here I will discuss recent results obtained using Liquid-Jet X-Ray Photoemission Spectroscopy on water interfaces for potassium halide solutions. In particular, the measurement of the photoelectron angular distributions allow for a higher spatial resolution than classic XPS measurements.

CPP 23.3 Tue 11:45 ZEU/LICH

Ion Correlations Drive Collective Adsorption of Hydronium Ions at the Air-Electrolyte Interface — •Elena Köhler Ruiz, Maximilian Becker, Louis Lehmann, and Roland Netz — Fachbereich Physik, Freie Universität Berlin, Germany

Acids exhibit distinct interfacial behavior at the air-water interface compared to simple monoatomic salts. While monoatomic ions are largely repelled from the interface, hydronium ions preferentially reside at the interface due to formation of an interfacial hydrogen-bond network. To investigate these contrasting behaviors, we perform molecular-dynamics simulations with thermodynamically optimized force fields, analyzing ionic distributions at the interface as well as resulting surface tensions and potentials. The simulated surface potentials reproduce the concentration-dependent trends observed in SFG experiments: At high concentrations, interfacial hydronium promotes co-adsorption of counterions, which results in a decrease of the surface potential with rising concentration, consistent with experimental observations. These findings highlight the critical role of ion-ion correlations at interfaces, which are not accounted for by modified Poisson-Boltzmann models.

CPP 23.4 Tue 12:00 ZEU/LICH

Calcium-amino acid complexation in water probed by Intermolecular Coulombic Decay — •Michele Pugini, Nicolas Velasquez, Harmanjot Kaur, Florian Trinter, Qi Zhou, Lukas Tomaník, Uwe Hergenhahn, and Bernd Winter — Fritz-Haber-Institut, Berlin

The Ca2+ ion is the most abundant metal ion in the human body, playing essential roles in numerous biological processes, many of which involve interactions with proteins. Gaining molecular-level insight into the nature of the interaction between Ca2+ ions and solvated amino acids is therefore crucial for understanding calcium's biological function. Intermolecular Coulombic decay (ICD), a non-local autoionization process, offers unique sensitivity to the local chemical environment and can selectively probe interactions within the first solvation shell of solvated Ca2+ ions.

Here, we demonstrate the sensitivity of resonant ICD3 to the chemical composition of the solvation shell, enabling the identification of Ca2+ associations with specific amino acids. Our model system is the amino acid proline. The interaction, if present, is revealed via the ICD electrons resulting from the ionization of the biomolecule upon the 2p to 3d excitation of Ca2+.

Our results unequivocally identify Ca2+-proline interactions, indicating substitution of water molecules in the ion's coordination shell by proline. These findings establish ICD as a sensitive probe of metal-biomolecule interactions and highlight its potential as a powerful spectroscopic tool for investigating biomolecular structure in solution.

CPP 23.5 Tue 12:15 ZEU/LICH

Distinguishing cavity and non-cavity solvation structures of the hydrated electron — •Sy Dat Ho and Benjamin Philipp Fingerhut — Department of Chemistry and Centre for NanoScience, Ludwig-Maximilians-Universität München, 81377 München, Germany

Solvated electrons in water are prototypical low-dimensional quantum systems that are coupled to a fluctuating, many-body environment. However, their hydration structure is still a matter of debate, with both cavity and non-cavity models having been suggested. First-principles molecular dynamics simulations are performed of excess-electron localization in liquid water, using hybrid-meta-GGA and hybrid-GGA density functionals that accurately reproduce bulk water structure. Perturbations to the local hydrogen bond structure of water due to interaction with the excess charge are identified, giving rise to specific signatures in transient radial distribution functions. These patterns are then compared with preliminary liquid-phase MeV-UED data obtained during an early science campaign at SLAC. In order to distinguish the structural changes induced by excess electrons in the diffraction patterns, long-time simulations at an unprecedented level of theory are required in order to minimise statistical noise. Our results clarify the coupling of hydrated electrons to solvent fluctuations and provide microscopic insight into polaron formation in disordered condensed phases.

CPP 23.6 Tue 12:30 ZEU/LICH

Mesoscopic Structures in Water/HFIP based Electrolytes — •Sophie Zeilinger[1,2] and Markus Mezger[1] — [1]Center for Nano Structure Research, Faculty of Physics, University of Vienna, AT-1090 Vienna — [2]Institute of Physical Chemistry, Faculty of Chemistry, University of Vienna, AT-1090 Vienna

Previous studies have shown that binary water/hexafluoroisopropanol (HFIP) mixtures exhibit nanoscale heterogeneties that strongly affect properties such as reaction rates. The complex hydrogen bonding network of the binary mixture together with the amphiphilic character of the HFIP molecule provides a sensitive environment in which subtle changes in interactions can generate nanoscale heterogeneties. Here, we study the structure formation in water/HFIP under the influence of hydrophilic and hydrophobic ions by Small Angle X-Ray Scattering (SAXS). Depending on water content, pH, salt concentration and temperature we observe monotonous and oscillatory density correlations with structural parameter on the nanometer length scale. These structures are explained by the coupling of coulombic interactions between charged hydrophilic and hydrophobic ions vs. local fluctuations in water/HFIP concentrations.

CPP 24: French-German Session: Simulation Methods and Modeling of Soft Matter IV

Time: Tuesday 11:30–12:45 Location: ZEU/0255

CPP 24.1 Tue 11:30 ZEU/0255

Systematic coarse-graining with density dependent potential: Application to small organic molecules, multicomponent mixtures and polymers — •Sayan Dutta[1,2,3], Maria C. Lesniewski[4], W. G. Noid[4], Denis Andrienko[5], and Arash Nikoubashman[2,3] — [1]Leibniz-Institut für Polymerforschung — [2]Technische Universität Dresden — [3]Johannes Gutenberg-Universität Mainz — [4]Pennsylvania State University, University Park, PA, USA — [5]Max-Planck Institut für Polymerforschung Mainz

Conventional coarse-graining (CG) approaches approximate the underlying many body interactions through effective pair potentials. Although this strategy works well for reproducing structural and thermodynamic properties in bulk systems, it often fails in heterogeneous systems, such as droplets or films, due to the inherently strong density fluctuations in those systems. To address this issue, we incorporated local-density-dependent potentials (LDPs) that treat these many-body contributions explicitly within a mean-field formalism. We develop a CG force-field framework that integrates LDPs, enabling accurate simulation of conjugated organic molecules, organic liquid mixtures, and polymeric systems. This approach provides a more accurate description of thermodynamic and interfacial properties of these systems. Further, it facilitates the establishment of structure-function description that helps in rational designing of functional materials.

CPP 24.2 Tue 11:45 ZEU/0255

A data-driven decoupled multiscale scheme for anisotropic finite strain magneto-elasticity — •Heinrich T. Roth, Philipp Gebhart, Karl A. Kalina, Thomas Wallmersperger, and Markus Kästner — TU Dresden, Dresden, Germany

Structured magnetorheological elastomers (MREs) are composite materials exhibiting magneto-mechanical coupling effects, such as the magnetostrictive and magnetorheological effect. They consist of magnetizable particles arranged in chain-like structures within a soft elastomer matrix. As explicitly resolving their microstructure in real-world samples is infeasible, a multiscale modeling approach is required.

In this work, we present a framework for the macroscale modeling of structured MREs using physics-augmented neural networks (PANNs) [1,2]. The framework begins with data generation, where a representative volume ele-

ment (RVE) undergoes macroscopic magneto-mechanical loadings in Finite Element (FE) simulations. The resulting homogenized microscale variables form a macroscale dataset for the training and testing of the PANN macromodel, which satisfies key physical principles [1]. Finally, the trained PANN model is used in a decoupled multiscale scheme as the material model for a macroscale FE simulation to examine the magnetostriction of a spherical sample.

We acknowledge support by the German Research Foundation DFG through Research Unit FOR 5599 on structured magnetic elastomers.

[1] H.T. Roth et al., arXiv:2510.24197, 2025. [2] K.A. Kalina et al., CMAME 421, 2024.

CPP 24.3 Tue 12:00 ZEU/0255

In Silico Self-Assembly of Magnetic Colloidal Polymers with Magnetization Dynamics — •Deniz Mostarac[1], Sofia Kantorovich[2], and Philip J. Camp[1] — [1]School of Chemistry, University of Edingburgh, EH9 3FJ Edinburgh , United Kingdom — [2]Computational and Soft Matter Physics, University of Vienna, Vienna, Austria

Polymer-like mesostructures formed by crosslinked magnetic nanoparticles (MNPs) have created a new class of stimuli-responsive materials magnetic colloidal polymers (MCPs) that show enhanced optical, thermal, mechanical, rheological, and adsorption properties compared to conventional magnetic fluids. The interplay between magnetic interactions and solvophilic/solvophobic forces produces complex, field-tunable self-assembly. In our previous work, we investigated isolated MCPs and showed that solvophobicity drives compact, magnetically frustrated conformations, with structural features determined by crosslink type and MNP properties. These distinctions strongly affect MCP dynamics under shear and external fields. In this contribution we study the self-assembly of solvophobic MCPs while explicitly modeling MNP magnetodynamics with finite anisotropy. Our simulations capture internal magnetization dynamics over long times and at system sizes sufficient for bulk behavior. We show that coupling between Brownian and Néel relaxation, together with nonlinear magnetization, yields distinct structural, magnetic, and dynamical features in MCP suspensions governed by solvophobicity and intrinsic NP magnetism.

CPP 24.4 Tue 12:15 ZEU/0255

Pulling knotted polymer rings and concatenated knotted polymer rings in order to understand the effects of entanglement on the mechanical properties of polymers materials — •Franco Ferrari[1], Neda Abbasi Taklimi[1], Marcin Piatek[1], and Luca Tubiana[2] — [1]CASA* and Institute of Physics, University of Szczecin, Szczecin, Poland — [2]Physics Department, University of Trento, Via Sommarive 14, Trento I-38123, Italy

The topological structure of polymers is expected to produce relevant effects on the mechanical properties of polymer systems. However, to assess the contribution of topology by experiment is difficult, mainly due to technical obstacles in controlling the entanglement during the synthesis process, in particular the formation of knots and concatenations. In this contribution presented are the results of numerical simulations focusing on the mechanical properties of topologically entangled polymer systems. First, the case of single knotted polymers pulled by an external force are discussed. Next, the stress-strain curves of a few concatenated knots with forces applied at different locations are shown. To check the validity of our simulations based on the Wang-Landau algorythm, two different methods are employed and their consistency is verified. The final goal of this research is to understand the mechanical properties of more complex polymer materials characterized by an uniform distribution of knots or concatenated knots of a given topological type.

CPP 24.5 Tue 12:30 ZEU/0255

Prediction of Ultra-Long Time-Scale Dynamics from Picoseconds to Seconds: Integral of First-Passage Times — •Qiyun Tang — School of Physics, Southeast University, Nanjing, China

The dynamics of non-equilibrium nanostructure formation span over 13 orders of magnitude in time, from molecular vibrations at picoseconds to macroscopic processes at seconds or longer. Predicting such ultra-long time-scale dynamics poses significant challenges for conventional molecular simulation methods. We recently proposed a new approach-Integral of first-passage times (IFS)-to predict the evolution of non-equilibrium nanostructures, and the resulting structural distributions align well with experimental observations [1]. Furthermore, we have verified that the dynamics predicted by IFS are consistent with direct simulations in cases of low free energy barriers, while under high free energy barriers, the ultra-long time-scale dynamics predicted by IFS agree with experimental measurements [2]. Utilizing this method, we have also systematically investigated the relationship between polymer adsorption dynamics and surface curvature [3,4]. The IFS method bridges microscopic picosecond-scale dynamics with macroscopic growth kinetics of nanostructures, offering an effective approach for designing and controlling non-equilibrium nanostructures.

[1]Q.Tang, C. Rossner, P. Vana, M. Müller, Biomacromolecules 2020, 21: 5008. [2]Q. Tang, Y. Huang, M. Müller, Phys. Rev. E 2024, 110: 044502. [3]J. Zhang, Q. Tang, Phys. Rev. Mater. 2024, 8: 105602. [4]Y. Huang, C. Tang, Q. Tang,*Nanoscale 2024, 16: 19806.

CPP 25: Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics II

Time: Tuesday 11:30–12:45 Location: ZEU/0260

CPP 25.1 Tue 11:30 ZEU/0260

Transiently Delocalised Hybrid Quantum States are the Gateways for Efficient Exciton Dissociation at Organic Donor-Acceptor Interfaces — •Filip Ivanovic[1], Samuele Giannini[2], Wei-Tao Peng[3], and Jochen Blumberger[1] — [1]Department of Physics and Astronomy, University College London, London, United Kingdom — [2]Department of Chemistry and Industrial Chemistry, University of Pisa, Pisa, Italy — [3]Department of Chemistry, Tunghai University, Taichung City, Taiwan

Organic solar cells (OSCs) have long been the subject of intensive research. Following the absorption of sunlight, localised excitations (excitons) are able to dissociate into separated charges at the interface between donor and acceptor components. Whilst this separation has been leveraged to achieve cell efficiencies above 20%, the exact mechanism by which this occurs remains without consensus.

Theoretical research has been centred on simulating such phenomena on experimentally relevant time scales, whilst sufficiently describing the underlying electronic structure. Here, we introduce our in-house non-adiabatic dynamics package, termed X-SH.

We elucidate the mechanism of ultrafast charge separation in an atomistic OSC junction, where separation is mediated by non-local hybridised states comprising both excitons and separated charges, and in-fact accelerated by non-interfacial exciton dissociation. We then demonstrate that tuning the hybridised states' accessibilities through the density of states can be translated into design rules informing the synthesis of yet more efficient OSCs.

CPP 25.2 Tue 11:45 ZEU/0260

Temperature-Dependent Spin-Sensitive Spectroscopy of Triplet-Exciton Dynamics in TADF OLEDs — •Ahmed Mohamed, Andreas Kohrmann, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

Thermally Activated Delayed Fluorescence (TADF) enables efficient harvesting of triplet excitons through reverse intersystem crossing (rISC) in OLEDs. Previous studies have shown that TADF device operation is dominated by triplet excitons, whose densities exceed singlet and charge carrier densities by several orders of magnitude. A major limitation to TADF efficiency is the non-radiative loss of triplet excitons. Here, we analyze the transient photoluminescence (trPL) and transient electroluminescence (trEL) decays of the blue TADF emitter ν-DABNA hosted in TDBA-Si or mCP. Temperature-dependent trPL/trEL kinetics were modeled using a rate-equation framework. Key triplet-exciton parameters, including the lifetime, diffusion coefficient, diffusion length, and activation energies were extracted by considering both 1^{st} and 2^{nd} order triplet-exciton decay pathways. The spin properties of the triplet exciton were additionally identified using photoluminescence-detected magnetic resonance (PLDMR) measurements on the organic layer stack. Together, kinetic and spin analysis of triplet excitons provide a comprehensive picture of non-radiative quenching to guide future improvements of TADF OLEDs

CPP 25.3 Tue 12:00 ZEU/0260

Modeling the ionization potential and electron affinity in organic semiconductors — •Alexey Gudovannyy and Frank Ortmann — Department of Chemistry, TUM School of Natural Sciences, and Atomistic Modeling Center, Munich Data Science Institute, Technical University of Munich, Germany

Ionization potential (IP) and electron affinity (EA) are essential quantities for characterizing and tuning transport properties of organic semiconducting materials. Computational prediction of these properties under realistic conditions of crystalline or polycrystalline forms remains challenging, as it requires a proper description of all interactions within the bulk material environment. In this work, we present an accurate protocol for computing molecular materials' IP and EA values, using computed gas-phase molecular values corrected via an improved multilevel scheme for describing the materials' environment, where an electronic structure is treated explicitly at the microscopic level, while at larger scales, a continuum model is applied. Special significance will be dedicated to the requirement of accurate reference gas-phase calculations, which we carried out within the GW framework and to demonstrating limitations of prevalent

Density Functional Theory (DFT) methods, while preserving feasible computational time demands. The main bottleneck of this approach is the need for an experimental or predicted crystal structure. We will also show how to incorporate reliable structure prediction into it, which opens up possibilities for purely in silico materials design.

CPP 25.4 Tue 12:15 ZEU/0260

Morphological Insights into Spray-Coated Organic Semiconductors — •Shuxian Xiong[1,2], Marie Betker[2,3], Simon Schraad[1,2], Yufeng Zhai[2], Benedikt Sochor[2], Sarathlal Koyiloth Vayalil[2,4], Peter Müller-Buschbaum[1], and Stephan V. Roth[2,3] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Department of Fibre and Polymer Technology, KTH, Stockholm, Sweden — [4]Applied Sciences Cluster, University of Petroleum and Energy Studies UPES, Dehradun, Uttarakhand, 248007, India

Ultrasonic spray coating offers improved scalability for large-scale applications, reduced material waste, and enhanced compatibility with various substrates, making it a more cost-effective solution for the mass production of photovoltaic devices. However, how to simply and efficiently build ordered structural networks is still a critical issue. We investigate the morphological transition of organic semiconductors and their effect on device performance using grazing incidence wide-angle X-ray scattering in traditional fullerene systems. By systematically optimizing spray flow rate and substrate temperature, we effectively tailored the film morphology, enhancing molecular crystallization of PTB7-Th and PCBM, resulting in an improvement in device performance of 9% in air, which is one of the highest device efficiencies currently achieved for spray-coated fullerene acceptor-based organic solar cells, and is equivalent to the device efficiencies of spin-coated fullerene acceptor-based organic solar cells.

CPP 25.5 Tue 12:30 ZEU/0260

Enhancing device performance parameters of organic photodiodes by understanding the thickness dependence of the reverse dark current — •Fred Kretschmer[1], Tianyi Zhang[1], Oskar J. Sandberg[2], Mathias Nyman[2], Karl Leo[1], and Johannes Benduhn[1] — [1]Institute of Applied Physics, TU Dresden, Dresden, Germany — [2]Faculty of Science and Engineering, Åbo Akademi University, Turku, Finland

In recent years, organic photodetectors (OPDs) have attracted interest due to their advantageous properties and rapidly advancing performance, making them promising not only as complements to inorganic photodetectors but also for emerging applications in bioimaging, health monitoring, and high-speed optoelectronics. A key figure of merit for comparing PDs is the specific detectivity (D^*), which quantifies the detector's ability to sense weak optical signals. Achieving high D^* relies on maximizing charge carrier extraction while minimizing internal noise. Under reverse bias, OPD performance is particularly influenced by shot noise, which is proportional to the dark current (J_D).

In this work, the variation of J_D with active-layer thickness across multiple energy-gap-tuned bulk-heterojunction systems was examined. Surprisingly, the dark current exhibits a thickness-dependent minimum, contrary to the general assumption that J_D only decreases with thickness. Using sensitive, temperature-dependent current-voltage measurements together with drift-diffusion simulations, the new minimum feature was confirmed, and improvements in the specific detectivity of OPDs were achieved.

CPP 26: French-German Session: 2D Materials, Thin Films and Interfaces II

Time: Tuesday 14:00–15:30 Location: HÜL/S386

Invited Talk CPP 26.1 Tue 14:00 HÜL/S386

Investigating lignin graphitisation depending on botanical source and extraction method — Lucie Dieval[1], Phuthiphong Ouitrakoon[2], Robert Hunter[2], Sébastien Schaefer[3], Louis Hennet[3], Erik Elkaim[4], Julie Ruellou[5], Milo S. P. Shaffer[2], Agnieszka Brandt-Talbot[2], and •Pascale Launois[1] — [1]LPS, CNRS/Université Paris Saclay, France — [2]Imperial College, UK — [3]ICMN, CNRS/University of Orléans, France — [4]Synchrotron SOLEIL, France — [5]ESRF, France

Lignins, plant-derived macromolecules, are promising carbon sources from a sustainable development perspective. Here, we study the transformations of various lignins into turbostratic carbon or graphite, consisting of stacked graphene sheets.

The lignin powders were heated at temperatures between 1000 and 2730°C. Analyses were performed ex-situ using X-ray scattering (XRS) and Raman spectroscopy, which confirmed XRS results. XRS data were analysed combining analyses in reciprocal space and in direct space with Pair Distribution Function. The dimensions of the carbonaceous crystalline domains formed from lignins are determined as a function of temperature, as well as the stacking mode of their graphene sheets. We find that all studied lignins transform into turbostratic carbon, with no evidence for intermediate stackings towards graphite. Different sizes of crystalline domains are evidenced depending on the lignin form. One lignin presents relatively large sizes both for the graphene layers and in the stacking direction at a temperature as low as 1300°C, a most promising finding for future applications.

CPP 26.2 Tue 14:30 HÜL/S386

Atomistic Origin of Photoluminescence Quenching in Colloidal MoS_2 and WS_2 Nanoplatelets — •Surender Kumar[1], Markus Fröhlich[2], Stefan Velja[1], Marco Kögel[2], Onno Strolka[2,3], André Niebur[3], Samuell Ginzburg[4], Muhammad Sufyan Ramzan[1], Jannik C. Meyer[2], Jannika Lauth[2,3], and Caterina Cocchi[1] — [1]Friedrich-Schiller-Universität Jena, Germany — [2]Eberhard Karls University of Tübingen, Germany — [3]Leibniz University of Hannover, Germany — [4]University of Cambridge, UK

Large chemical tunability and strong light-matter interactions make colloidal transition metal dichalcogenide nanostructures particularly suitable for light-emitting applications. However, ultrafast exciton decay and quenched photoluminescence limit their potential. Combining femtosecond transient absorption spectroscopy with first-principles calculations on MoS_2 and WS_2 nanoplatelets, we reveal that the observed sub-picosecond exciton decay originates from edge-located optically bright hole traps [1]. These intrinsic trap states stem from the metal *d*-orbitals and persist even when the sulfur-terminated edges are hydrogen-passivated. Notably, WS_2 nanoplatelets show more localized and optically active edge states than their MoS_2 counterparts, and zigzag edges exhibit a higher trap density than armchair edges. The nanoplatelet size dictates the competition between ultrafast edge-trapping and slower core-exciton recombination, and the states responsible for exciton quenching enhance catalytic activity.

[1] S. Kumar, et al., arXiv:2511.19077 (2025)

CPP 26.3 Tue 14:45 HÜL/S386

Data-driven exploration of thermal and elastic properties in covalent organic framekworks — •Aleksander Szewczyk[1], Leonardo Medrano Sandonas[1], David Bodesheim[1], Bohayra Mortazavi[2], and Gianaurelio Cuniberti[1] — [1]TUD Dresden University of Technology, 01062 Dresden, Germany — [2]Leibniz Universität Hannover, Welfengarten 1A, 30167 Hannover

Covalent organic frameworks (COFs) are a class of advanced materials that can be precisely engineered for diverse applications, including catalysis, flexible electronics, and sensors. However, COFs synthesised experimentally often exhibit a variety of structural defects and grain boundaries, which affect their properties. Because of their large and complex structure, COFs pose a considerable challenge for traditional *ab-initio* methods. Machine learning interatomic potentials (MLIPs) can be used to significantly accelerate property calculations, while retaining near *ab-initio* accuracy. Our team have parametrised an MLIP using the MACE architecture and a dataset of non-equilibrium confirmations of 2D COFs. We assessed the transferability of the MACE model computing atomic forces and phonon dispersions of unseen COFs, and compared these results to ReaxFF and reference data by Density Functional Theory using VASP code. Using the parametrised model, we explore the effect of defects and grain boundaries on thermal and elastic properties of COFs.

CPP 26.4 Tue 15:00 HÜL/S386

PNIPAM Microgel-Stabilized Foam Films: Effect of Crosslinking Content — •Luca Mirau, Joanne Zimmer, Kevin Gräff, Matthias Kühnhammer, and Regine von Klitzing — Institute for Condensed Matter Physics, TU Darmstadt, Germany

Aqueous foams find widespread application in fields such as cosmetics, the food industry, oil recovery and fire-fighting. Their stabilization requires the presence of surface-active molecules or colloidal particles. In this study, thermoresponsive microgels (MGs) composed of poly(N-isopropylacrylamide) (PNIPAM) with varying crosslinker contents are applied as foam stabilizers, resulting in temperature-sensitive foams. Foam films serve as the fundamental building blocks of foams. The structuring of MGs within these films is analyzed using the Thin Film Pressure Balance (TFPB) technique. Foam films are formed within a pressure chamber, and their thickness is determined through interferometric methods under a light microscope. The foam films display an inhomogeneous structure, characterized by network-like, several 100nm thick regions containing MGs, interspersed with thin MG-depleted zones less than 100nm thick. We show how the cross-linker density of the microgels affect the MG layering within these thick network regions, influencing the film thickness. Another question we answer is how the MG-free areas are stabilized.

CPP 26.5 Tue 15:15 HÜL/S386

Irreversible protein adsorption on mobile surfaces: control and modelling of surface density and in-plane mobility through molecular crowding — Wanchung Chiang[1], Lionel Bureau[1], Ralf Richter[2], Galina Dubacheva[1], and •Delphine Debarre[1] — [1]Grenoble-Alpes University, France — [2]University of Leeds, UK

Adsorption of proteins onto surfaces has been the focus of a wealth of experimental, theoretical and numerical studies but surprisingly little is known on the dynamics of protein adsorption on fluid surfaces.

In this study, we consider irreversible adsorption of streptavidin, a protein with a very strong affinity for its ligand biotin, onto a lipid bilayer incorporating biotin-terminated lipids, a widely-used model to build biomimetic surfaces. We show that after the initial, rapid adsorption phase, a slower, logarithmic continuous adsorption can lead to surface densities much larger than in the absence of surface diffusion. Simultaneously, we quantify the lateral diffusion of the adsorbed proteins, which drops sharply and can be tuned continuously over two orders of magnitude depending on surface density.

We then adapt free-volume theories to two dimensions to rationalize our findings and bridge the gap between in-plane diffusion and adsorption dynamics. Beyond a better understanding of adsorption onto mobile surfaces, our data paves the way towards biomimetic surfaces incorporating mobility control of functional groups.

CPP 27: Focus Session: Water – from Atmosphere to Space III (joint session CPP/DY)

Time: Tuesday 14:00–15:30 Location: ZEU/LICH

Topical Talk CPP 27.1 Tue 14:00 ZEU/LICH

Why water in plants survives negative pressure — Marin Šako[1,2], Emanuel Schneck[3], Roland Netz[4], and •Matej Kanduč[1] — [1]Jožef Stefan Institute, Ljubljana, Slovenia — [2]University of Ljubljana, Faculty of Mathematics and Physics, Ljubljana, Slovenia — [3]Physics Department, Technische Universität Darmstadt, Darmstadt, Germany — [4]Fachbereich Physik, Freie Universität Berlin, Berlin, Germany

It may seem surprising that we can lower the pressure in a liquid to negative values, far below the saturated vapor pressure at which a vapor phase should form. In water, such deeply metastable states are possible only when it is exceptionally pure and free of nucleation sites. It is therefore even more striking that plants transport water at negative pressures down to −100 atm without cavitation, even though xylem sap is anything but pure: it contains dissolved ions, sugars, lipids, and other organic molecules. How is this possible?

In this talk, I will show how molecular simulations and theory can explain this surprising behavior. We find that amphiphilic molecules such as lipids can adsorb onto hydrophobic surface crevices — places that would normally trap nanobubbles. Once coated, these surface defects can no longer stabilize bubbles, which allows water to stay intact even under strong tension. This mechanism offers a molecular-level explanation for how trees transport water to heights of over 100 meters without cavitation. More broadly, it illustrates how soft-matter physics and interfacial molecular organization can control the mechanical stability of liquids under extreme conditions.

CPP 27.2 Tue 14:30 ZEU/LICH

Cholesterol Controlled Photo-Switching Activity of Azobenzene Glycoconjugates in Lipid Membranes — •Prashant Hitaishi[1,2], Svenja C. Hövelmann[1,2], Michael Röhrl[3], Nicolas Hayen[1], Ella Diebell[1], Ali Ashtiani[1], Carlotta Mager[1], Thisbe Lindhorst[3], and Bridget M. Murphy[1,2] — [1]Institute of Experimental and Applied Physics, Kiel University, Leibnizstraße 19, Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, Hamburg, Germany — [3]Otto Diels-Institut für Organische Chemie, University of Kiel, Germany

Reversible photo-switchable molecules enable precise optical control of soft interfaces and are attractive for smart surfaces and light-triggered drug delivery. Azobenzene glycoconjugates (Azo) undergo reversible trans-cis isomerization under alternating UV and visible illumination, thereby modulating their conformation and interactions with lipid membranes. Here, Azo is incorporated into DPPC monolayers containing 0, 15, or 30 mol% cholesterol to mimic biologically relevant membrane compositions. Langmuir monolayer isotherm studies combined with time-resolved illumination cycles and X-ray measurements are used to quantify Azo-induced changes in membrane structure and relaxation kinetics. Increasing cholesterol slows Azo photo-switching, indicating a more constrained, rigid nanoenvironment, and shows that membrane composition can be used to tune light responsiveness in lipid interfaces for designing azobenzene-based responsive biomaterials.

CPP 27.3 Tue 14:45 ZEU/LICH

Photoelectron Angular Distributions of Ions Influenced by Surfactants at the Solution-Vapor Interface — •Shirin Gholami[1], Tillmann Buttersack[1], Clemens Richter[2], Rémi Dupuy[3], Daniela Torres-Díaz[1], Christophe Nicolas[4], Uwe Hergenhahn[1], and Hendrik Bluhm[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]SPECS Surface Nano Analysis GmbH, Berlin, Germany — [3]Sorbonne Université, CNRS, Paris, France — [4]Synchrotron SOLEIL, Paris, France

Aqueous liquid-vapor interfaces play key roles in atmospheric and oceanic processes. The ocean-air boundary forms the largest aqueous-vapor interface, covering over 70 % of Earth's surface. In addition to Na^+ and Cl^-, Mg^{2+} and SO_4^{2-} are the most abundant ions in ocean water.

Here, we investigate how Mg^{2+} and SO_4^{2-} ions behave at the aqueous solution-vapor interface in the presence of charged surfactants. Using sub-monolayer coverages of octylamine $-CNH_3^+$ and octanoate $-COO^-$, we examine how these surfactants modify the distance of the ions from the interface. Liquid-jet X-ray photoelectron spectroscopy in combination with photoelectron angular distributions provides Å-scale depth sensitivity, enabling us to quantify ion-surfactant interactions.

Our results show that differently charged surfactants shift the interfacial positioning of Mg^{2+} and SO_4^{2-}, and that specific ion-ion interactions influence their interfacial propensity.These findings reveal how surfactants govern the depth distribution of ions, providing insight into oceanic and atmospheric processes.

CPP 27.4 Tue 15:00 ZEU/LICH

Contact line dynamics on moving fibers measured by X-ray holography — •Louisa E. Kraft[1,2], Jens Lucht[3], Fiona Berner[1,2], Hannes P. Hoeppe[3], Tobias Eklund[1,2], Yizhi Liu[1], Markus Osterhoff[3], Tim Salditt[3], Hans-Jürgen Butt[1], and Katrin Amann-Winkel[1,2] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Johannes Gutenberg University, Institute for Physics, Mainz, Germany — [3]Georg-August-University, Institute of X-ray Physics, Göttingen, Germany

The wetting properties of solid surfaces are important for many natural and industrial processes, especially with respect to dynamic wetting. The wetting dynamic of solid surfaces, in particular the quantitative description of the dynamic contact angles, is still under debate. Dynamic contact angle variations connect macroscopically measured quantities with microscopic processes. Most studies rely on optical or confocal microscopy which limits the experimental access to the sub-microscopic region where these processes take place. We present data from X-ray holography experiments, imaging the three-phase contact line on moving glass fibers with an improved spatial resolution of about 450 nm combined with a temporal resolution of 10 Hz. We used the GINIX nanofocusing setup at the P10 beamline at PETRA III (DESY, Hamburg). The used glass fibers were pulled out of a liquid bath filled with varying aqueous solutions while changing the lateral velocity. We could clearly observe a decrease of the receding dynamic contact angle with increasing fiber velocity confirming the predictions of dynamic wetting theory.

CPP 27.5 Tue 15:15 ZEU/LICH

Properties of micrometre-sized supercooled water droplets — Claudia Goy[1], •Frédéric Caupin[2], Felix Lehmkühler[1], and Robert E. Grisenti[3,4] — [1]Deutsches Elektronen Synchrotron DESY, Hamburg, Germany — [2]Université Claude Bernard Lyon 1, Villeurbanne, France — [3]GSI, Darmstadt, Germany — [4]J. W. Goethe-Universität, Frankfurt am Main, Germany

Water displays a wide range of anomalous behaviors, many of which become particularly pronounced in the supercooled state, where its properties deviate strongly from those of other liquids. A prevailing hypothesis suggests that, at low temperatures, water may locally adopt two distinct structural motifs. This presentation will discuss results from temperature-dependent experiments that probe the physical and chemical properties of liquid water. The studies employ evaporatively cooled liquid jets in vacuum, investigated with techniques such as Raman spectroscopy and X-ray spectroscopy. These approaches enable a detailed examination of inter- and intramolecular vibrational modes, providing insight into the molecular dynamics of cooling water and optical properties, including the refractive index. Together, these experimental methods offer a comprehensive view of the temperature-dependent behavior of water, shedding light on the complex interactions that drive its anomalies. Through these studies, we aim to elucidate the mechanisms governing water's unique behavior in the supercooled regime and contribute to a deeper understanding of its structural transformations and physical properties.

CPP 28: Active Matter IV (joint session DY/BP/CPP)

Time: Tuesday 14:00–15:30 Location: ZEU/0160

CPP 28.1 Tue 14:00 ZEU/0160

Automated decision-making by chemical echolocation in active droplets — •Aritra K. Mukhopadhyay[1], Ran Niu[2], Linhui Fu[2], Kai Feng[2], Christopher Fujta[1], Qiang Zhao[2], Jinping Qu[2], and Benno Liebchen[1] — [1]Technische Universität Darmstadt, Darmstadt, Germany. — [2]Huazhong University of Science and Technology, Wuhan, China.

Motile microorganisms like bacteria and algae combine self-propulsion, cooperation, and decision-making at the micron scale. Inspired by these biological systems, synthetic microswimmers are emerging as human-made counterparts capable of self-propulsion. Recent breakthroughs provide a platform to integrate additional functionalities, bridging the gap between biology and synthetic systems. We propose and experimentally demonstrate a mechanism that enables synthetic microswimmers, including autophoretic colloids, droplet swimmers, and ion-exchange-driven modular swimmers, to make autonomous navigational decisions. These swimmers generate chemo-hydrodynamic signals that interact with boundaries, producing echoes that encode structural information about the environment. These echoes trigger automatic responses, such as synthetic chemotaxis, allowing swimmers to avoid dead ends and autonomously find paths through complex mazes. We show the mechanism remains robust across different maze geometries, ensuring reliable navigation without external cues. Our findings illustrate how simple physical principles can endow synthetic systems with advanced navigation functionalities.

CPP 28.2 Tue 14:15 ZEU/0160

Dead or alive?—Probing scale-dependent liveliness in multiscale active matter — •Joscha Mecke[1] and Klaus Kroy[2] — [1]Institute for Advanced Study, Shenzhen University, Shenzhen, China — [2]Institut für Theoretische Physik, Universität Leipzig, Leipzig, Germany

If you have ever watched live and dead trouts swimming upstream, side by side, you may have wondered how closer inspection of their mesoscale activity might help to tell them apart. But probing spatially heterogeneous activity in living matter is a major challenge. We demonstrate the emergence of multiple effective ("active") temperatures in nonequilibrium molecular- and Brownian-dynamics simulations of an active polymer. Energy injection at different length scales leads to mode coupling, inter-modal energy transfer, and entropy production. We put forward a generalised Langevin equation for a labelled monomer, which, by application of a harmonic potential, can serve as a spectroscopic device. Upon varying the trap stiffness, we can selectively scan through the emergent effective temperatures and thereby resolve the scale-dependent activity. Our approach thus provides a minimally invasive spectroscopic tool to generate quantitative maps of liveliness, across multiple scales.

CPP 28.3 Tue 14:30 ZEU/0160

Tuning the velocity of thermophoretic microswimmers with thermo-sensitive polymers — Franziska M. Braun, Aritra K. Mukhopadhyay, Samad Mahmoudi, Benno Liebchen, and •Regine von Klitzing — Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstrasse 8, 64289 Darmstadt

Understanding and controlling the motion of self-propelled particles in complex fluids is crucial for applications in targeted drug delivery, microfluidic transport, and the broader field of active matter. Here, we investigate the thermophoretic self-propulsion of partially gold-coated polystyrene Janus particles (Au-PS) in temperature-responsive linear Poly(N-isopropyl acrylamide) (PNIPAM) solutions across various PNIPAM concentrations and temperatures. Particle velocities are examined at three representative temperatures: far below, near but below and above the LCST. In pure water, Au-PS Janus particles propel with the PS hemisphere leading, driven by their intrinsic thermophoretic response. Conversely, the positive Soret coefficient of PNIPAM results in depletion forces that induce motion of the Janus particle towards the hot Au side. The experiments reveal a non-monotonic dependence of particle velocity on temperature, with a maximum near the LCST. Interfacial processes like ion movement in the electric double layer and PNIPAM adsorption at the Au-PS particles are separated from processes that are coupled to the bulk solution. Theoretical calculations are in good agreement with the experimental findings and are essential for the understanding of the complex interplay of microswimmers with thermoresponsive polymers.

CPP 28.4 Tue 14:45 ZEU/0160

Non-reciprocal multifarious self-organization — •Saeed Osat[1] and Ramin Golestanian[2] — [1]Institute for Theoretical Physics IV, University of Stuttgart, Heisenbergstraße 3, 70569 Stuttgart, Germany — [2]Max Planck Institute for Dynamics and Self-Organization (MPI-DS), 37077 Goettingen, Germany

Biological systems exhibit a unique ability to design diverse structures from a shared set of building blocks, with a plethora of proteins made from a limited set of amino acids as a prime example. Furthermore, these systems often use building blocks efficiently by introducing transformations between different structures. A structure might undergo structural transformations to form a new structure with different functional purposes, without the need to discard the current structure and start anew. To unravel this mystery, one must examine the underlying non-equilibrium processes that make this shape-shifting behavior feasible.

Here, we leverage non-reciprocal interactions between building blocks to provide a foundation for designing dynamic structures. We used a multifarious self-assembly (MSA) model, which is the molecular counterpart of the Hopfield associative memory. By upgrading the MSA model to its non-equilibrium counterpart with non-reciprocal interactions, we introduce the ability to not only self-assemble different structures on demand but also facilitate shifts and transformations that lead to shape-shifting behavior.

Invited Talk CPP 28.5 Tue 15:00 ZEU/0160

Designing topological edge states in bacterial active matter — Yoshihito Uchida[1], Daiki Nishiguchi[2,1], and •Kazumasa A. Takeuchi[1] — [1]The University of Tokyo, Tokyo, Japan — [2]Institute of Science Tokyo, Tokyo, Japan

Besides its potential relevance to the life sciences, active matter also manifests as a novel, intrinsically non-equilibrium kind of matter, endowed with characteristic transport properties distinguished from conventional matter. A challenge is how to control and design transport in active matter. A potentially useful, emerging concept here is topological transport developed in condensed matter physics, which was extended to active matter successfully, but experimental realizations have thus far relied on the chirality of the active particles, which limits design capabilities.

Here we report a controlled realization of topological edge states in dense bacterial suspension, induced by microfabricated geometry instead of the bacteria's chirality. First we demonstrate that we can rectify bacterial collective motion by a channel with asymmetric shape. Then we construct networks made of asymmetric channels and show that we can control the emergence of topological edge states through the network design. Through modelling and experiments, we discuss what properties of the network and the bacterial flow are crucial to the observed topological phenomenon. We expect our results may pave the way for establishing a control and design principle of topological transport in such active matter systems.

Ref) Y. Uchida, D. Nishiguchi, and K. A. Takeuchi, to appear.

CPP 29: Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods III

Time: Tuesday 14:00–15:30 Location: ZEU/0255

CPP 29.1 Tue 14:00 ZEU/0255

Towards Evolved Sensing Applications for Organic Photonic Devices Utilizing Room-Temperature Phosphorescence — •Sebastian Kaiser, Sebastian Schellhammer, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics (IAP), Technische Universität Dresden

Photonic devices function through the absorption and emission of light, making them independent of electricity or other influences. This trait is vital for sustainable advances in imaging, sensing, information storage, and anticounterfeiting. Programmable luminescent tags (PLTs) exemplify this by utilizing the oxygen-sensitivity of organic room-temperature phosphorescence (RTP) for controllable switching of the device's light output under UV illumination. [1, 2] Optimizing the homogeneity and reproducibility of photonic thin-film devices, paired with use-case-tailored layer compositions, allowed us to develop a new, advanced UV light-sensing application. The thin-film nature of PLTs, especially their flexibility and transparency, combined with a freely scalable sensor area, enables a broader range of use cases than common detectors can achieve. The combination of these unique device characteristics opens the way for new sensing applications for purely photonic devices.

[1] Gmelch et al., Science Advances 2019. aau7310

[2] Tsiko et al., Communications Chemistry 2025, 025-01620-0

CPP 29.2 Tue 14:15 ZEU/0255

Synergistic and unique information reveals multicentre bonding and geometry — •Kyunghoon Han, Miguel Galleogos Gonzalez, and Alexandre Tkatchenko — University of Luxembourg, Luxembourg, Luxembourg

Classical bonding measures and entropy maps are mostly pairwise, obscuring cooperative effects. We introduce a Partial Information Decomposition of bond character built from standard density-functional and coupled-cluster data. Fragment electron- and spin-number distributions along a coordinate define a simple label (covalent, ionic, multicenter), and information about that label is separated into redundant (shared), unique (single-fragment), and synergistic (joint-only) parts. Treating bond character as a geometric response, small perturbations yield a synergy profile that pinpoints where cooperation emerges and how it evolves. The profile rises at the onset of sharing in diatomic hydrogen, is maximal for the central bond of bicyclo[1.1.1]propellane only when the bridgeheads and the three methylene groups are taken together, and peaks at the square geometry of cyclobutadiene before dropping with bond alternation. Benchmarks against density, orbital, energy, and machine-learning descriptors show where PID adds explanatory power and, for ordinary two-center bonds far from dissociation, why it is near-zero with detectable exceptions only when the two atoms are the same.

CPP 29.3 Tue 14:30 ZEU/0255

Utilizing Immediate Phosphorescence in Organic Photonic Devices for Rewritable Information Storage and Oxygen Sensing — •Lucy Winkler, Sebastian Schellhammer, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics (IAP), Technische Universität Dresden

Programmable luminescent tags (PLTs) are photonic devices that offer simple and versatile solutions for reversible information storage and food labeling by using the oxygen-sensitive phosphorescent emission from organic emitters embedded in polymer matrices [1]. Conventional PLTs fabricated by spin-coating under ambient conditions exhibit oxygen-quenched phosphorescence in their initial state, requiring photoactivation to consume oxygen in the active layer and switch on emission. However, these PLTs show inconsistent activation between the initial and subsequent writing processes, significantly limiting their controlled reusability for practical applications [2]. To better understand activation cycles and identify potential improvements, different fabrication workflows in oxygen-free environments were tested. While activation behavior remains similar to conventional devices, these fabrication approaches enable creation of activated PLTs with an initial switched-on state that could serve as simple oxygen detectors, for example, in vacuum packaging integrity monitoring.

[1] Thomas, H. et al. Adv. Mater. 36, 2310674 (2024).
[2] Tsiko, U., et al. Commun Chem 8, 274 (2025).

CPP 29.4 Tue 14:45 ZEU/0255

Solution to the current paradox of anomalous underscreening in electrolytes — •Esther Ohnesorge, Thomas Tilger, Michalis Tsintsaris, Hayden Robertson, and Regine von Klitzing — Department of Physics, Technische Universität Darmstadt, Darmstadt, 64289, Germany

Since colloidal dispersions have a significant importance in our daily life, it is of special interest to get a deeper understanding of which interfacial forces govern their stability and how this stability can be tailored.

For aqueous electrolyte solutions, DLVO theory is a powerful and well-established framework to describe these interactions at low and intermediate ionic strengths. In contrast, the situation at high ionic strength is less understood and the main methods for direct force measurements give inconsistent results. Whilst the surface force apparatus (SFA) provides clear evidence for a re-entrance of repulsion in the highly concentrated regime (termed underscreening) for a wide range of different electrolytes [1], similar observations were not possible with the atomic force microscope (AFM) to date [2]. In this presentation we will examine the reason of these fundamental differences. Specifically, in an attempt to explore experimental screening lengths across a wide suite of electrolyte concentrations, we demonstrate the experimental parameters dominating the occurrence of anomalous underscreening and a comprehensive understanding of this long-debated phenomenon. [1] DOI: 10.1103/PhysRevLett.119.026002 [2] DOI: 10.1016/j.jcis.2022.05.004

CPP 29.5 Tue 15:00 ZEU/0255

Thermal properties of a knotted diblock copolymer ring — •Neda Abbasi Taklimi[1], Franco Ferrari[1], Marcin Radoslaw Piatek[1], and Luca Tubiana[2] — [1]Institute of Physics, University of Szczecin, Wielkopolska15, 70-451 Szczecin, Poland — [2]INFN-TIFPA, Trento Institute for Fundamental Physics and Applications, Via Sommarive 14, I-38123 Trento, Italy

The phase transitions and geometrical properties of diblock copolymers have been studied extensively; however, few studies have addressed knotted structures under varying monomer distributions and solvent quality. Here, we present a computational study of how topological constraints and block lengths affect the behavior of a single diblock copolymer ring. We used the Wang-Landau Monte Carlo algorithm and a coarse-grained model on a simple cubic lattice with an implicit solvent to explore thermal and structural properties. In the AB model, A-type monomers are self-repulsive, B-type monomers are self-attractive, and AB interactions are neutral; the solvent is good for A-type and poor for B-type monomers at low temperatures.

We computed key properties, including heat capacity, radius of gyration of individual blocks and the whole ring, number of contacts (AA, BB, AB), and knot length. Our results reveal several phase transitions for specific monomer distributions and topologies. Subtle changes in monomer distribution lead to transitions between knotlocalization and delocalization at low temperatures, driven by the competition between entropic and energetic contributions to the free energy.

CPP 29.6 Tue 15:15 ZEU/0255

A Systematic Multiscale Study of Bio-Based Polymers for Novel Food Packaging Systems — •Andoni Ugartemendia, Alessandro Mossa, and Giorgia Brancolini — Institute of Nanoscience, CNR-NANO S3, via G. Campi 213/A, 41125 Modena, Italy

Recently, monolayer materials of bio-based polymers have gained increased attention to develop more sustainable packaging systems.[1] In this regard, rational in silico design has become essential to predict novel polymers and reduce experimental workload. However, the computational modeling of these materials poses a great challenge since their dynamics span over different time scales.[2] To bypass this issue, in this work we propose a modular multiscale computational protocol to study linear polymers from ab initio to coarse grained (CG) dynamics. In the first part, we derive a full atomistic force field (FA-FF) from DFT data and carry out FA-MD simulations for its validation. In the second step, all structural properties are passed to a database to parametrize a CG-FF with the iterative Boltzmann inversion (IBI).[3] Lastly, large scale CG-MD simulations are run for a final validation of the CG-FF. This methodology is applied first to PET, a polymer widely used in the packaging industry, as well as to emerging bio-based polymers such as PEF and PLLA.

[1] V. Guillard, et al., Front. Nutr., 2018, 5, 121. [2] R. B. Bird, R. C. Armstrong, O. Hassager, Dynamics of Polymeric Liquids. Volume 1: Fluid Mechanics, 2nd ed. (Wiley-Interscience, United States, 1987). [3] A.P. Lyubartsev, et al., J. Chem. Theory Comput. 2013, 9, 1512.

CPP 30: Complex Fluids, Colloids, Micelles and Vesicles I

Time: Tuesday 14:00–15:30 Location: ZEU/0260

Invited Talk CPP 30.1 Tue 14:00 ZEU/0260

Solvent effects on amphiphile self-assembly in Deep Eutectic Solvents — •Karen Edler — Centre for Analysis and Synthesis, Chemistry Department, Lund University, Sweden

Deep eutectic solvents (DES) are mixtures of hydrogen bond donors and acceptors that form strongly hydrogen-bonded room temperature liquids. These mixtures are straightforward to prepare, using cheap, bioderived components, with lower volatility than most organic solvents, so are potential new green solvents for applications from drug delivery to battery electrolytes. We are interested in micelle templating of inorganic nanomaterials and formulations for delivery of actives, using these versatile solvents.

Changing the H-bonding components and their ratios alters the physicochemical properties of DES, leading to changes in solubility of other species in these solvents. This also alters the self-organisation of surfactants in these mixtures. We have investigated how specific DES components and their molar ratios impact upon solubility and structuring in surfactant solutions, using small angle X-ray and neutron scattering and rheology. Factors such as polarity, the presence of water, and the intermolecular interactions, both between solvent components and with the surfactant headgroups, play a role in the size and morphology of the micelles formed. We aim to develop design rules for novel complex solutions with applications in templating, rheology control and encapsulation using these interesting new solvent systems.

CPP 30.2 Tue 14:30 ZEU/0260

Brick by Brick - Magnetic Particle Transport — •Margaret Rosenberg[1], Jonas Bugase[2], Christian Janzen[2], Rico Huhnstock[2], Arno Ehresmann[2], and Hartmut Löwen[1] — [1]Heinrich-Heine University Düsseldorf, Universitätsstraße 1, Düsseldorf — [2]Institute of Physics , University of Kassel, Kassel

Facilitated by advances in particle synthesis, anisotropic and anisometric magnetic micro- and nanoparticles have been intensely studied in recent years, as the

particles' lack of symmetry can give rise to unique, tailor-able interactions. However, the modeling of off-equilibrium processes in non-trivial magnetic landscapes is still relatively under-explored. This contribution will seek to understand the ratchet-like transport process of a magnetically coated polymer block ("brick") across a stripe-patterned magnetic surface via a sequence of time-dependent external magnetic fields, from a simulation perspective. In particular, we explore the rotational behavior unlocked by the anisotropic particle shape, and discuss the connection to ongoing experiments.

CPP 30.3 Tue 14:45 ZEU/0260

Role of acids in stabilizing Reverse Micelles: the case of Dodecyl Sulfate — •Qixuan Li and Marialore Sulpizi — Faculty of Physics and Astronomy, Ruhr-University Bochum

The anionic surfactant Sodium dodecyl sulfate (SDS) can form reverse micelles (RMs) in two non-miscible components above the critical micelle concentration [1]. Although the RMs in salt or alkali solution has been investigated in previous studies [2,3], less is known on the working mechanism of acids in SDS RMs. Here, we employ all-atom (AA) and coarse-grained (CG) molecular dynamics to investigate the effects of chloroauric acid (HAuCl4), fluoroboric acid (HBF4) and phosphoric acid (H3PO4) solutions on the stability of the RMs through spontaneous self-assembly in toluene. We find that investigated acids can stabilize micellar structure, particularly H3PO4 due to the stable hydrogen-bonds it forms with the SDS headgroups. In addition, HAuCl4 can significantly influence micelle shape because of its strong polarizability at the water-toluene interface, while HBF4 causes the highest interfacial tension as a result of its significant hydrophilicity. Moreover, scission free energy calculations from CG simulations [4,5] reveal important differences, which along with the viscosity can explain how different acids affect the size of RMs. Our findings can help to rationalize the impact of different acids on the RMs stability and morphology and, in turn, on the metallic nanoparticles synthesis where the RMs are used as nanoreactors.

CPP 30.4 Tue 15:00 ZEU/0260

Microsecond-Resolved Tracking of Ultrasound-Responsive Colloids: From Rigid Silica Probes to Acousto-Responsive Microgels — Parsa Kassaiyan, Regine von Klitzing, and •Amin Rahimzadeh — Technische Universität Darmstadt, Hochschulstrasse 8, 64289 Darmstadt, Germany

Dynamic Light Scattering (DLS) is a powerful tool for characterizing dispersed particles, providing access to their size, size distribution, and dynamical behavior. Here, we integrate high-frequency ultrasound excitation into a conventional DLS setup to resolve the microsecond-scale motion of colloidal particles subjected to intense acoustic fields. This enables simultaneous extraction of particle size and ultrasound-induced oscillation parameters such as vibration frequency, amplitude, and acoustic response, through analysis of the scattered-light intensity correlation function. Compact silica particles serve as robust reference probes: their size remains unaffected by ultrasound, allowing us to map local acoustic energy dissipation by tracking their oscillatory motion at varying distances from the ultrasound source. Building on this reference system, we investigate acousto-responsive PNIPAM microgels. We find that microgels undergo a pronounced ultrasound-induced volume phase transition, shrinking due to rapid dehydration driven by absorption of high-frequency acoustic energy. Our approach thus provides both microsecond-resolved characterization of particle dynamics and a direct pathway to understanding, and exploiting, the acousto-responsiveness of microgels.

CPP 30.5 Tue 15:15 ZEU/0260

Influence of End Groups on the Aggregation of Polymers: A Neutron Scattering Study — •Jonathan Linus Samuel Garthe[1,2], Sylvain Prévost[3], and Matthias Karg[1] — [1]Physical Chemistry of Functional Polymers, Martin Luther University Halle-Wittenberg, Halle (Saale), Germany — [2]Physical Chemistry: Colloids and Nanooptics, Heinrich Heine University Düsseldorf, Düsseldorf, Germany — [3]Large Scale Structures, Institut Laue-Langevin, Grenoble, France

The solution structure of polymers depends strongly on polymer concentration, solvent quality, and molecular weight. Additionally the nature of chemically different terminal groups influences the phase behavior of polymers with strong differences depending on the average chain length. We investigated the solution behavior and the occurrence of micelle-like structures for (semi)-dilute solutions. We synthesized PNIPAM homopolymers that are hydrophobically terminated. Via aminolysis we also cleaved the hydrophobic end groups allowing for direct comparison of the same homopolymers with and without hydrophobic end group. Small-angle neutron scattering was used to study the structure of the polymers in solution. Our studies demonstrated that a subdominant micelle formation occurs for samples with molecular weights below 100 kDa. The aggregation number of these micelles scales inverse with the molecular weight. At low concentrations, these micelles exist as individual structures. Upon increasing the concentration micelles aggregate, leading to a distinct structure factor contribution in the scattering profile.

CPP 31: Responsive and Adaptive Systems

Time: Wednesday 9:30–11:30 Location: ZEU/0255

Invited Talk CPP 31.1 Wed 9:30 ZEU/0255

Hydrogels with a Pinch of Embodied Intelligence — •Andreas Walther — Department Chemie, JGU Mainz

Smart is good, but intelligent is better. The next frontier in soft matter research is to design life-like materials with embodied intelligence, featuring the integrated sensor-processor-actuator paradigm. Our work explores how hydrogels and soft robotic systems can be endowed with autonomous operation and decision-making capacity by embedding chemical reaction networks, enzymatic feedback loops, and mechanical gating principles. Such metagels and metamaterials are capable of self-strengthening behavior, strain-gated responses, and non-reciprocal motion, moving far beyond the limits of traditional responsive materials. By intertwining chemical, mechanical, and structural information, these systems provide a blueprint for programmable, adaptive matter that approaches the complexity and functionality of biological tissues.

CPP 31.2 Wed 10:00 ZEU/0255

Secondary crosslinking of thermoresponsive microgels for smart microgel-based membranes — •Jonas Runge[1,2], Stefanie Uredat[1,2], Aditi Gujare[1,2], Domenico Truzzolillo[2], Julian Oberdisse[2], and Thomas Hellweg[1] — [1]Physical and Biophysical Chemistry, Bielefeld University, Germany — [2]Laboratoire Charles Coulomb, Université Montpellier, France

Responsive microgels are crosslinked polymer networks of colloidal size, which undergo a so-called volume phase transition induced by a certain stimulus like e.g. temperature or pH. Temperature sensitive microgels undergo a strong decrease in size at the volume phase transition temperature (VPTT). Smart membranes are based on responsive polymers and allow to open pores triggered by an external stimulus [1]. Our project on smart microgel-based membranes (SmartBRANE) aims to incorporate an UV-crosslinker and form membranes by activating the UV-crosslinker [2]. The working temperature of low-temperature fuel cells is in the range of 80-100 °C. Since the VPTT of common acrylamides is close to the physiological temperature, we synthesized a hydrophilic acrylamide monomer (NIPMAMol) with an extrapolated VPTT of 85°C. In this work, we copolymerize NIPMAMol with NIPAM and the UV-crosslinker HMABP to increase the VPTT of the then formed membrane. The thermoresponsive properties of the microgels are characterized with PCS. The distribution of the UV-crosslinker within the microgels particles and the formed membrane is investigated with contrast-matching SANS experiments. [1]Runge,Gujare,Uredat, PCCP, 2024, 26, 2732.[2]Dirksen, RSC Advances, 2021, 11(36), 22014.

CPP 31.3 Wed 10:15 ZEU/0255

Photoresponsive Control of Fullerene Diffusion in Azo-BT Nanotraps — Dmitry A. Ryndyk[1,2] and •Olga Guskova[1] — [1]IPF Dresden, Dresden, Germany — [2]TU Dresden, Dresden, Germany

We present a light-switchable azobenzene-bithiophene (Azo-BT) self-assembled monolayer (SAM) on Au(111) that operates as a reversible nanotrap for C60. Using density-functional theory and QM molecular dynamics, we quantify C60 adsorption on planar layers and diffusion on the SAM and within a fixed 12 A slit-like pore. Direct adsorption on the cis layer is about twice as favorable as on the trans layer due to stronger dispersion interactions with exposed thiophene rings, whereas the densely packed trans layer presents mainly hydrogen contacts and weaker binding. In the slit geometry, the trans (and mixed) layers provide an open pore that captures C60, while photoisomerization to cis closes the slit and prevents release. Diffusion analysis shows that specific interaction sites along the slit walls and the effective degree of confinement - arising from local potential variations within the fixed 12 A slit - govern diffusion pathways and escape barriers. External electric fields or charging of the Au/Azo-BT/C60 complex enable active expulsion, offering design principles for light- and field-responsive nanocarbon trapping interfaces. The financial support from DFG (grant number 509039598) is highly appreciated.

CPP 31.4 Wed 10:30 ZEU/0255

Reversible Photoswitching of Arylazopyrazole-functionalized Polyacrylamide Thin Films under Water Vapor — •David P. Kosbahn[1], Morgan P. Le Dû[1], Simon A. Wegener[1], Feifei Zheng[2], Robert Cubitt[3], René Steinbrecher[4], André Laschewsky[4,5], Christine M. Papadakis[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for

Functional Materials, Garching, Germany — [2]TUM School of Natural Sciences, Soft Matter Physics Group, Garching, Germany — [3]Institut Laue-Langevin, Grenoble, France — [4]Institut für Chemie, Universität Potsdam, Potsdam-Golm, Germany — [5]Fraunhofer Institut für Angewandte Polymerforschung, Potsdam-Golm, Germany

This study investigates the swelling behavior of p(AAPEAm-co-DMAm) films in both isomeric states of the novel photoswitchable molecule arylazopyrazole (AAP). The impact of reversible switching using two different wavelengths on swelling of the polymer in water vapor is examined, with the aim of controlling water uptake, expansion, and nanoscale morphology. This material shows potential for applications in reversible light sensors, photo-actuators, and drug delivery systems. We use time-resolved FTIR spectroscopy to monitor group vibrations during switching, gaining insights into molecular interactions throughout the isomerization processes. Additionally, in situ time-of-flight neutron reflectometry on a thin film provides time- and depth-resolved data on the water distribution along the surface normal. The results shed light on the influence of arylazopyrazole moieties on the polymer's microscopic properties.

CPP 31.5 Wed 10:45 ZEU/0255

Modeling the Viscoplastic Deformation of Azopolymers Under the Influence of Structured Light — •Nikolai Liubimtsev and Marina Saphiannikova — Leibniz Institute of Polymer Research Dresden, Germany

A distinctive feature of side-chain azopolymers is their ability to convert structured light into a well-defined stress field [1]. This field results from the alignment and elongation of polymer backbones along the light-polarization direction, which acts as a nematic director. Linearly or elliptically polarized irradiation induces uniaxial or biaxial chain orientation, and the stress tensor is proportional to the rate of change of the second-order orientation tensor, predicted from the spatial distribution of light intensity and polarization [1]. Using viscoplastic photoalignment modeling, we achieve excellent agreement with experimentally observed reshaping of azopolymer microstructures. Three-dimensional light fields - such as tightly focused Gaussian beams or q-plate patterns - produce directional photodeformations. These fields are incorporated into ANSYS either analytically or by directly mapping intensity, polarization, and ellipticity at each material point, the latter being especially useful for arbitrary SLM-generated patterns. Financial support from DFG grant GR 3725/10-1 is gratefully acknowledged.

References: [1] I. K. Januariyasa, F. Reda, N. Liubimtsev, et al., Stress-driven photo-reconfiguration of surface microstructures with vectorial light fields, arXiv:2506.06857 (2025), accepted for publication in Light: Science and Applications.

CPP 31.6 Wed 11:00 ZEU/0255

Impact of surface chemistry on the adsorption and dynamics of stimuli-responsive polymers — Baptiste Chabaud[1], Wanchung Chiang[1], Lionel Bureau[1], Ralf Richter[2], Rachel Auzély[1], Delphine Debarre[1], and •Galina Dubacheva[1] — [1]Université Grenoble Alpes, Grenoble, France — [2]University of Leeds, Leeds, UK

Stimuli-responsive polymers at interfaces underpin smart coatings, sensors and bioinspired materials, yet how surface chemistry controls their binding and dynamics remains poorly understood. We probe the interfacial behavior of redox- and thermosensitive polymers on well-defined model surfaces using QCM-D, SPR, ellipsometry, electrochemistry and fluorescence microscopy. For redox-active host/guest systems, we show that grafting strategy, linker flexibility and host/guest density govern the stability, specificity and reversibility of polymer assemblies. Kinetic analysis further reveals that small changes in surface chemistry, such as linker design or dilution with inert molecules, strongly tune multivalent superselectivity, enabling sharp discrimination of receptor densities. Using supported lipid bilayers as fluid interfaces, we correlate lateral mobility with contraction, dehydration and 2D aggregation of thermoresponsive polymer brushes. Overall, we identify interfacial density, mobility and flexibility as key parameters for controlling stimuli-responsive polymer assemblies and outline design rules for supramolecular and bio-inspired systems with high specificity and precision.

CPP 31.7 Wed 11:15 ZEU/0255

Modeling of magnetic hysteresis in magneto-active elastomers — •Pawan Patel[1,2], Dirk Romeis[1], and Marina Saphiannikova[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V, Hohe Straße 6, 01069, Dresden, Germany — [2]Faculty of Mechanical Science and Engineering, Dresden University of Technology, 01062, Dresden, Germany

Magneto-active elastomers (MAEs) are soft polymer composites containing magnetizable microparticles. MAEs exhibit field-dependent mechanical and magnetic properties. When subjected to an external magnetic field, MAEs display magneto-mechanical coupling effects such as tunable stiffness and reversible shape changes. This study presents a multiscale theoretical model to describe the magnetic hysteresis behavior of MAEs, focusing on the role of microstructure evolution during magnetization and demagnetization of microparticles. The total energy of the system is formulated as the sum of magnetic and micromechanical contributions, while macroscopic deformation of the cylindrical sample is constrained. The model incorporates both pure dipole–dipole interactions and near field effect to account for multipole higher-order particle interactions. The results reveal that magnetic hysteresis in soft magnetic MAEs arises primarily from microstructural rearrangements, where the spatial configuration of particles differs between increasing and decreasing magnetic fields. Simulations demonstrate that parameters such as particle volume fraction, sample geometry, and micromechanical stiffness significantly influence the hysteresis loop width.

CPP 32: Focus Session: Water – from Atmosphere to Space IV (joint session CPP/DY)

Time: Wednesday 9:30–10:45 Location: ZEU/0260

Topical Talk CPP 32.1 Wed 9:30 ZEU/0260

Synchrotron X-Ray Studies on Structural Transitions in Water and Alcohol containing Ice Analogues — •Christina M. Tonauer — Institute of Physical Chemistry, University of Innsbruck, Austria — Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany

To this date, 21 different crystalline and at least 3 distinct amorphous forms of water ice have been discovered. In addition to the structural versatility of pure water ice phases, water forms solid guest-host systems, so-called 'clathrate hydrates' where water builds cage-like structures around guest molecules of various sizes (e.g., Ar, CO2, methane, ethanol).

Ices in space are exposed to various forms of (external) stress, e.g., impacts, cosmic rays, UV/Vis radiation as well as endogenous thermal fluctuations, thereby undergoing structural changes. By studying such structural transitions in ice analogues upon heating (and/or radiation), conclusions can be drawn about the conditions at various extraterrestrial environments.

Therefore, we here present temperature-resolved wide- and small-angle synchrotron X-ray scattering data of vapor-deposited water-ethanol mixtures of various concentrations, collected at PETRA 3/DESY. While the SAXS data allows for monitoring of changes of the morphology of the microporous sample, the WAXS data reveals the formation sequence of two different hydrates, offering new insights into the crystallisation of astrophysical ices.

CPP 32.2 Wed 10:00 ZEU/0260

Water in exoplanetary atmospheres: from molecular spectra to Water Worlds — •Sergey Yurchenko — Department of Physics and Astronomy, University College London, Gower Street, WC1E 6BT London, United Kingdom

Water vapour is one of the key tracers of atmospheric physics and chemistry on exoplanets, from hot Jupiters to temperate sub-Neptunes and so-called Water Worlds. In this contribution I will give an overview of the role of H_2O across this diversity of atmospheres, focusing on how we infer its presence from transmission and emission spectra. I will review both low-resolution transit spectroscopy and high-resolution cross-correlation techniques, and show how they are applied to data from space- and ground-based facilities, including JWST, Hubble and VLT, as well as future observations with the ELT and ESA's Ariel mission. Special emphasis will be placed on the way clouds and hazes imprint themselves on the observed spectra.

I will summarise the current observational status of water detections and non-detections – including recent and sometimes controversial claims for habitable-zone planets. A central theme of the talk will be the importance of accurate laboratory and theoretical data for water and related species. I will highlight how comprehensive molecular line lists and cross sections from the ExoMol and HITRAN databases, together with other laboratory measurements, underpin the modelling and retrieval of exoplanet spectra over a wide range of temperatures, pressures and compositions, thereby linking detailed molecular physics to the emerging picture of water in exoplanetary atmospheres.

CPP 32.3 Wed 10:15 ZEU/0260

Structures of Ices by Quantum Crystallography and PDF — Krzysztof Wozniak[1], •W. Sławiński[1], G. Łach[2], R. Gajda[1], M. Chodkiewicz[1], P. Rejnhardt[1], M. Arhangelskis[1], Ch. Ridley[3,4], and C. L. Bull[3,5] — [1]Deptm. of Chem., Univ. of Warsaw,Poland — [2]Deptm. of Phys., Univ. of Warsaw, Poland — [3]ISIS Neutron and Muon Source, STFC, RAL, Harwell Campus, UK. — [4]Spallation Neutron Source, Oak Ridge Nat. Lab., Oak Ridge, Tennessee 37830, USA — [5]Univ. of Edinburgh, UK.

Ice is the solid form of water (H*O). The most familiar form of ice is the hexagonally structured ice Ih. However, water can crystallize into at least 21 distinct

phases, unique in structure, depending on T and P and route of formation. In this contribution, will present details of structures of ices (VI[3], VII[1,2], Ih [4]) obtained with quantum-crystallographic Hirshfeld Atom Refinement against single crystal X-ray and electron diffraction data. We will also present the first quantitative characterisation of disorder in D2O ice VII and VI obtained through a combination of Pair Distribution Function (PDF) analysis, Reverse Monte Carlo (RMC) modelling, and high-pressure neutron scattering. Our results provide a detailed decomposition of both the average and local atomic structures of Ice VII, revealing a previously unquantified level of structural disorder. References [1] R. Gajda et al., IUCRJ, 12(3) (2025) 288-294; [2] W. A. Sławiński et al., Hidden complexity in D2O Ice VII, Acta Mat., (2025) submitted; [3] M. L. Chodkiewicz et al., IUCRJ, 9 (2022) 573-579; [4] M. L. Chodkiewicz et al., IUCRJ, 11(5) (2024) 730-736.

CPP 32.4 Wed 10:30 ZEU/0260

Water dynamics in conductive PEDOT:PSS/cellulose nanocomposite films in dependence of relative humidity and temperature — •Lucas Kreuzer[1], Marie Betker[2], Marcell Wolf[1], Jacques Ollivier[3], Daniel Söderberg[4], and Stephan V. Roth[2,4] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), TUM, Garching, Germany — [2]Deutsches Elektronen Synchrotron, Hamburg, Germany — [3]Institut Laue-Langevin, Grenoble, France — [4]Department of Engineering Mechanics, Royal Institute of Technology KTH, Stockholm, Sweden

PEDOT:PSS is a conductive and water-soluble polymer blend widely used in organic electronics. However, pure PEDOT:PSS films absorb significant amounts of water, causing swelling, degradation, and eventually a decrease in conductivity. Integrating PEDOT:PSS with cellulose nanofibrils (CNFs) overcomes these issues by limiting water absorption and enhancing mechanical stability. However, a minor amount of water is still absorbed, leading to a change in film morphology: high humidity induces de-wetting of PEDOT:PSS from the CNFs, reducing conductivity, whereas drying generally leads to a re-wetting of PEDOT:PSS, thereby restoring conductivity. To investigate further the role of water, quasi-elastic neutron scattering is applied, which reveals two water species in the films: mobile bulk water and slower hydration water. Upon drying, bulk water is released completely, while hydration water remains in the films, supporting the re-wetting of PEDOT:PSS. Moreover, at higher temperatures, different diffusive behavior was found for bulk and hydration water.

CPP 33: Complex Fluids, Colloids, Micelles and Vesicles II

Time: Wednesday 10:00–11:15 Location: ZEU/LICH

Invited Talk CPP 33.1 Wed 10:00 ZEU/LICH

Shape-induced superstructure formation in concentrated ferrofluids — •Sabrina Disch — University of Duisburg-Essen, Essen, Germany

The response of magnetic nanoparticles to applied static and dynamic magnetic fields is the subject of intense research in view of its fundamental technological importance [1]. The field-assisted self-organization of shape-anisotropic nanoparticles in dispersions is particularly desired for liquid crystalline or optically anisotropic materials and as a prerequisite for self-organization into long range ordered arrangements [2]. A strong structure-directing influence of the particle shape on the symmetry of mesocrystalline arrangements has been established for nanocubes with a varying degree of cubicity [3].

In this contribution, we give a detailed account on the impact of nanoparticle shape and size on the interparticle correlations in colloidal dispersions of maghemite nanoparticles. Despite the similar particle size, magnetic moment, and volume concentration (>5 vol-%), we observe a significantly distinct aggregation behavior of nanospheres and nanocubes using small-angle neutron scattering [4]. The field-dependent arrangement of cuboidal nanoparticles into mesocrystalline assemblies and their geometric orientation will be discussed as observed by field-dependent small-angle scattering experiments.

[1] Q. A. Pankhurst et al., J. Phys. D: Appl. Phys. 36, R167 (2003).
[2] S. Disch, E. Wetterskog et al., Nano Letters 11, 1651 (2011).
[3] E. Wetterskog, S. Disch et al., Nanoscale 8, 15571 (2016).
[4] P. Bender, S. Disch et al., J. Appl. Cryst. 55, 1613 (2022).

CPP 33.2 Wed 10:30 ZEU/LICH

Modeling artificial cells to control the local chemical environment — •Nils Göth and Joachim Dzubiella — Applied Theoretical Physics—Computational Physics, Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, 79104 Freiburg, Germany

Living cells change and respond to their environment. Synthesized artificial cells (hollow microgels) show in experiments pH-responsive behavior by a pH-dependent membrane permeability and change their pH-environment by a chemical reaction [1]. Here, we report a simple model for such artificial cells based on the feedback mechanism between permeability and pH. We introduce the model on the basis of recent experiments [1] and study the effects of experimentally tunable parameters. The model captures not only the effects observed in the experiments, but further predicts the behavior of mixtures of two different kinds of artificial cells. Thus, we provide guidance for future experiments in the field of collective behavior of artificial cells.

[1] Krehan et al., Chem 11, 102409 (2024).

CPP 33.3 Wed 10:45 ZEU/LICH

Evaporation-driven assembly of colloidal monolayers and multilayers — •Qingguang Xie[1] and Jens Harting[1,2] — [1]Helmholtz-Institut Erlangen-Nürnberg for Renewable Energy (IET-2), Forschungszentrum Jülich, Erlangen, Germany — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Drying of colloidal suspension films is a common approach to synthesize colloidal monolayers and multilayers for applications such as photovoltaics and catalysis. The fundamental understanding of the complex processes involved in film drying is essential for controlling and optimizing the deposition structure. We numerically investigate the drying dynamics of both thin and thick colloidal suspension films. For thin films, we focus on the influence of substrate and particle wettability on assembled monolayers. High substrate wettability promotes hexagonally packed monolayers, while low wettability leads to droplet formation and particle clustering. Furthermore, we reveal that higher particle wettability can mitigate the impact of substrate wettability and facilitate the formation of highly ordered monolayers. We propose theoretical models predicting the surface coverage fraction dependent on particle volume fraction, initial film thickness, particle radius, as well as substrate and particle wettability, and validate these models with simulations. In a further step, we investigate the drying of thick films with different particle-particle interactions. Weak interactions led to densely packed structures, while strong interactions led to more porous structures due to aggregation.

CPP 33.4 Wed 11:00 ZEU/LICH

Microscopic liquid marbles for force sensing using AFM — •Tomas P. Corrales[1], Constanza Rodriguez[1], Catalina Navarrete[1], Diego Cortés[2], Michael Kappl[2], and Syuji Fujii[3] — [1]Universidad Tecnica Federico Santa Maria — [2]Max-Planck-Institut für Polymerforschung, Mainz, Germany — [3]Osaka Institute of Technology, Osaka, Japan

An AFM cantilever is an exceptional tool for measuring friction and adhesion forces at the nanoscale. We have recently shown the possibility of fixing microscopic liquid droplets on the end of a tipless AFM cantilever, which was used to measure friction forces of a Teflon surface (D. Cortes et al., Physical Review Letters 135, 048203, 2025). In this new work, we have set out to extend this approach by fixing microscopic liquid marbles at the end of an AFM cantilever. Liquid marbles are prepared from hydrophobic nanoparticles of CaCO3. We first spray a mixture of water glycerol over a powder of these CaCO3 nanoparticles, which creates a collection of microscopic liquid marbles. Afterwards, we attach these droplets to a hydrophobic tipless AFM cantilever with a hydrophilic sticky point. With this system we explore liquid marble friction, adhesion and stability.

CPP 34: Focus Session: Water – from Atmosphere to Space V (joint session CPP/DY)

Time: Wednesday 11:00–12:00 Location: ZEU/0260

CPP 34.1 Wed 11:00 ZEU/0260

Scalable Machine Learning Model for Energy Decomposition Analysis in Aqueous Systems — •Thomas Kühne — CASUS/HZDR, Görlitz, Germany

Energy decomposition analysis (EDA) based on absolutely localized molecular orbitals provides detailed insights into intermolecular bonding by decomposing the total molecular binding energy into physically meaningful components. Here, we develop a neural network EDA model capable of predicting the electron delocalization energy component of water molecules, which captures the stabilization arising from charge transfer between occupied absolutely localized molecular orbitals of one molecule and the virtual orbitals of another. Exploiting

the locality assumption of the electronic structure, our model enables accurate prediction of electron delocalization energies for molecular systems far beyond the size accessible to conventional density functional theory calculations, while maintaining its accuracy. We demonstrate the applicability of our approach by modeling hydration effects in large molecular complexes, specifically in metal-organic frameworks.

CPP 34.2 Wed 11:15 ZEU/0260

Advances in absolute-scale electronic structure measurements of liquid water and aqueous solutions — •Florian Trinter — Fritz-Haber-Institut, Berlin, Germany

Recent advances in liquid-jet photoelectron spectroscopy (LJ-PES) have enabled the precise determination of absolute electronic energetics of liquid water and aqueous solutions, both in the bulk and at interfaces. By implementing refined vacuum and Fermi-level referencing procedures, rooted in condensed-matter concepts, vertical ionization energies (VIEs) and solution work functions can now be measured with high accuracy. We show that binding energy determinations near the ionization threshold are strongly influenced by quasi elastic electron scattering and indirect ionization processes. Vibrational excitation and autoionization via super-excited states lead to spectral distortions at electron kinetic energies below ~14 eV, necessitating careful data interpretation to extract intrinsic properties. Applying these methods to neat water and aqueous solutions of sodium iodide (NaI) and tetrabutylammonium iodide (TBAI), we reveal solute-specific effects: NaI primarily alters water's bulk structure, increasing the $1b_1$ binding energy with concentration, while TBAI affects surface potentials through interfacial dipole formation, leading to an apparent binding energy decrease. Additionally, we determine the work function of neat water as 4.73 ± 0.09 eV and quantify its reduction in TBAI solutions. These findings establish a framework for quantitative studies of molecular interactions and electronic-structure modifications in aqueous systems, with implications for electrochemical and interfacial science.

CPP 34.3 Wed 11:30 ZEU/0260

Liquid-vapor critical behavior of the TIP4P/2005 water model: Effects of NaCl solutes and hydrophobic confinement — •Mayank Sharma and Peter Virnau — Institute of Physics, Johannes Gutenberg University Mainz, 55128 Mainz, Germany

The liquid-vapor critical behavior of water is strongly influenced by both ionic solutes and confinement. Molecular dynamics simulations of aqueous NaCl solutions using the TIP4P/2005 water model and the Madrid-2019 ion parameters reveal a systematic increase in the liquid-vapor critical temperature and pressure with salt concentration, consistent with experimental trends. In contrast, confinement between parallel hydrophobic plates leads to a depression of the critical point. The critical temperature was determined using the Binder cumulant crossing in the NVT ensemble, based on a recently developed method originally applied to an active Brownian particle system [1]. The reliability of this approach was verified through complementary NPT simulations using histogram reweighting. We further demonstrate the pronounced sensitivity of the estimated critical point to the van der Waals cutoff distance, underscoring the importance of properly accounting for long-range interactions. The present results capture qualitative shifts in the critical point of water arising from ionic interactions and confinement, and the Binder-cumulant framework used here is readily extendable to other critical phenomena, including the putative liquid-liquid critical point of water.

[1] J.T Siebert et al., Phys. Rev. E 98, 030601 (2018).

CPP 34.4 Wed 11:45 ZEU/0260

Cooperative molecular dynamics and nuclear quantum effects in bulk water — •Margarita Russina — Helmholtz-Zentrum Berlin for Materials and Energy, Berlin, Germany

The cooperative dynamics in water remain difficult to access due to the lack of long-range order and the short lifetimes of molecular correlations. Neutron scattering is well suited to probe such phenomena on the nanoscale but has been hindered by the weak coherent signal of H2O. Using a novel neutron polarization-analysis approach, we directly measure the coherent scattering in H2O and D2O with high accuracy [1]. Beyond self-diffusion and molecular rotation, we identify a picosecond cooperative process in liquid water, likely associated with rearrangements of several neighboring molecules and the reorganization of hydrogen bonds. This process may act as a precursor to large-scale molecular transport. In the intermediate wave-vector range Q < 1 1/Å, the coherent signal in H2O is enhanced compared to the expectation for rigid, noninteracting, randomly oriented molecules. Since this Q-range corresponds to distances of several molecular spacings, our results provide evidence that intermolecular correlations in water extend beyond short-range correlations and involve more distant neighbors, giving rise to cooperative dynamical fluctuations. Such an enhancement can be rationalized by correlated preferential molecular orientations, hydrogen-bond rearrangements, and nuclear quantum effects. In contrast, D2O follows a more hydrodynamic behavior consistent with reported differences in the molecular bonding and symmetry of H2O and D2O. [1] M. Russina et al., J. Phys. Chem. Lett. (2025).

CPP 35: Glasses and Glass Transition (joint session DY/CPP)

Time: Wednesday 11:15–12:45 Location: ZEU/0118

Invited Talk CPP 35.1 Wed 11:15 ZEU/0118

Topological defects in 2D amorphous ensembles — •Peter Keim — Heinrich-Heine-Universität Düsseldorf

Topological defects are key to understand melting of crystals in two dimensions. A dilute gas of bound thus virtual pairs of dislocations cause the softening of a crystal in the vicinity of melting. If thermal energy is high enough to unbind dislocation pairs, translational order is destroyed and the crystal to melts due to the lack of shear resistance. In an amorphous solid, the concept of topology seems useless for the first glance due to the absence of order. Here, we discuss, how the definition of virtual dislocations can be generalized for a two-dimensional glass. Based on positional data of a binary colloidal monolayer we determine the fugazity of generalized virtual dislocations and measure elasticity close to the glass transition: Youngs modulus gets 16π at melting in surprisingly close analogy to Kosterlitz-Thouless-Halperin-Nelson-Young (KTHNY) - theory for melting of 2D crystals.

CPP 35.2 Wed 11:45 ZEU/0118

Glass transition and universal scaling in ultra-low crosslinked microgels — Alessandro Martinelli[1], Rajam Elancheliyan[1], Andrea Scotti[2], Alexander V. Petrunin[3], •Domenico Truzzolillo[1], and Luca Cipelletti[1,4] — [1]Laboratoire Charles Coulomb (L2C), UMR 5221 CNRS-Universitè de Montpellier, F-34095 Montpellier,France — [2]Division of Physical Chemistry, Lund University, SE-22100 Lund, Sweden — [3]Institute of Physical Chemistry, RWTH Aachen University, Landoltweg 2, 52074 Aachen,Germany — [4]Institut Universitaire de France, F-75231 Paris, France

We investigate the glassy dynamics of Ultra-Low Crosslinked (ULC) poly(N-isopropylacrylamide) (PNIPAM) microgels. The glass transition is reached by varying either the temperature (modulating microgel swelling) or the colloidal number density. Our Dynamic Light Scattering (DLS) measurements confirm that the dynamic slowdown is solely governed by the effective volume fraction (φ), with ULC microgels behaving as fragile glass formers. Small-Angle X-ray Scattering data further indicates that the center-to-center inter-microgel distance is insensitive to temperature, scaling geometrically with mass fraction, while the height of the first peak of the static structure factor decreases with increasing concentration, suggesting structural melting above glass transition. We finally we report on the striking emergence of a universal dynamic behavior for the relaxation time (τ_α) dependence on the scattering vector (q) across the entire supercooled and glass regimes, allowing the data to collapse onto a master curve, whose features will be discussed.

CPP 35.3 Wed 12:00 ZEU/0118

Strain-rate dependent rheological memory in a model glass former — •Monoj Adhikari and Jürgen Horbach — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany

We investigate the shear response of deeply supercooled liquids far below the mode coupling critical temperature of a model glass former. Our system is based on the Kob-Andersen binary Lennard-Jones mixture (KABLJM) model but incorporates polydispersity, allowing us to combine SWAP Monte Carlo (MC) with Molecular Dynamics (MD) simulations. This hybrid approach enables equilibration at temperatures far below the Mode-Coupling critical temperature, T_{MCT}, while maintaining an equation of state similar to the original binary KABLJM model. We examine the response of these equilibrated samples to shear deformation at finite temperature and strain rate. By combining MD with SWAP MC during shear, we demonstrate that states with stress far below the yield stress can be accessed, making Newtonian fluid behavior observable even at temperatures well below T_{MCT}. To characterize the Newtonian fluid states obtained from this hybrid approach, as well as the solid-like states from standard MD, we employ a strain-rate switching protocol on the steady states. When applying this protocol to the stationary states, we observe intriguing memory effects. In the transient regime, stress overshoots appear when increasing the strain rate, whereas a striking stress undershoot emerges when decreasing it, mirroring recent experimental observations in polymer glasses.

CPP 35.4 Wed 12:15 ZEU/0118

An Analytical Relation between Thermodynamics and Dynamics in a Trap-like Model of Supercooled Liquids — •Simon G. Kellers, Anshul D. S. Parmar, and Andreas Heuer — Institute of Physical Chemistry, University of Münster, Corrensstraße 28/30, 48149 Münster, Germany

Recent studies on 2D non-network glass formers, enabled by the million-fold acceleration of Swap Monte Carlo, have revealed clear deviations from Gaussian behavior in the inherent-structure (IS) density of states and linked these features to the fragile-to-strong crossover (FSC) and the emergence of a low-energy depletion regime.

Here, we establish such a connection by introducing a direct analytical relation between thermodynamic PEL statistics and dynamical properties within a trap-like description of supercooled liquids. We illustrate this relation using a binomial distribution of IS states and show that it naturally yields a characteristic trap size for polydisperse systems. This trap size reflects the effective number of degrees of freedom that collectively determine the depth and barrier of a metabasin participating in an activated relaxation event, thereby offering a physically transparent measure of cooperativity.

By combining this analytical framework with simulation data for a polydisperse 2D glass former, we obtain a coherent and quantitatively consistent landscape-based interpretation of the FSC.

[1] Andreas Heuer, J. Condens. Matter Phys. 2008, 20, 373101
[2] Anshul D. S. Parmar, Andreas Heuer, 2023 arXiv preprint arXiv:2307.10143

CPP 35.5 Wed 12:30 ZEU/0118

Single particle vs. collective diffusion dynamics in a glassforming ternary Lennard-Jones mixture — •Anna Pini and Jürgen Horbach — Institut für Theoretische Physik II: Soft Matter, Heinrich Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf

Ternary fluid mixtures exhibit a rather complicated diffusion dynamics compared to their binary counterparts. Apart from three self-diffusion coefficient, there are three interdiffusion coefficients. In this work, we study a ternary ABC Lennard-Jones mixture using molecular dynamics computer simulation. It is based on the Kob Andersen binary Lennard-Jones mixture (KABLJM) [1] to which we have added a third C component. While C-C and A-C interactions are respectively identical to A-A and A-B interactions, B-C interactions are different from those between A and B particles. We study the glassy dynamics of this system at a high density of $\rho = 1.2$ and compare it to that of the original KABLM. While the self-diffusion coefficient show a similar temperature dependence for the binary and the ternary system, the behavior of the interdiffusion coefficients in the ternary system is significantly different from that in the binary one; in particular, unlike the binary system, the Darken equation does not hold in the ternary one. [1] W. Kob and H. C. Andersen, Phys. Rev. Lett. **73**, 1376 (1994).

CPP 36: Round Table Discussion: The Future of Neutrons in France and Germany (joint session CPP/BP)

Organized by Benoit Coasne and Christine M. Papadakis.

Time: Wednesday 11:45–12:45 Location: ZEU/LICH

Discussion CPP 36.1 Wed 11:45 ZEU/LICH

Round Table: Novel Opportunities for France/Germany Cooperation in Neutron Science — •Julian Oberdisse[1], •Frank Schreiber[2], •Arnaud Desmedt[3], •Stephan Förster[4], •Jacques Jestin[5], •Pascale Launois[6], •Christian Pfleiderer[7], and •Sabrina Disch[8] — [1]Laboratoire Charles Coulomb, U Montpellier, France — [2]Institut für Angewandte Physik, Universität Tübingen, Germany — [3]Laboratoire Léon Brillouin (LLB), Gif-sur-Yvette, France, — [4]Jülich Centre for Neutron Science (JCNS), FZ Jülich, Germany — [5]Institut Laue-Langevin (ILL), Grenoble — [6]Laboratoire de Physique des Solides d'Orsay, France — [7]Heinz Maier-Leibnitz Zentrum (MLZ), Garching, German — [8]University of Duisburg-Essen, Germany

With current and upcoming major changes in European neutron science and facilities, Germany and France are expected to play a strong role. This emerging new landscape for neutron science offers opportunities to reshape and reinvent the traditionally strong bonds between our two countries – both in terms of science cooperation and technical collaboration. The hosts Julian Oberdisse and Frank Schreiber look forward to a diverse panel discussion with the directors of the French and German neutron facilities as well as the chairs of the French and German neutron associations.

CPP 37: Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics III

Time: Wednesday 15:00–16:45 Location: ZEU/LICH

Invited Talk CPP 37.1 Wed 15:00 ZEU/LICH

Predicting molecular ordering in deposited molecular films — •Denis Adrienko — Max Planck Institute for Polymer Research, Mainz, Germany

Thin films of molecular materials are commonly employed in organic light-emitting diodes, field-effect transistors, and solar cells. The morphology of these organic films is shown to depend heavily on the processing used during manufacturing, such as vapor co-deposition. However, the prediction of processing-dependent morphologies has until now posed a significant challenge, particularly in cases where self-assembly and ordering are involved. In this work, a method is developed based on coarse-graining that is capable of predicting molecular ordering in vapor-deposited films of organic materials. The method is tested on an extensive database of novel and known organic semiconductors. A good agreement between the anisotropy of the refractive indices of the simulated and experimental vapor-deposited films suggests that the method is quantitative and can predict the molecular orientations in organic films at an atomistic resolution [1]. The methodology can be readily utilized for screening materials for organic light-emitting diodes.

[1] C. Scherer, N. Kinaret, K.-H. Lin, M. N. Qaisrani, F. Post, F. May, D. Andrienko, Adv. Energy Mater., 14, 2403124, 2024

CPP 37.2 Wed 15:30 ZEU/LICH

A Universal Soft Upper Limit to the Seebeck Coefficient in Organic Thermoelectrics — •Dorothea Scheunemann[1], Zelong Li[2], Dennis Derewjanko[1], Yuqian Liu[2], Martijn Kemerink[1], and Guangzheng Zuo[2] — [1]Heidelberg University, Germany — [2]Fudan University, Shanghai, P.R. China

Organic thermoelectrics have the potential to convert waste heat into electricity by utilizing lightweight and flexible polymers. Despite over a decade of intensive research, significant progress remains limited. A key factor is the trade-off between conductivity (σ) and Seebeck coefficient (S), which dictates the extent to which the power factor ($PF = \sigma S^2$) can be optimized. Here, we combine an experimental data set for different polymers at variable doping levels to show that the S vs. σ curve is universal up to the maximum PF, followed by a material-dependent roll-off, when S and σ are normalized to their values at maximum PF. Furthermore, it is demonstrated that there is a soft upper limit for S ($\sim$200μV/K), at which the optimal power factor is achieved. Combining tight-binding and kinetic Monte-Carlo modeling, we quantitatively explain this behavior in terms of quasi-free charges moving in a renormalized density of states of Gaussian shape, where the renormalization accounts for the screened interaction with the ionized dopants. These findings suggest that the trade-off only exists at the single-material level, which subsequently gives rise to practical design rules.

CPP 37.3 Wed 15:45 ZEU/LICH

Nanoscale Dry-Processed Phosphorescent Films for Programmable Photonic Applications — •Yana Bui Thi, Sebastian Schellhammer, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics, Technische Universität Dresden

Room-temperature phosphorescence (RTP) of organic materials provides a versatile basis for applications in environmental detection, security features, and optical data storage. Many of these concepts, including programmable luminescent tags (PLTs) [1], rely on precise control of triplet states, which poses certain challenges in terms of stability and processing. While polymer matrices are commonly used to suppress non-radiative decay, their processing limitations have restricted the miniaturization and control of devices. Here, we introduce ultra-thin RTP tags that are produced entirely solvent-free and use organic materials as active layer. These nm-sized stacks exhibit higher efficiency and can be more than twenty times thinner than polymer-based structures. We characterize the

resulting activation dynamics, stability, and reusability and discuss how the processing enables improved uniformity and the possible integration with structuring techniques. These results demonstrate a path toward compact, low-energy, and precisely controllable luminescent tags for future photonic technologies.

[1] Gmelch et.al. High-Speed and Continuous-Wave Programmable Luminescent Tags Based on Exclusive Room Temperature Phosphorescence (RTP). Adv Sci. 2021 (23):e2102104.

CPP 37.4 Wed 16:00 ZEU/LICH

Probing the percolating charge transport network in organic semiconductors by noise spectroscopy — •Sebastian Klein, Priya Viji, Constantin Tormann, Clemens Göhler, and Martijn Kemerink — IMSEAM, Heidelberg University, Germany

In disordered organic semiconductors (OSCs), a suppression of shot noise is expected due to the internal charge carrier transport mechanisms, which is relevant for, e.g., their application in photodetectors. The charge transport in OSCs, which occurs by hopping between localized sites, can be described by percolation theory, from which it follows that so-called hard hops form the bottleneck that charge carriers have to overcome to progress through the device. The tunneling through one singular hard hop is a random uncorrelated poissonian process which leads to OSCs displaying shot noise. Since multiple hard hops sit in series in the charge transport path in macroscopic OSCs, it is expected that shot noise in OSC is suppressed, inversely proportional to the number of hard hops, which in turn depends on disorder, temperature and thickness of the OSC. This suppression is quantified by the Fano factor, which we directly measure by current cross-correlation noise spectroscopy. Temperature- and current-bias-dependent Fano factor measurement results are compared with kinetic Monte Carlo simulations. From the measurements and simulations, it can consistently be concluded that Fano factor measurements give direct and otherwise inaccessible insight into the internal structure as well as the disorder and correlation length of OSC.

CPP 37.5 Wed 16:15 ZEU/LICH

Charge transfer dynamics in PBDB-T blends studied by time-resolved optical spectroscopy — Beatriz Molinaro Guerra[1], Federico Cilento[2], Maria Luiza Miranda Rocco[1], and •Wibke Bronsch[2] — [1]Institute of Chemistry, Federal University of Rio de Janeiro, 21941-909, Rio de Janeiro-RJ, Brazil — [2]Elettra-Sincrotrone Trieste S.C.p.A., 34149 Basovizza, Trieste, Italy

Charge transport processes in conjugated polymers are an important key for the production of more efficient organic optoelectronic devices, such as organic solar cells. Specially, the study of electron charge transfer dynamics in excited states may help us to understand charge transport properties in these materials. We studied the ultrafast response of different blends of PBDB-T polymers with small molecules after NIR excitation. Time-resolved optical spectroscopy measurements with broad-band probe pulses performed in the T-ReX facility at Elettra reveal clear changes in the ultrafast response when comparing the results for the pure molecule films and the blends, suggesting that charges are transferred between the two components of the blend on the femto- to picosecond timescale. After exciting the HOMO-LUMO transition of the ITIC molecule, the exciton population decay time drastically reduces due to the presence of the PBDB-T polymer, while the decay constant at photon energies in the range corresponding to the PBDB-T HOMO-1-LUMO transition increases. This behavior indicates hole injections in PBDB-T after primary excitation of ITIC, as it was also discussed for PBBF:ITIC blends [1]. [1] Liu et al. Advanced Science 6, 1802103 (2019).

CPP 37.6 Wed 16:30 ZEU/LICH

Analysis of Charge Carrier Dynamics in Organic Solar Cells via Optical Impedance Spectroscopy — •Elias Wassmer, Jan Phillip Ott, Brian Hinz, Clemens Göhler, and Martijn Kemerink — IMSEAM, Heidelberg University, Germany

Understanding the complex dynamics of charge carriers in organic solar cells (OSCs) is essential to identify the mechanisms that lead to voltage, current and fill factor losses. In this work, we investigate these dynamics by combining conventional electrical impedance spectroscopy (EIS) with the newly implemented optical impedance spectroscopy (OIS). In OIS, in addition to a constant background illumination, a small alternating light signal is applied to investigate the photogenerated charge carriers under quasi-steady-state conditions. The results of both EIS and OIS of PM6:Y6 OSCs across a range of operating conditions are used to compare the two methods and allow us to track changes during device degradation. To interpret the measured impedance spectra, two established models are applied: an equivalent-circuit model, which maps the behaviour of the OSC onto a network of resistances and capacitances, and a rate-equation model that describes carrier generation, recombination and extraction through differential equations. Comparing these modelling approaches allows us to evaluate how well the charge-carrier dynamics are captured by each model and how this relates to the physical processes inside the OSCs. Our results show that the equivalent-circuit model is insufficient for describing OIS, indicating that a more physically motivated rate-equation model is needed to reproduce photogenerated carrier dynamics.

CPP 38: Biopolymers, Biomaterials and Bioinspired Functional Materials I (joint session CPP/BP)

Time: Wednesday 15:00–16:45 Location: ZEU/0255

Invited Talk CPP 38.1 Wed 15:00 ZEU/0255

Engineering, processing and application of recombinant spider silk proteins — •Thomas Scheibel — Universität Bayreuth, Lehrstuhl Biomaterialien, Prof.-Rüdiger-Bormann-Str. 1, 95440 Bayreuth

Proteins reflect one fascinating class of natural polymers with huge potential for technical as well as biomedical applications. One well-known example is spider silk, a protein fiber with excellent mechanical properties such as strength and toughness. We have developed biotechnological methods using bacteria as production hosts which produce structural proteins mimicking the natural ones. We employ silk proteins in application forms such as fibers, hydrogels, particles or films with tailored properties, which can be employed especially for biomaterials applications. In case of implants or catheters cell adhesion plays a crucial role for the overall function of the to-be-used material. To change the properties of in-use polymers and to adopt their biocompatibility, we established coatings based on engineered spider silk proteins. Spider silk hydrogels can be employed as new bioinks for biofabrication. Their elastic behavior dominates over the viscous behavior over the whole angular frequency range with a low viscosity flow behavior and good form stability. Cell-loaded spider silk constructs can be easily printed without the need of additional cross-linkers or thickeners for mechanical stabilization. Our bio-inspired approach serves as a basis for new materials in a variety of medical, biological, or technical applications.

CPP 38.2 Wed 15:30 ZEU/0255

Inferring Structure-Property Relationships with Artificial Intelligence: A Lignin Case Study — •Matthias Stosiek and Patrick Rinke — Department of Physics, Atomistic Modelling Center, Munich Data Science Institute, Technical University of Munich

The potential of lignin as an abundant, underutilized biopolymer is increasingly being realized. A key challenge for the targeted production of lignins remains the poorly understood relation between lignin properties and its complex structure. Artificial intelligence (AI) methods could reveal such structure-function relationships but remain elusive in biomaterials research.

95 structurally diverse lignins are extracted from birch wood combining the Aqua Solv Omni (AqSO) biorefinery process and AI-guided data acquisition [1, 2]. Each lignin sample is characterized with 2D NMR spectroscopy and complemented with measurements of key lignin properties such as antioxidant activity.

To establish structure-function relationships, we correlate regions of the NMR spectra with corresponding property measurements. With a feature importance analysis, we identify structural relevant features for each property and provide a chemical interpretation. For instance, we find that more β-O-4 bonds lead to lower surface tension in water indicating a more linear lignin structure. Our structure-inference approach is designed to be general and applicable to a wide range of materials and characterization data.

[1] D. Diment et al., ChemSusChem, e202401711 (2024). [2] M. Alopaeus, M. Stosiek et al., Sci Data 12, 996 (2025).

CPP 38.3 Wed 15:45 ZEU/0255

A minimalist view on biopolymer phase separation and aging — •Jasper Michels — Max Planck Institute for Polymer Research, Mainz, Germany

Phase separation of proteins is a ubiquitous process by which cells regulate biological processes. In aberrant cases, such as encountered in neurodegeneration, initially liquid condensates age to become more solid-like. Understanding the interplay between phase separation and aging seems essential in the development of new therapeutic strategies. We apply minimal models that aim to capture the essence of biological transitions in terms of driving forces and thermodynamics. Models discriminating between mono- and multivalent directed association on the one hand and non-specific interactions on the other appear surprisingly versatile in reproducing and predicting biopolymer phase behavior, while at the same time providing essential mechanistic insight. We will review our efforts, combining theory with experiments and demonstrating how relatively simple descriptions can (re)produce complex multi-component phase behavior. We will also present a dynamic version of the model, which provides for a thermodynamically fully consistent and intuitive description of the experimentally observed

changes in viscoelasticity during aging. Our calculations explain how the stickiness of the proteins changes with time and concentration and how the coupling between association and solvation determines condensate viscoelasticity.

CPP 38.4 Wed 16:00 ZEU/0255

Cellulose-colloid hybrid materials for refractive index tuning — •Stephan V. Roth — Deutsches Elektronen-Synchrotron DESY, Hamburg, Sweden — KTH Royal Institute of Technology, Stockholm, Sweden

Cellulose nanofibrils (CNF) with tailored (negative) surface charge are ideal for stable, nanoporous, structure-guiding network for thin film composite materials. Colloid materials offer the possibility for tunable structural colors, templates for metamaterials, and refractive index tuning. Here, core-shell-colloids with a hydrophobic core and positively charged, hydrophilic shell are used as additive in CNF thin films to tune their refractive index. The imbibition and self-assembly of the colloids as a function of colloid diameter in the CNF network was quantified, with colloids smaller than the pores in the CNF network penetrating into the thin film. Subsequent heat treatment allows for nanoscale composite formation on the level of the ~ 10 nm sized CNF bundles, while humidity treatment homogenizes the colloid distribution. Furthermore, the influence of the colloid size on the CNF structure inside the thin film was investigated and related to the mechanical properties of the colloid-CNF composite.

CPP 38.5 Wed 16:15 ZEU/0255

A universal material basis for biocompatible printed electrolytes in Organic Electrochemical Transistors (OECTs) — •Moritz Flemming, Paul Zechel, Rakesh Nair, Laura Teuerle, Hans Kleemann, and Karl Leo — Institute of Applied Physics, Technische Universität Dresden

Organic Electrochemical Transistors (OECTs) stand out for their interplay between ionic and electronic conduction, making them ideal analogues to biological synapses for neuromorphic computing or biosensors. Furthermore, they can be printed into integrated circuits on flexible substrates, allowing for low-cost and high throughput fabrication of full electronic systems. However, most OECT electrolytes for integrated circuits still lack biocompatibility and suffer from rheology-related printing challenges. This talk presents a novel material basis that can be combined with an ionic liquid to fabricate a biocompatible electrolyte for OECTs. It allows rheological adjustments to enable the use of electrolyte in both inkjet and screen printing. Furthermore, the electrolyte is UV-curable, enabling it to transition into solid-state structures after printing. Extended ink and device lifetimes for screen-printed structures enable the fabrication of state-of-the-art OECTs that can operate in ambient air more than 30 days after fabrication. Ultimately, a fully biocompatible and screen-printed OECT on a leaf substrate is demonstrated.

CPP 38.6 Wed 16:30 ZEU/0255

Nonequilibrium dynamics of the helix-coil transition in polyalanine — •Maximilian Conradi[1], Fabio Müller[1], Suman Majumder[2], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, IPF 231101, 04081 Leipzig, Germany — [2]Amity Institute of Applied Sciences, Amity University Uttar Pradesh, Noida 201313, India

As a continuation of our previous work, the nonequilibrium pathways of the collapse of the helix-forming biopolymer polyalanine are investigated in an explicit solvent. To this end, the full time evolution of the helix-coil transition is simulated using molecular dynamics simulations. We compare the phenomenology of the transition between the two studies and investigate the dynamics.

CPP 39: French-German Session: Nanomaterials, Composites and Hybrids I

Time: Wednesday 15:00–16:45 Location: ZEU/0260

Invited Talk CPP 39.1 Wed 15:00 ZEU/0260

A polarizable model for atomistic simulations of metals and graphitic material/ liquid interfaces — Krishan Kanhaiya[1], Hendrik Heinz[2], and •Marialore Sulpizi[1] — [1]Department of Physics and Astronomy, Ruhr-University Bochum, Universitätsstraße 150, 44801 Bochum, Germany — [2]Department of Chemical and Biological Engineering, University of Colorado at Boulder, Boulder, CO 80301

Polarization significantly affects the interaction and adsorption energy of molecules on metal surfaces. The ability to describe at a metal surface the classical "image charge" potential is a direct result of its polarizability, which needs to be modelled correctly to accurately simulate interfacial phenomena e.g. in electrochemistry or catalysis. Recently, we have introduced a polarizable model for metals which permits to describe also electrified interfaces. Here we extend the idea to graphitic material introducing flexible dummy electrons to represent the polarizable π-electron cloud. The model accurately predicts surface and hydration energy, water contact angle as well as experimental and DFT data on molecular adsorption on surfaces. A considerable improvement is obtained in the prediction of water-graphite interfacial friction, which is obtained at the level of electronic structure calculations.

CPP 39.2 Wed 15:30 ZEU/0260

Lamellar Domain Spacing of Copolymers with Nonlinear Block Architectures — Andrzej Grzyb[1], Jarosław S. Kłos[2], Aykut Erbaş[3], Michael Lang[4], and •Jarosław Paturej[1] — [1]Institute of Physics, University of Silesia, Katowice, Poland — [2]Faculty of Physics, A. Mickiewicz University, Poznań, Poland — [3]UNAM, Bilkent University, Ankara, Turkey — [4]Leibniz-Institut für Polymerforschung Dresden e.V., Germany

Topological modification of block copolymer (BCP) conformations offers a promising approach for developing self-assembled periodic nanostructured materials with smaller domain sizes, which are essential for a range of technological applications. Cyclic polymers, with their inherently more compact conformations, present an effective strategy for achieving this miniaturization. In this work, through a combination of analytical theory and coarse-grained molecular dynamics simulations, we establish a relationship between different nonlinear topologies and the corresponding domain size of lamella-forming BCPs. Our investigations includes BCP architectures with one or two cyclic segments such as tadpoles, diblock and triblock 8-shaped polymers, and diblock nonconcatenated and concatenated rings. We demonstrate that the primary reduction in lamellar domain size is driven by the more compact arrangement of monomers in the cyclic architectures, with an additional contribution from the nonconcatenation of cyclic segments. This is corroborated by theoretical predictions for both domain size reduction and BCP conformations across different architectures.

CPP 39.3 Wed 15:45 ZEU/0260

Self-Healing Composite Structures for Aerospace Applications — •Merve Ozkutlu Demirel[1], Eray Kostur[1,2], Yigitalp Okumus[1], Bilal Altin[1], Melih Seckin[1], and Yahya Oz[1] — [1]Turkish Aerospace, R&D and Advanced Technologies Directorate, 06980 Ankara, Turkiye — [2]Cukurova University, Department of Mechanical Engineering, 01330 Adana, Turkiye

Self-healing composite structures offer a promising solution for enhancing durability and reducing maintenance costs in aerospace platforms. In this study, a self-healing mechanism based on a microvascular channel network was developed. Composite laminates were fabricated using carbon fabric and epoxy resin. Polyamide monofilaments with a diameter of 450 um were integrated into a hand lay-up process by placing them between composite layers. After curing, these fibers were removed to create hollow channels. Various channel configurations were manufactured and evaluated through bending tests. 5-Ethylidene-2-norbornene was selected as healing agent because its operating temperature range is similar to flight temperature conditions. The healing agent was injected into the channels, while the Grubbs catalyst that would start the polymerization reaction was uniformly dispersed within the polymer matrix. Upon crack formation, the healing agent is expected to flow into the damaged region and polymerize upon contact with the catalyst, thereby filling the crack. Compact tension tests were performed to analyse the healing performance. The results demonstrated that the microvascular channel approach exhibits strong potential for aerospace applications.

CPP 39.4 Wed 16:00 ZEU/0260

Increasing the Mechanical Stability of Carbon Nanomembranes Using a Holey Carbon Interlayer — •Luzie Lina Heinrichs, Zhen Yao, Yang Yang, and Armin Gölzhäuser — Faculty of Physics, Bielefeld University, 33615 Bielefeld, Germany

Carbon nanomembranes (CNMs) are atomically thin, with sub-nanometre pores that enable strong gas selectivity and fast, efficient water transport. However, their limited mechanical robustness has constrained their integration into practical filtration technologies.

In this study, we introduce a reinforced CNM architecture that incorporates an intermediate holey support layer. We fabricate and compare single-layer, double-layer, and holey film reinforced composite CNMs. Water permeation measurements using a cup test, combined with nanoindentation characterisation, show that the reinforced architecture preserves high water permeability while markedly improving mechanical stability. The effective Young's modulus reaches ~25 GPa, approximately five times higher than that of an unreinforced double layer.

By combining mechanical robustness with efficient single-file water transport and precise selectivity, the holey-layer-reinforced CNMs provide a promising route toward real-world applications, especially in seawater desalination.

CPP 39.5 Wed 16:15 ZEU/0260

Particle distribution and thermoresponsive properties of PNIPAM brush/gold nanoparticle composite films — •Elias Hallenbach, Marvin Glock, Hayden Robertson, and Regine von Klitzing — TU Darmstadt, Institute for Condensed Matter Physics, 64289 Darmstadt, Germany

Metal/polymer nanocomposites are versatile hybrid materials and find use in many fields such as photonics, biomedical engineering and catalysis. A promising realization of this type of hybrid material is the controlled self-assembly of gold nanoparticles (AuNPs) inside a polymer brush, which induces color changes upon exposure to environmental changes, enabling sensor applications. Polymer brushes can serve as a matrix for the immobilization of AuNPs. Particle uptake into the brush matrix is affected by parameters such as thickness, particle size and grafting density [1]. Nanoparticle uptake has proven to be highest at intermediate grafting densities [2]. In the present study thermoresponsive Poly(*N*-Isopropylacrylamide) brushes with varying grafting densities were synthesized directly from a silicon substrate. Nanocomposite materials were fabricated by dip-coating of polymer brushes into an AuNP suspension. Characterization of nanocomposites was performed by (in situ) spectroscopic ellipsometry, atomic force microscopy and (in situ) X-ray reflectometry. The relation between particle distribution and temperature-induced structural changes will be discussed.

[1] S. Christau et al., *Polymers* **2014**, *6*, 1877-1896.
[2] R.R. Bhat, J. Genzer, *Appl. Surf. Sci.* **2006**, *252*, 2549-2554.

CPP 39.6 Wed 16:30 ZEU/0260

Morphology-controlled electrical and thermal conductivity of filled diblock copolymers: effect of filler shape. — •Alexander Chervanyov — University of Münster, Münster, Germany

We investigate the electrical and thermal conductivity of an electrically insulating diblock copolymer (DBC) matrix filled with conductive cylindrical and spherical nanofillers modeling carbon nanotubes (CNTs) and carbon black (CB), respectively. The composite transport properties are examined as functions of the underlying DBC morphology, the selective affinities of CNTs and CB for the dissimilar DBC blocks, and inter-filler interactions that determine the positional and, for CNTs, orientational correlations. Using a combined phase-field description of the DBC host and Monte Carlo simulations of anisotropic CNT fillers, we show that the localization and alignment of CNTs within the microphase-separated domains are highly sensitive to the above parameters. The simulated CNT and CB network structures are used to compute the electrical and thermal response of the composite. We quantitatively elucidate how the morphological transitions in the DBC correlate with structural rearrangements of the filler networks. Furthermore, we demonstrate that both the order-disorder transition and the order-order transitions between distinct DBC morphologies lead to pronounced changes in composite conductivity, driven by morphology-induced restructuring and alignment of the conductive pathways formed by CNT and CB.

Financial support of Deutsche Forschungsgemeinschaft (DFG) through Grant No. CH 845/2-3, is gratefully acknowledged.

CPP 40: Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics IV

Time: Wednesday 17:00–18:30 Location: ZEU/LICH

CPP 40.1 Wed 17:00 ZEU/LICH

Morphological Disorder Boosts Charge Separation in Single-Component OPDs — •Michel Panhans[1], Jakob Wolansky[2,3], Karl Leo[2], Johannes Benduhn[2,3], and Frank Ortmann[1] — [1]TUM School of Natural Sciences and Atomistic Modeling Center, Munich Data Science Institute, Technische Universität München, 85748 Garching b. München, Germany — [2]Dresden Integrated Center for Applied Physics and Photonic Materials, Technische Universität Dresden, 01069 Dresden, Germany — [3]DZA, Görlitz, Germany

Single-component organic photodetectors (OPDs) provide a simplified alternative to donor-acceptor heterojunctions, yet their operation mechanisms remain theoretically underexplored. We investigate the molecular origin of charge generation in vapor-deposited DCV2-5T by modeling the excitonic density of states with an effective exciton Hamiltonian that incorporates electronic coupling, Coulomb interaction, and structural disorder. Disorder is introduced through lateral shifts between π-stacked molecules, which notably modulates electronic and excitonic couplings. Simulations show that intermediate disorder reproduces the experimental external quantum efficiency, while strong disorder enhances hybridization between excitonic states. This hybridization enables exciton delocalization via a superexchange-like mechanism, increasing the probability of charge separation. Counterintuitively, disordered domains exhibit stronger coupling than crystalline ones, suggesting that reduced structural order can facilitate charge generation. These insights highlight morphology-dependent excitonic interactions as a design principle for self-driven OPDs.

CPP 40.2 Wed 17:15 ZEU/LICH

Limiting factors to free charge generation in low-bandgap organic blends for photovoltaic applications and beyond — •Manasi Pranav[1], Atul Shukla[1,2], and Dieter Neher[1] — [1]University of Potsdam, Potsdam, Germany — [2]University of Queensland, Brisbane, Australia

Despite possessing similar theoretical limits, state-of-the-art organic solar cells outshine low-bandgap organic blends (absorption edge beyond 1000 nm) in their exciton harvesting efficiency. An understanding of these free charge generation mechanisms is needed to tap into the potential of such low-bandgap non-fullerene acceptors (NFAs) for photovoltaic and photodetector applications. To this end, we probe the pathways of exciton dissociation and charge-transfer state separation in multiple D:NFA systems with varying absorption edges, and varying extents of energy-transfer or charge-transfer prior to free charge generation. This is done by combining transient and steady-state optoelectronic techniques, to resolve the losses incurred between photon absorption and carrier extraction. For some of these systems, namely in blends using Y6 derivatives with extended pi-conjugation, we find that the kinetic competition between geminate charge-transfer state decay and its separation is a major limiting role in the overall photon harvesting capability of the devices. As part of ongoing work, these investigations aim to reveal the underlying geminate loss pathways, which limit overall internal quantum efficiency of the blends and, in turn, limit the figures of merit of the resulting devices.

CPP 40.3 Wed 17:30 ZEU/LICH

Consistency of Electron-Vibrational Coupling Across Methods? A Comparative Study — •Maximilian F. X. Dorfner, Konrand Merkel, and Frank Ortmann — Department of Chemistry, TUM School of Natural Sciences, and Atomistic Modeling Center, Munich Data Science Institute, Technical University of Munich, München, Germany

Characterizing electron-vibrational interaction in materials is a non-trivial theoretical task, owing to the differing definitions of coupling constants and the variety of available methods for computing these. This diversity naturally raises questions about the consistency and reliability of the methods used and their interrelation.

To address this issue, this contribution presents a systematic comparison of electron-vibrational coupling calculations. We summarize our findings on the relationship between density functional theory approaches and quasi-particle methods [1], study the influence of different exchange and correlation functionals, and investigate the impact of various ab initio methodologies [2] on the resulting electron-vibrational coupling constants.

Our findings provide guidelines and data for validating methodologies and estimating theoretical errors in coupling constant calculations.

[1] M.F.X. Dorfner and F. Ortmann, J. Chem. Theory Comput. 2025, 21, 5, 2371-2385; [2] K. Merkel, M.F.X. Dorfner and F. Ortmann, J. Phys. Mater. 8 045014

CPP 40.4 Wed 17:45 ZEU/LICH

Enhanced Photo-multiplication Effect through Synergistic Hole Blocking and Traps Engineering in OPDs — •Awais Sarwar[1], Louis Conrad Winkler[1,2], Karl Leo[1], and Johannes Benduhn[1,2] — [1]IAPP, TU Dresden, Germany — [2]DZA, Görlitz, Germany

Photomultiplication-type organic photodetectors (PM-OPDs) are highly effective for detecting weak light. However, they often face a significant trade-off: high gain usually results in excessive noise and slow response times. To overcome these limitations, we introduce a vacuum-deposited broadband photodetector architecture that utilizes the synergistic integration of hole-blocking layers and precise traps engineering. By strategically controlling the charge injection barriers and trap distribution, this design effectively separates the gain mechanism from the noise floor. The resulting device achieves a peak external quantum efficiency (EQE) exceeding 1100 per cent, while maintaining a specific detectivity of 4.4*10e12 Jones at a bias of -2 V. Unlike slow trap-dominated systems, our optimised architecture keeps a cutoff above 25 kHz. Vacuum-deposited PM-OPDs offer high sensitivity and fast response, ideal for real-time sensing.

CPP 40.5 Wed 18:00 ZEU/LICH

Wavelength-dependent charge carrier extraction of organic solar cells under operational conditions — •Lara Bartnick, Martijn Kemerink, and Clemens Göhler — IMSEAM, Heidelberg University, Germany

Organic solar cells (OSCs) have recently achieved power-conversion efficiencies of about 20%, making them increasingly promising for renewable energy ap-

plications despite still falling behind silicon photovoltaics. To understand the mechanisms that limit their performance, highly sensitive external quantum efficiency (EQE) measurements are essential, as they show how efficiently photons of different energies generate extractable charge carriers across the UV- to near-infrared spectrum.

We have measured the EQE of current standard PM6:Y6 OSCs under different initial conditions including bias voltage in both reverse and forward direction, bias illumination, and temperature, to investigate how open-circuit voltage- and fill-factor losses can be attributed to wavelength-dependent charge carrier generation efficiencies. These measurements reveal that the spectral shape of the EQE is highly sensitive to biasing conditions. By relating the voltage dependent EQE to collection fields, we have been able to identify charge carrier extraction losses under typical working conditions, which are dependent on the incident photon energy. These findings, as well as wavelength- and voltage-dependent exciton generation and recombination rates, contribute to understanding the loss mechanisms and charge extraction behaviour of OSCs.

CPP 40.6 Wed 18:15 ZEU/LICH

Current Generation in Photomultiplication-type Organic Photodetectors — •Louis Conrad Winkler[1,2], Jonas Kublitski[1,3], Awais Sarwar[1], Hrisheekesh Thachoth Chandran[1], Wolfgang Tress[4], Urs Aeberhard[5], Karl Leo[1], and Johannes Benduhn[1,2] — [1]IAPP, TU Dresden, Germany — [2]DZA, Görlitz, Germany — [3]Departamento de Fisica, UTFPR, Curitiba, Brazil — [4]ZHAW, Winterthur, Switzerland — [5]FLUXiM, Winterthur, Switzerland

Organic photodetectors (OPDs) utilizing intrinsic gain promise enhanced performance in regard to faint light detection. While this gain mechanism boosts the external quantum efficiency (EQE), the associated noise often negates the net improvement of the specific detectivity D*. Nonetheless, the simplified readout circuitry and associated cost savings hold high potential for the market. Crucially, the origin of this photomultiplication (PM) effect is currently attributed to tunnel injection of charge carriers, driven by internal band bending due to trapped charge carriers. Here, we challenge this prevailing tunnel injection model based on comprehensive experimental evidence. We propose an alternative mechanism that offers a unified explanation for the gain observed across diode-like OPD architectures and validate it by drift-diffusion simulations. This model successfully provides general predictive capabilities regarding the magnitude and dependencies of the photocurrent gain. We rigorously tested this proposed mechanism across 29 diverse material systems, including both vacuum-processed and solution-processed devices.

CPP 41: Biopolymers, Biomaterials and Bioinspired Functional Materials II (joint session CPP/BP)

Time: Wednesday 17:00–18:45 Location: ZEU/0255

CPP 41.1 Wed 17:00 ZEU/0255

Coarse-grained simulations of network-forming DNA nanostructures — •Takahiro Yokoyama[1,2] and Arash Nikoubashman[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany

DNA nanotechnology offers exceptional nanoscale designability through precise control of DNA sequences. These individual DNA strands can form predetermined building blocks, which then hierarchically assemble into super-structures such as nanotubes, nanocapsules, or nanostars. The latter can assemble further into (percolated) networks, where sequence-level design enables systematic control of the rheological and mechanical network properties. This multi-scale self-assembly can lead to cascading effects, where even a single unpaired nucleotide on the building block level can act as a highly flexible hinge that dramatically alters the network mechanics. To understand how such variations on the nucleotide-scale affect the network properties, we designed a series of DNA networks by systematically altering the arm number and junction flexibility of the star-shaped building blocks using coarse-grained molecular simulations of the oxDNA model. Our study revealed that the bulk modulus of the network decreased with increasing number of DNA arms; this counter-intuitive behavior stems from the addition of flexible junctions on the single-star level, which preferentially absorb deformation and soften the overall network. This result highlights the importance of precise nanoscopic design on the order of one nucleotide to obtain optimal network properties.

CPP 41.2 Wed 17:15 ZEU/0255

Characterizing interactions between glycoproteins and RNA at the lipid membrane interface — •Horacio V. Guzman[1] and Viviana Monje[2] — [1]Biophysics & Intelligent Matter Lab, Material Science Institute of Barcelona, CSIC, Spain — [2]Department of Chemical and Biological Engineering, State University of New York at Buffalo, 308 Furnas Hall, Buffalo, USA

Biological membrane interfaces interacting with proteins, nucleic acids, and glycans are integral to many cellular processes. The interplay between membrane lipids and biopolymers is highly sensitive to their flexibility grade, secondary structure, and electrostatics. Consequently, the cell membrane interface experiences changes in local lipid distribution and fluctuation in local properties. Projecting biophysical and structural membrane and biopolymer properties onto a two-dimensional plane simplifies the quantification of molecular signatures by reducing the dimensional space and identifying relevant entropic and short-range interactions at the interface of interest, as well as, characterizing interaction patterns and spatial correlations of complex lipid bilayers as they interact with biopolymers. We compare lipid-lipid interaction patterns in membrane-only systems to the corresponding systems containing small proteins and RNA fragments, respectively. These analyses quantify the effect of peripheral biopolymers on local lipid composition, structure, packing, deformation ratio of the biopolymer, and surface topology of the membrane upon adsorption. Such characterization is crucial for starting with the next-generation rational design of lipid vesicles and lipid-coated RNA drug delivery systems.

CPP 41.3 Wed 17:30 ZEU/0255

Nanoscale characterization of piezoelectric nanofibers blended with Salmon Gelatin — •Martín Chavarría-Vidal[1], Dragica Bezjak[2], María Saavedra-Fredes[1], Benjamín Schleyer-Thiers[1], Ilka Hermes[3], and Tomás P. Corrales[1] — [1]Universidad Técnica Federico Santa María, Valparaíso, Chile — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [3]Leibniz Institute of Polymer Research, Dresden, Germany

We electrospin salmon gelatin (SG) mixed in a polyvinyl alcohol (PVA) matrix containing chitosan (Ch). Furthermore, we used a coaxial electrospinning approach to blend these nanofibers together with polyvinylidene fluoride (PVDF). Such biomaterials could lead to the potential development of biocompatible and piezoelectric heart patches. After electrospinning our polymers, we observe by SEM two size distributions. Mechanical characterization of the large nanofibers obtained by AFM reveals two Youngs moduli peaks, centered at 1.77 GPa and 209 MPa. Small nanofibers also show a two component mechanical moduli distribution with peaks at 565 MPa and 1.33 GPa (10.1016/j.bbadva.2025.100168). EDS shows that both distributions contain Fluor. However, complimentary PFM measurements indicate that large nanofibers have a piezoelectric response comparable to pure electrospun PVDF, while the small ones do not exhibit such response. These measurements lead us to believe that the large nanofibers are mainly β-phase PVDF, while the smaller ones are composed of PVA/SG/Ch with α-phase PVDF (10.1177/15589250221125437).

CPP 41.4 Wed 17:45 ZEU/0255

Structural investigations using in situ SAXS on flexible bio-based vitrimeric carbon nanocomposites — •Sarathlal Koyiloth Vayalil[1,2], Vaishnav B[2], Viranchika Bijalwan[2], Sravendra Rana[2], and Ajay Gupta[2] — [1]Deutsches Elektronen Synchrotron DESY, Hamburg, Germany — [2]Applied Science Cluster, UPES, Dehradun, India

In this work, in situ small- and ultra-small-angle X-ray scattering has been employed to investigate the real-time structural evolution of 3D-printed vitrimeric thiol-acrylate photopolymers and their carbon-based nanocomposites designed for healable strain-sensing and soft-robotic applications. Flexible bio-acrylate based vitrimers reinforced with graphene/CNT fillers at varying concentrations are examined to elucidate temperature-dependent phase segregation and enable direct visualization of nano- and microscale filler morphologies, their spatial distribution, and their evolution across key thermal transitions (Tg and Tv of the polymer matrix). The effects of the stress/strain and cyclic-thermal cycles on the filler aggregates affecting the composites conductivity in carbon-filled samples are also evaluated. These insights into nano- and microscale morphology, reinforcement, and conductive behavior help us understand the dynamic structure-property relationships governing vitrimer-based conductive networks

CPP 41.5 Wed 18:00 ZEU/0255

Nanomechanical testing of suspended single nanofibers and humidity-induced glass transition — •Benjamin Schleyer-Thiers[1], Diego Benavente[2], Yusser Olguin[2,3], and Tomas P. Corrales[1,3] — [1]Physics department of Universidad Tecnica Federico Santa Maria, Valparaiso, Chile — [2]Technological and Scientific Center (CCTVal), Valparaiso, Chile — [3]Biotechnology Center Daniel Alkalay Lowitt

In this work we will study the interaction of water molecules with polymeric nanofibers made from hygroscopic biopolymers and contrast them in environ-

ments with variable relative humidity. For this, we will suspend single nanofibers over micropatterns etched on silicon. In this suspended configuration, we shall perform three-point bending tests utilizing the environmental Atomic Force Microscope (AFM) and detect bending forces of the nanofiber, at different relative humidities. As bending tests are performed over the suspended nanofiber, the position-dependent stiffness can be plotted to find its mechanical modulus through bending models. The stiffness of single nanofibers drops with the increase in relative humidity, hinting a glass transition induced by this environmental condition. To test this behavior, we attempt to perform fracture experiments on a micro structured grid made by photolithography.

CPP 41.6 Wed 18:15 ZEU/0255

Probing light-induced drug release to lipid monolayers — •Ipsita Pani, Michael Hardt, and Björn Braunschweig — Institute of Physical Chemistry, University of Münster, Corrensstraße 28-30, Münster 48149, Germany

Light-induced drug release using photoresponsive nanocarriers is increasingly explored for targeted therapeutic applications. While most studies characterize release in bulk aqueous environments, drug release across aqueous-organic interfaces is equally important, as these interfaces represent the entry point into cells. We recently demonstrated light-induced drug release to air-water interface.[1] In cancer therapeutics, passive diffusion of anticancer drugs across lipid membranes is a key transport mechanism, yet direct quantitative data on drug-lipid interactions and their effect on release remain limited. Here, using arylazopyrazole photosurfactant nanocarriers and doxorubicin as a representative anticancer drug, we investigate how interfacial lipid composition governs light-induced drug release. By combining Langmuir monolayers with interface-specific vibrational sum frequency generation (SFG) spectroscopy, we quantitatively estimate drug release at lipid-adsorbed interfaces as a model membrane. To systematically probe headgroup effects, we employ four dimyristoyl lipids-DMPC, DMPG, DMPS, and DMPE which share identical acyl chains but differ in charge and polarity. These results elucidate how lipid-drug interactions modulate release efficiencies at membrane-like interfaces, providing insights key to the design of photoresponsive nanocarriers for targeted drug delivery. [1] Pani et al. Chem. Sci., 2024, 15, 18865-18871.

CPP 41.7 Wed 18:30 ZEU/0255

Hetero-aggregation of microplastic particles — Thomas Witzmann[1], Anja F. R. M. Ramsperger[2], Hao Liu[2], Yifan Lu[3], Holger Schmalz[2], Lucas Kurzweg[4], Tom C. D. Börner[4], Kathrin Harre[4], Andreas Greiner[2], Christian Laforsch[2], Holger Kress[2], Christina Bogner[3], Stephan Geckle[2], Andreas Fery[1], and •Günter K. Auernhammer[1] — [1]Leibniz-Institut für Polymerforschung Dresden, Germany — [2]Universität Bayreuth, Germany — [3]Universität zu Köln, Germany — [4]Hochschule für Technik und Wirtschaft Dresden, Dresden

Microplastic particles (MPP) in the environment are surrounded by a layer known as an 'eco-corona'. This is made up of natural organic matter (NOM), such as biomolecules, humic substances, and other natural molecules. NOM substantially alters the surface properties of MP particles, thereby influencing their interaction with other surfaces in an aqueous environment and their aggregation behaviour. We studied the interactions of eco-corona-covered MP particles on the nanoscale using colloidal probe-AFM. Measurements were performed at different ionic concentrations to mimic changing environmental conditions. We found that the eco-corona can pull on the silica colloidal probe via polymer bridging. This mechanism leads to aggregation and, consequently, sedimentation in the environment. By comparing our AFM results with experiments and simulations at different length scales, we consistently found that this type of heteroaggregation is conducive to stable aggregate formation and retains MPPs in sediments.

CPP 42: French-German Session: Nanomaterials, Composites and Hybrids II

Time: Wednesday 17:00–18:45 Location: ZEU/0260

Invited Talk CPP 42.1 Wed 17:00 ZEU/0260

Mesopores filled with (poly)ionic liquids: phase transitions under confinement, and structure seen by SAXS and SANS — •Julian Oberdisse and Anne-Caroline Genix — Laboratoire Charles Coulomb, U Montpellier France

Understanding the molecular structure of mesoporous solid ionic systems is crucial for optimizing macroscopic properties, in particular ionic transport for energy applications, as well as mechanical flexibility. These systems can be synthesized efficiently under "one-pot" conditions, which rely on mesopore formation through microphase separation of templating ionic liquids.

In the present study, the phase transitions of the embedded ionic liquid have been studied by wide-angle scattering, QENS, DSC, and BDS, as a function of confinement. Then, poly(ionic liquid)s have been added in order to incorporate both connectivity and modify mechanical strength. We report on the structural analysis of ionic liquid and poly(ionic liquid) embedded in ionosilica matrices, employing a combination of small-angle scattering of neutrons and X-rays, isotopic substitution, and physico-chemical solvent-based extraction methods. Data analysis is based on molecular modelling with an original, quantitative comparison of the scattering curves under different contrasts. In agreement with NMR, it is shown that these mesoporous systems have an unexpected molecular structure, with the ionic liquid counterions penetrating the ionosilica matrix surrounding the mesopores. The poly(ionic liquid) forms patches decorating the pore walls, with tunable conformation sensitive to solvent conditions.

CPP 42.2 Wed 17:30 ZEU/0260

Plasmonic core-shell microgels: The role of the core size — •Déborah Feller[1,2], Julian Oberdisse[3], Sylvain Prévost[4], and Matthias Karg[1] — [1]Physical Chemistry of Functional Polymers, Martin Luther University Halle-Wittenberg, Halle (Saale), Germany — [2]Physical Chemistry: Colloids and Nanooptics, Heinrich Heine University Düsseldorf, Düsseldorf, Germany — [3]Laboratoire Charles Coulomb (L2C), Université de Montpellier, CNRS, Montpellier, France — [4]Large Scale Structures, Institut Laue-Langevin, Grenoble, France

Gold-poly-N-isopropylacrylamide (Au PNIPAM) core-shell microgels are interesting due to the localized surface plasmon resonance (LSPR) of the cores. The LSPR position strongly depends on the core size. Compared to other core-shell microgels, Au cores can be precisely overgrown in the shell in situ. Although cores grow in size, the overall hydrodynamic diameter of the microgels does not change. It is not known how the structure of the shell changes during the overgrowth.

Here, we are analyzing Au-PNIPAM microgels with two crosslinker densities. The cores are overgrown from 14 nm in diameter to nearly 100 nm. We perform small-angle X-ray and neutron scattering (SAXS/SANS) to study the respective form factors. SAXS provides information about the cores and SANS about the shell. We also investigate temperature-dependent changes in the microgel by SANS. Additionally, extinction spectra are recorded to study the optical properties. We perform simulations of the different microgels to get information on the internal structure of the shell and the polymer distribution.

CPP 42.3 Wed 17:45 ZEU/0260

Consequences of the near-field effect in highly filled magneto-active elastomers — •Dirk Romeis and Marina Saphiannikova — Leibniz-Institut für Polymerforschung Dresden

In many theoretical models for magneto-active elastomers (MAEs) the interactions among magnetic/magnetizable particles are approximated via dipole models. In highly filled samples, as well as in structured MAEs, the particles are often very close to each other. In such situation the dipole approximation largely underestimates the interactions among magnetizable particles. Yet, for only 2 spherical particles the analytic solution is quite complex, resulting in a slowly converging series expansion. When considering many particle systems only computationally elaborate methods like a finite element approach can provide numerical solutions. Based on a compact fitting function for the 2-body problem, we suggest an accurate approximation for many-body systems including the near-field effect beyond dipole interactions. Considering these corrections due to the near-field effect in comparison to the dipole approximation, we further investigate the role of cluster formation and dispersion of particles in MAEs when an external magnetic field is applied or switched off.

CPP 42.4 Wed 18:00 ZEU/0260

Magneto-active elastomers with magnetically hard vs soft particles: molecular dynamics simulations — •Júlio P. A. Santos and Sofia Kantorovich — University of Vienna, Faculty of Physics, Kolingasse 14-16, 1090 Vienna, Austria

Magneto-active elastomers (MAEs) [1-2], or magnetorheological elastomers (MREs), are composite materials whose properties - such as stiffness, surface roughness (wettability), and shape - can be controlled by low-energy magnetic fields, making them ideal for soft robotics. MAEs consist of an elastic matrix embedded with magnetic micro- or nanoparticles, magnetically either hard (MH) or soft (MS). For high concentrations of MH particles, one can use a complex arrangement of springs that randomly bond nearby MH particles [3]. However, this model oversimplifies particle behavior (as permanent point dipoles) - critical for modeling physically relevant MAEs.

We address these issues in ESPResSo [4], employing molecular dynamics to study the impact of MS particles on the surface relief of a MAE layer and to provide a critical comparison between MH- and MS-based MAEs. At zero field, MS particles do not interact magnetically, whereas MH particles form long chains within the layer. Increasing the field slowly promotes dipolar interactions between the MS particles and rapidly promotes Zeeman interactions with the ap-

plied field, leading to chains that preferentially align parallel to it. In contrast, MH chains must break before reorienting in the direction of the magnetic field, due to the greater importance of dipolar interactions relative to Zeeman, requiring larger applied fields for signficant surface structural changes.

CPP 42.5 Wed 18:15 ZEU/0260

Microstructure analysis of intermediate states in the structure formation process of magnetorheological elastomers — •Nils Magin and Stefan Odenbach — TU Dresden

A composite of magnetic particles and an elastic polymer matrix is referred to as a magnetorheological elastomer. The size and concentration of magnetic particles, as well as the elasticity of the matrix, are the determining factors in the magnetorheological (MR) effect of such materials. Materials exhibiting significant MR properties are commonly referred to as MR elastomers. The application of an external homogeneous magnetic field during the polymerisation process enables the structuring of particles in the initially liquid polymer matrix, resulting in the fabrication of an anisotropic (or structured) material. In order to facilitate a more profound comprehension of the structural formation, the application of the magnetic field is initiated at discrete phases of the polymerisation process. This process gives rise to intermediate states in the structuring that can be observed. The microstructure is examined using computer X-ray tomography and image processing. Furthermore, the influence of the magnetic field, particle concentration, and sample height on the microstructure is discussed. We acknowledge support by the German Research Foundation DFG through Research Unit FOR 5599 on structured magnetic elastomers.

CPP 42.6 Wed 18:30 ZEU/0260

Approximate doubling of the magnitude of maximized magnetorheological effects — Lukas Fischer[1,2] and •Andreas M. Menzel[1] — [1]Otto von Guericke University Magdeburg, Magdeburg, Germany — [2]The University of Osaka, Osaka, Japan

In its static limit, the magnetorheological effect of magnetic elastomers implies changes of elastic moduli by external magnetic fields. Induced magnetic interactions between magnetizable inclusions in a soft, elastic, polymeric matrix affect the overall mechanical stiffness.

First, we optimized the spatial arrangement of the magnetizable inclusions to achieve the strongest change in overall elastic moduli, either for maximized overall stiffening or softening [1]. We focused on both, Young and shear moduli.

Second, in combination, we simultaneously optimized the structural organization to achieve maximized stiffening when an external magnetic field is applied in one direction, but maximized softening when the field is applied along a perpendicular direction [2]. In our case, switching between these two field directions can approximately double the magnitude in overall change of elastic moduli.

Once experimental realizations of prescribed structuring become possible, our strategy provides a direct route to further extend the potential of the materials.

We acknowledge support by the German Research Foundation DFG through Research Unit FOR 5599 on structured magnetic elastomers.

[1] L. Fischer, A. M. Menzel, PNAS Nexus **3**, pgae353 (2024).

[2] L. Fischer, A. M. Menzel, arXiv:2507.22777 (2025).

CPP 43: Biomaterials and Biopolymers (joint session BP/CPP)

Time: Thursday 9:30–12:45 Location: BAR/SCHÖ

CPP 43.1 Thu 9:30 BAR/SCHÖ

Characterization and Application of Honey-PVA Electrospun Scaffolds in Tissue Engineering — •Catalina Navarrete-Vera[1], Karen Yáñez[2], Cristian Acevedo[2], and Tomas Corrales[1,2] — [1]Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso, Chile — [2]Centro de Biotecnología Daniel Alkalay Lowitt, Universidad Técnica Federico Santa María, Chile

Tissue engineering seeks to develop functional biomaterials that integrate seamlessly with biological systems. Electrospinning with static collectors enables the production of nanostructured scaffolds suitable for cell regeneration (10.1021/acsomega.3c06436). Incorporating natural components, such as honey, valued for its regenerative, anti-inflammatory, and antimicrobial properties, offers a route to bioactive wound-dressing alternatives (10.1016/j.carbpol.2019.05.004).

In this study, Manuka and Ulmo honeys were each combined with PVA to generate nanofibers and scaffolds via electrospinning. AFM force spectroscopy was used to assess individual fiber mechanics, and SEM and cell-culture assays were employed to evaluate morphology and biocompatibility. Both formulations produced fibers of similar diameter (100-300 nm) and nanomechanical stiffness (~200 MPa), while honey-containing scaffolds improved cell growth over controls. These results indicate that Ulmo honey is a promising alternative to Manuka honey for tissue-engineering applications.

CPP 43.2 Thu 9:45 BAR/SCHÖ

Additive Manufacturing in Wound Care Innovation from Sugarcane Bagasse — •Ahmed El-Hussein Elnewishy[1], Muhammad Mounir[1], Mona Tarek[1], and Ita Junkar[2] — [1]Biotechnology Program, Faculty of Science, Galala University — [2]Department of Surface Engineering, Jožef Stephan Institute, Ljubljana, Slovenia

Three-dimensional (3D) printing technology is capable of creating highly complex, customizable objects, offering unique advantages for various biomedical applications through methods such as inkjet-based, extrusion-based, and light-assisted techniques. This study focuses on using direct ink writing for additive manufacturing to print antibacterial wound dressings, addressing a critical gap in the current wound care market. The management of chronic and acute wounds presents significant challenges facing human health and overall wellness. Current wound dressing fails to meet patients needs in terms of high adhesion, poor gas exchange, low moisture retention, and the use of systemic and synthetic antibiotics. Additionally, the presence of unused agricultural waste and weak waste management increase greenhouse gas emissions, thus contributing to global warming. To address these issues, we utilized agricultural waste, specifically sugarcane bagasse, to create biopolymer 3D printing ink for wound dressings. We extracted cellulose from sugarcane bagasse and antibacterial bioactive compounds from plant extracts. The synthesized ink was then printed and post treated to enhance mechanical properties. We evaluated the cytotoxicity, antibacterial activity, and morphological structure of the patches using scanning electron microscopy.

CPP 43.3 Thu 10:00 BAR/SCHÖ

FCS-Based RNA Payload Quantification and FLIM Analysis of pH-Dependent Lipid Phase Transitions in Lipid Nanoparticless — •Bernhard Kirchmair[1], Judith Müller[1], Thomas Kellerer[2], Ekaterina Kostyurina[1], and Joachim Rädler[1] — [1]Ludwig-Maximilians-Universität München, Germany — [2]Max Planck-Institut für Biochemie, Martinsried, Germany

Lipid nanoparticles (LNPs) emerged as one of the most promising delivery systems for transfecting mammalian cells with synthetic messenger RNA (mRNA). However, LNPs show a substantial heterogeneity both in shape and cargo and the precise mRNA payload and stoichiometric ratios in multi-component nucleic acid delivery remain poorly quantified. In this project we investigate how mRNA payload depends on LNP size and surface composition using fluorescence correlation spectroscopy (FCS) supported by dynamic light scattering, enabling estimation of particle concentration and RNA copies per LNP. Fluorescence cross-correlation spectroscopy further allows measurement of siRNA/mRNA ratios in mixed cargos. To link payload properties to endosomal escape rates and hence delivery efficiency, we probed pH-dependent lipid phase transitions using fluorescence lifetime imaging (FLIM) and fluorescence anisotropy, capturing changes both in bulk lipid phases and in intact LNPs. These measurements build a framework to monitor structural changes relevant to endosomal escape and can be applied to other LNP formulations and cargo types. Quantitative knowledge about content and ratios will ultimately support the delivery of genetic programs for regulated gene expression.

CPP 43.4 Thu 10:15 BAR/SCHÖ

pH-dependent phase transitions in ionizable lipid mesophases — •Ekaterina Kostyurina[1], Susanne Liese[2], Akhil Sudarsan[2], Julian Philipp[1], and Joachim Rädler[1] — [1]Faculty of Physics, Ludwig-Maximilians University, 80539 Munich, Germany — [2]Faculty of Mathematics, Natural Science, and Materials Engineering, Institute of Physics, University of Augsburg, 86159 Augsburg, Germany

Lipid Nanoparticles (LNPs) have proven valuable in modern medicine as a medium for RNA delivery. Nanoparticles containing cationic ionizable lipid (CIL), cholesterol and structural lipids complex with nucleic acids into size-controlled particles that transport nucleic acid molecules across cell membranes via the endocytic uptake pathway. The delivery efficiency of a drug or vaccine is directly related to the efficiency of the endosomal release. Here, we study pH-dependent structural transitions of the CIL core phase which are believed to play an essential role in this process. We use bulk phases of ionizable lipid/cholesterol as a model system of the LNP core which allows us to study the structure of the lipid phases with high precision using X-ray diffraction. We show that the commonly used ionizable lipids overcome the inverted micellar-inverted hexagonal phase transition within the pH range typical for endosomal life cycle, and connect structural properties of the phases with LNP efficacy. Furthermore, we are aiming to understand the thermodynamics of these phase transitions by combining experimental measurements with theoretical modeling. This will help to

better understand the structure-activity relation of LNPs and to increase the delivery efficiency in clinically relevant LNP delivery systems.

CPP 43.5 Thu 10:30 BAR/SCHÖ

To gel or not to gel? Assembly phase changes of engineered spidroin proteins induced by temperature and time — •Isabell Tunn[1,2,3], Dmitry Tolmachev[2,4], Adam L. Harmat[2,4], Nea B. Möttönen[1,2], Alberto Scacchi[2,4,5], Maria Sammalkorpi[2,4], and Markus B. Linder[1,4] — [1]Department of Bioproducts and Biosystems, Aalto University, Finland — [2]Academy of Finland Center of Excellence in Life-Inspired Hybrid Materials (LIBER), Aalto University, Finland — [3]Fraunhofer Institute for Applied Polymer Research (IAP), Germany — [4]Department of Chemistry and Materials Science, Aalto University, Finland — [5]Department of Mechanical and Materials Engineering, University of Turku, Finland

Bioinspired silk-like proteins offer exciting possibilities for developing the next generation of advanced materials - from medicine to food packaging. Here, we investigate the temperature- and time-dependent assembly behaviour of engineered silk-like proteins into hydrogels conducting experiments and molecular dynamics simulations.* Phase transitions are controlled by entropic changes in flexible glycine-rich regions and hydrophobic interactions of alanine-rich α-helical regions. High-temperature gelation proceeds through interactions between alanine-rich domains, leading to β-sheet formation while time-induced gelation occurs via protein percolation mainly driven by dimerization of terminal domains. These findings provide guidelines for engineering protein-based materials with tailored assembly properties and gel characteristics, advancing the rational design of biomimetic soft materials. *https://doi.org/10.1016/j.ijbiomac.2025.147712

CPP 43.6 Thu 10:45 BAR/SCHÖ

Power-Law Analysis of Force Relaxation and Creep Compliance in Nanoindentation of Glassy Gelatin in Humid Air — Paul Zech, Martin Dehnert, Mario Zerson, and •Robert Magerle — Fakultät für Naturwissenschaften, TU Chemnitz

Gelatin-based materials are widely used in food technology, drug delivery systems, and tissue engineering. Water acts as a plasticizer, softening gelatin and reducing its glass transition temperature. Using AFM-based nanoindentation experiments, we examined the mechanical response of a gelatin film to nanoindentations under constant strain (force relaxation) or constant stress (creep compliance) at a wide range of tip approach velocities and relative humidity levels. Scaling analysis using a fractional rheology model reveals that force relaxation and creep compliance exhibit universal power-law behavior. Temporal evolution depends only on the tip indentation time, which defines the externally imposed timescale of the process, and the power-law exponent α, which characterizes the degree of viscoelasticity. At relative humidity > 85%, the α values differ between the force relaxation and creep compliance data. This indicates differences in the underlying molecular processes.

15 min. break

Invited Talk CPP 43.7 Thu 11:15 BAR/SCHÖ

Directed evolution of material-producing bacteria — •André Studart — Complex Materials, Department of Materials, ETH Zürich

Engineers often use high temperatures, pressures and polluting chemicals to make synthetic materials. By contrast, biology produces remarkable materials like wood and bone using widely available chemicals in water and at ambient temperature. The ability of organisms to create materials under mild conditions relies on the intricate biological machinery of living cells. Notably, natural selection processes have evolved such machinery for hundreds of millions of years to fulfill the demands of biological environments. Can we harness the machinery and evolutionary processes of biology to create materials more sustainably while still meeting engineering needs ? To explore this question, we utilized a microfluidic platform to evolve material-forming microorganisms towards cell mutants that meet the high productivity needed in industrial processes. Using cellulose-producing bacteria as an example, we show that this directed evolution approach enabled the isolation of a bacterial mutant that produces up to 70% more cellulose than its native counterpart. The overproducing bacterial strain offers an attractive alternative to wood to meet the growing demand for cellulose in the textile, medical and packaging industries. Beyond cellulose, the proposed technology offers a compelling approach to isolate bacteria for the bio-fabrication of other sustainable materials, such as silk, polyesters and clay-based bricks.

CPP 43.8 Thu 11:45 BAR/SCHÖ

Controlling Axonal Outgrowth of Organoids by 3D Nanoprinted Scaffolds — •Tobias Müller[1], Malte Siegmund[1], Emma Wollesen[1], Kim Krieg[2], Ole Pless[2], Jan Hahn[3], Robert Zierold[1], and Robert Blick[1] — [1]Center for Hybrid Nanostructures, University of Hamburg, 22761 Germany — [2]Fraunhofer ITMP, Discovery Research Screening Port, 22525 Germany — [3]Section Facility Mass Spectrometry and Proteomics, University Medical Center Hamburg-Eppendorf, 20246 Germany

Cortical organoids are promising models for neurodegenerative disease research, yet their integration into defined neural networks remains challenging. We use two-photon polymerization (2PP) to fabricate three-dimensional scaffolds that direct axonal outgrowth and support organoid integration into engineered circuits.

Scaling structures from single neurons to millimeter-scale organoids introduces adhesion and imaging challenges. We address this by combining tailored scaffold geometries with a polydimethylsiloxane (PDMS)-based anchoring strategy, critical-point drying and quantitative analysis of electron microscopy images. Walls, stairs and microwires enhance organoid-scaffold interactions, promoting axonal outgrowth along intended paths and reducing extension into non-target regions.

These results demonstrate that 2PP-fabricated microarchitectures can guide axon growth and stabilize organoid-substrate contact, enabling more controlled organoid-based neuronal networks and advancing brain-on-a-chip approaches.

CPP 43.9 Thu 12:00 BAR/SCHÖ

Stimulus-induced biomechanical perturbations via smart hydrogel microstructures — •Katja Zieske — Max Planck Institute for the Science of Light, Erlangen, Germany

Cells reside within complex three-dimensional extracellular matrices, where mechanical interactions play essential roles in tissue development, and disease progression. To mimic these interactions, we developed a lab-on-a-chip platform that applies spatially and temporally controlled mechanical perturbations using intelligent hydrogel microstructures.

First, we optimized material composition and photopolymerization parameters and demonstrated reliable, stimulus-dependent expansion and contraction of the hydrogel microstructures within microfluidic chambers. Using these microstructures, we then applied compressive forces to Matrigel and collagen networks. Finally, we applied mechanical perturbations to cellular systems.

By mimicking cellular pushing forces with hydrogel microstructures, this lab-on-a-chip system provides a versatile tool for studying mechanical remodeling of biopolymers and cellular systems.

CPP 43.10 Thu 12:15 BAR/SCHÖ

Functionally Connecting High- and Low-Density Neuronal Networks Using 3D-Nanoprinted Structures — •Emma Wollesen, Malte Siegmund, Tobias Müller, Josephine Hoppe, Robert Zierold, and Robert Blick — Center for Hybrid Nanostructures, University of Hamburg, 22761 Hamburg, Germany

Tracing the propagation of interneural communication from high- to low-density networks is essential for exploiting information processing at the single-cell level. Given the multitude of synaptic connections, high-density networks of hiPSC-derived neurons may generate bursts of action potentials, a key communication mode that can be analyzed at the single-cell level in receiving low-density networks. Here, we move toward such a cultivation platform by evaluating 3D nanoprinted (3DN) structures fabricated by two-photon polymerization for their efficiency in facilitating connected high- and low-density networks. We demonstrate the prerequisite formation of hiPSC-derived low-density neuronal networks in tower-shaped 3DN structures. For augmentation with high-density networks, a stomach-shaped structure and connecting elements were fabricated. A minimum structure height of 30 micrometers proved critical for clear network demarcation. For future region-specific chemical stimulation, millimeter-scale structures for media reservoir separation were conceptualized, and fabrication feasibility was confirmed, requiring a 10 micrometer overlap and a suitable shear angle at structure interfaces. These results extend established 3DN platforms for low-density networks and support the integration of neural networks into Brain-on-a-Chip applications.

CPP 43.11 Thu 12:30 BAR/SCHÖ

Multiplex sensing of respiratory viruses using surface plasmon resonance spectroscopy — •Ghazaleh Eshaghi[1], David Kaiser[1], Hamid Reza Rasouli[1], Dominik Gary[2], Tobias Fischer[2], Katrin Frankenfeld[2], Abhishek Sharma[3], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena — [2]Forschungszentrum für Medizintechnik und Biotechnologie (fzmb) GmbH, 99947 Bad Langensalza, Germany — [3]BioNavis Ltd., Hermiankatu 6-8H, 33720 Tampere, Finland

We present label-free and real-time biosensing of three major respiratory viruses using the Multi-Parametric Surface Plasmon Resonance (MP-SPR) technique. In this approach, MP-SPR SPR Au sensors are functionalized with ultrathin (~1 nm) azide-terminated carbon nanomembranes (N3-CNMs), enabling covalent attachment of virus-specific antibodies and thereby providing selective immobilization of target antigens on the sensor surface. We demonstrate specific detection of SARS-CoV-2, Influenza A, and Respiratory Syncytial Virus (RSV) antigens with negligible cross-reactivity and high reproducibility in both PBS-P buffer (physiological pH) and clinically relevant nasopharyngeal swab matrices. For SARS-CoV-2, Influenza A, and RSV antigens, we determine dissociation constants (KD) of 7.0 * 0.5 nM, 86 * 4 pM, and 3.0 * 0.2 pM, respectively, with corresponding limits of detection (LOD) of ~65 pM, ~80 pM, and ~2 pM.

CPP 44: Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics V

Time: Thursday 9:30–11:15 Location: ZEU/LICH

Invited Talk CPP 44.1 Thu 9:30 ZEU/LICH

Shedding light on wide bandgap perovskites — •Michael Saliba — Institute for Photovoltaics (ipv), University of Stuttgart, Germany

Low bandgap perovskite solar cells are approaching the Shockley-Queisser limit for single-junction solar cells. Less progress, however, was made for wider bandgap perovskites, which are of interest, e.g., for multijunction photovoltaics. These wide bandgap perovskites are often comprised of fully inorganic components, which are hard to dissolve in conventional solvent systems and require more sophisticated synthesis as well as crystallisation techniques. In this talk, I will discuss strategies to address these challenges by providing a library of hitherto unexplored wider bandgap perovskites using combinatorics.

Unfortunately, the newly formulated liquid precursors often exhibit complex crystallization behaviour struggling to expel the typically used DMSO solvent. To delay the crystallization time, two strategies are proposed to remove the strongly complexating DMSO molecules through a) modified processing of the liquid thin-film and b) a coordination solvent with a high donicity and a low vapor-pressure leading to a marked improvement in the overall film quality. Lastly, interface manipulation, especially on top of the formed perovskite, is becoming a central topic to advance further. Light annealing is introduced to modify the perovskite surface resulting in a reduced surface recombination.

CPP 44.2 Thu 10:00 ZEU/LICH

Perovskite Solar Cells under Orbit-Like Thermal Cycling — •Simon Alexander Wegener[1], Christoph Gernot Lindenmeir[1], Thomas Baier[1], Xiaojing Ci[1], Sigrid Bernstroff[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]Elettra-Sincrotrone Trieste S.C.p.A., Basovizza, Trieste, Italy

Perovskite solar cells offer strong potential for space power systems due to their high visible-light absorbance, thin active layers, and efficiencies comparable to silicon. These features provide exceptional power-to-weight ratios, and solution processing reduces manufacturing and launch costs relative to multi-junction gallium arsenide cells. Initial demonstrations have confirmed their operability in space. Key challenges remain, particularly the extreme temperature swings in low Earth orbit. Our work examines these stresses using operando grazing-incidence wide-angle X-ray scattering (GIWAXS) to track structural changes in the perovskite during illumination and temperature cycling. Synchrotron radiation enables the necessary temporal resolution to study the multilayer device stack, which combines materials with differing mechanical and thermal properties. Complementary photoluminescence measurements reveal associated changes in optical and electrical behavior. Across -125°C to +100°C, the perovskite shows changes in crystal phase, anisotropic strain, and optoelectronic response. These findings clarify the coupled mechanical and electronic effects driving performance loss and enable strategies to enhance durability of perovskite solar cells for space applications.

CPP 44.3 Thu 10:15 ZEU/LICH

Depth Resolved Structural Analysis on CsPbI3 Nanocrystal Nucleation Seed Induced Pervskite Thin Films — •Altantulga Buyan-Arivjikh[1], Lukas Wolz[1], Ajeet Kumar[2], Yanan An[1], Christopher Everett[1], Guangjiu Pan[1], Jiinsheng Zhang[1], Zhuijun Xu[1], Matthias Schwartzkopf[3], Stephan V. Roth[4], Jürgen Hauer[1], Johanna Eichhorn[1], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, 85748 Garching, Germany — [2]Department of Chemical Physics, Lund University, 22100 Lund, Sweden — [3]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [4]Department of Fibre and Polymer Technology KTH, SE-10044 Stockholm, Sweden

Lead-halide perovskites have attracted significant attention due to their favorable optoelectronic properties, simple processing, and the availability of precursor materials. Their performance is strongly governed by the crystallinity and morphology of the typically polycrystalline thin films. Among strategies to optimize these features, nanocrystal seeding has emerged as a promising route. Here, we show improved crystallographic orientation and reduced defect density in printed FAPbI3 thin films through the introduction of CsPbI3 nanocrystal nucleation seeds. Incidence-angle-varied GIWAXS enabled depth-resolved structural analysis, revealing seed incorporation and corresponding modifications of the energy landscape through the film thickness.

CPP 44.4 Thu 10:30 ZEU/LICH

***In-Situ* KPFM Growth Studies of Pentacene as a Model Hole Transport Material on 2D/3D Heterostructured $Cs_2AgBiBr_6$ for Perovskite Solar Cells** — •Tim P. Schneider and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

Forming low-dimensional perovskite interlayers in perovskite solar cells by applying ammonium salt solutions is a well-known method to improve devices. This has already been approved for the $Cs_2AgBiBr_6$ double perovskite in solar cell geometry by a 2D-modification with BABr or PEABr salts achieving respective low-dimensional phases at the interface. Using pentacene as a model hole conductor, its film growth and contact formation to the different double perovskite phases was investigated via *in-situ* growth studies using Kelvin Probe force microscopy (KPFM). Measuring the morphology and work function at intermittent steps during film deposition allowed to observe their evolution depending on the average pentacene film thickness. Image processing of the resulting KPFM images facilitated to assign different morphological features (from substrate or pentacene) present in the height images to different contributions to the work function and, especially, clearly identified the pentacene grains within other similar morphological features. A much more homogenous growth of pentacene on 2D/3D heterostructured $Cs_2AgBiBr_6$ was observed, forming evenly shaped grains or dendritic islands. This was further accompanied by a more confined work function, speaking for an enhanced contact alignment between the double perovskite and pentacene.

CPP 44.5 Thu 10:45 ZEU/LICH

Gas quenching under ambient condition for efficient and stable perovskite solar cells with surface passivation — •Zhaonan Jin[1], Xiongzhuo Jiang[1], Zerui Li[1], Xiaojing Ci[1], Guangjiu Pan[1], Lixing Li[1], Jinsheng Zhang[1], Xinyu Jiang[2], Sarathlal Koyiloth Vayalil[2,3], Kun Sun[4], Stephan V.Roth[2,5], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]DESY, Hamburg — [3]UPES, India — [4]HZB, Berlin — [5]Department of Fibre and Polymer Technology, KTH, Stockholm, Sweden

Wide-bandgap perovskite solar cells play a key role in tandem solar cells, which aim to overcome the Shockley-Queisser limit for single-junction solar cells. In this work, we develop and optimize a gas quenching method under ambient conditions for the fabrication of wide-bandgap (1.77 eV) perovskite films. To improve the performance of PSCs, three different organic spacer cations, including aromatic amino molecules (PEAI), aliphatic amino with long alkyl chain molecules (OAI), and short alkyl chain molecules (BAI), are applied and investigated as surface passivation materials. As a result, the 2D perovskite layers form on top of 3D perovskite films. The n-i-p devices with PEAI passivation exhibit a champion PCE of 16.26% along with a high Voc of 1.21 V, exceeding the control device (PCE = 13.42%, Voc = 1.15 V), and maintaining 88% of its initial PCE after 120 minutes of continuous illumination. This work offers a guide for the fabrication of wide-bandgap PSCs under ambient conditions and the choice of organic spacer cations for passivation.

CPP 44.6 Thu 11:00 ZEU/LICH

Solvated PbI2 Clusters Preceding the Crystalization of Lead Halide Perovsites - UV/VIS In Situ Study — •Maximilian Spies[1], Leonard Krapf[1], Fabian Eller[2], Eva M. Herzig[2], and Anna Köhler[1] — [1]Soft Matter Optoelectronics, University of Bayreuth — [2]Dynamics and Structure Formation, University of Bayreuth

The solution-based fabrication of reproducible, high-quality lead iodide perovskite films demands a detailed understanding of the crystallization dynamics. This dynamic is primarily determined by the precursor solution chemistry and processing conditions. We conducted a systematic in-situ study to elucidate the formation mechanism of perovskite films and the role of additives in the pre-crystallization phase. Using UV absorption spectroscopy during spin coating allows us to track the evolution of iodoplumbate complexes and a solvated pre-crystalline phase (PDS) present in the precursor solution. This PDS phase is proportional to the precursor concentration, even during spin coating. Notably, using different precursor solvents changes the PDS phase evolution substantially. However, when introducing additives we see no difference in this pre-crystalline evolution, suggesting that additives only affect the perovskite film formation at a later stage

CPP 45: Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates I (joint session CPP/BP)

Biomolecular condensates play a central role in many cellular processes and provide a fascinating example of self-organized, highly dynamic systems. Physical methods, particularly from statistical physics and soft matter, have emerged as valuable tools for understanding and predicting their fundamental properties. Conversely, the complexity and diversity of biological systems open new perspectives and challenges for physical modeling. This focus session will highlight current research at the interface of physics and biology, with an emphasis on theoretical modeling and simulation of the physics of biomolecular condensates.

Organized by Arash Nikoubashman, Tyler Harmon and Lukas Stelzl.

Time: Thursday 9:30–11:15 Location: ZEU/0260

Topical Talk CPP 45.1 Thu 9:30 ZEU/0260

Wetting transitions in biomolecular coacervates — •Susanne Liese[1], Tiemei Lu[2], Evan Spruijt[3], and Christoph Weber[1] — [1]University of Augsburg — [2]University of Oxford — [3]Radboud University

Biomolecular coacervates are liquid-like droplets that can interact with membranes and self-organize into complex structures. Understanding the principles governing their shapes and higher-order assemblies is crucial for controlling compartmentalization in biological and synthetic systems.

We present a theoretical framework describing the shape and organization of biomolecular coacervates interacting with membranes and each other. Large coacervate droplets adopt morphologies determined by the balance of surface tensions, from partial adhesion to full engulfment. Scaled membrane tension and droplet-membrane interactions predict transitions between spherical, lens-shaped, partially wrapped, and endocytosed droplets, with composition-dependent contact angles linking molecular properties to macroscopic shapes.

For multiphase coacervates, we model the impact of interfacial species on droplet organization. Enrichment of an interfacial component at phase boundaries drives partial wetting between droplets, promoting the formation of dimers and extended chains. Numerical simulations show that surface tension minimizes the contact area, straightening droplet arrangements and generating polymer-like behavior with bending stiffness and segment-length constraints.

CPP 45.2 Thu 10:00 ZEU/0260

Elastic regulation of biomolecular condensates — •Oliver Paulin and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany

In recent years, biomolecular condensates have emerged as a vital component of sub-cellular organisation. Here, we discuss the role that elastic interactions can play in regulating condensate size, count, and mechanical properties. First, we focus on the impact of 'external' elasticity that arises from a confining mesh such as the cytoskeleton. We find that the additional energetic cost of network deformations induced by condensate growth limits condensate size, and can even suppress condensate formation entirely. Additionally, when condensate size is comparable to characteristic heterogeneities of the network, non-local interactions may arrest thermodynamic coarsening and drive the formation of stable patterned states with an energetically selected length scale. Second, we study how 'internal' elasticity, resulting from the intrinsic viscoelasticity of condensate material, can inhibit condensate growth, but also impart condensates with mechanical strength. For the case in which condensate growth is driven by active incorporation of new material, we demonstrate how a delicate balance of material properties provides condensates with solid-like mechanical strength, without compromising their liquid-like ability to form and grow rapidly. For both examples, we construct dynamic continuum models that couple phase separation with elastic deformation, analysing the key parameters that control condensate form, and identifying how cells can use elasticity to fine-tune condensate behaviour to fulfil a specific function.

CPP 45.3 Thu 10:15 ZEU/0260

Phase Separation of a Nucleator in a Self Straining Active Filament Network — •Jakob Schindelwig[1], Quentin Bodini-Lefranc[1,2], and Sebastian Fürthauer[1] — [1]Institute of Applied Physics, TU Wien, Lehargasse 6, 1060 Vienna, Austria — [2]Ecole polytechnique, Institut Polytechnique de Paris, Route de Saclay, 91120 Palaiseau, France

Many membraneless compartments of cells, such as stress-granules, form via liquid-liquid phase separation. In cells many compartments of the same type and similar sizes can coexist. Since this is inconsistent with equilibrium phase separation physics, we ask if active mechanics could explain this observation. We develop a model coupling dynamics of the droplet material to an active self-straining filament network. This model shows (i) arrested coarsening , (ii) oscillations, (iii) scale selection. We establish that our model is physiologically plausible by comparing to recent work on a phase separating nucleator of actin.

CPP 45.4 Thu 10:30 ZEU/0260

Active Transport as a Mechanism of Microphase Selection in Biomolecular Condensates — •Le Qiao, Peter Gispert, and Friederike Schmid — Institut für Physik, Johannes Gutenberg-Universität Mainz, D55099 Mainz, Germany

Cells control the size and organization of biomolecular condensates formed by liquid-liquid phase separation (LLPS), yet the underlying physical principles remain incompletely understood. We propose a transport-driven mechanism in which undirected motor-mediated motion along cytoskeletal filaments redistributes phase-separating components, generating an effective non-equilibrium long-range repulsion that arrests coarsening. This is explored using a minimal reaction-diffusion-transport model that captures the interplay between binding-release kinetics, diffusion, and active transport. A linear stability analysis and three-dimensional simulations reveal a transition from macroscopic to microphase separation at remarkably low binding/release fractions, corresponding to minute fractions of motor-bound proteins. Tuning motor binding rates b or transport velocities enables sublinear control of condensate dimensions ($L \sim b^{1/4}$) from nanometers to micrometers. This mechanism provides a simple physical route for spatially programmable condensate organization in living cells and active materials.

CPP 45.5 Thu 10:45 ZEU/0260

Positive feedback in chemically active droplets — •Xi Chen[1], Jens-Uwe Sommer[1,2], and Tyler Harmon[1] — [1]Leibniz Institute of Polymer Research, Dresden, Germany — [2]Dresden University of Technology

Biomolecular condensates are dynamic compartments that can be maintained far from equilibrium by active chemical reactions. Active condensates can be driven by phase-dependent reaction fluxes, for example via localized enzymatic activity, and thereby exhibit emergent behaviors that cannot be realized in equilibrium condensates. We analyzed condensates with positive feedback between phase separation and reactions: droplets enhance reactions, and the resulting products stabilize the droplets. We show that this feedback produces pronounced hysteresis, making droplets resilient to cellular fluctuations. We show the hysteresis persists across a broad range of reaction schemes and parameter choices, indicating that it is a robust feature of droplets with positive feedback. Condensates that form to satisfy transient cellular needs may benefit from such hysteresis, because it ensures that they persist long enough to carry out their functions despite fluctuating conditions.

CPP 45.6 Thu 11:00 ZEU/0260

Chemically driven simulations of enzymatic phosphorylation in protein condensates — •Emanuele Zippo[1], Dorothee Dormann[1,2], Thomas Speck[3], and Lukas Stelzl[1,2] — [1]Johannes Gutenberg University Mainz, Mainz, Germany — [2]Institute of Molecular Biology (IMB), Mainz, Germany — [3]University of Stuttgart, Stuttgart, Germany

The condensation and aggregation of intrinsically disordered proteins (IDPs) in cells are governed by enzyme-driven, non-equilibrium processes. Kinases such as Casein kinase 1 delta (CK1d) phosphorylate proteins using ATP as chemical fuel, tuning intermolecular interactions and modulating condensate assembly. The neurodegeneration-linked protein TDP-43 undergoes CK1d-mediated hyperphosphorylation, proposed as a cytoprotective mechanism through condensate dissolution, yet the mechanisms underlying kinase-condensate interactions remain unclear. Using coarse-grained molecular dynamics simulations, we investigate how CK1d phosphorylates TDP-43 and how this reaction drives the structural reorganization and dissolution of its condensates. To ensure thermodynamic consistency in such fuel-driven simulations, we employ an automatic, generally applicable Markov state modeling framework. Post-translational modifications (PTMs), such as phosphorylation, can actively regulate condensate stability and suppress Ostwald ripening, offering a mechanism to control mesoscale structure in soft materials. Understanding such reaction-structure coupling in non-equilibrium environments is key to explaining cellular self-organization and designing biomimetic systems.

CPP 46: Poster II

Focus Session: Water - from Atmosphere to Space (with DY); French-German Session: Membranes and Porous Materials; Gels, Polymer Networks and Elastomers; Biopolymers, Biomaterials and Bioinspired Functional Materials (with BP); Complex Fluids and Colloids, Micelles and Vesicles (with DY); Charged Soft Matter, Polyelectrolytes and Ionic Liquids; Responsive and Adaptive Systems; Nanomaterials, Composites and Hybrids; Crystallization; Molecular and Polymer Dynamics, Friction and Rheology; Simulation Methods and Modeling of Soft Matter; Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods

Time: Thursday 9:30–11:30 Location: P5

CPP 46.1 Thu 9:30 P5

Pressure-induced amorphization of aqueous PEG solutions — •Leah Dorothea Schwerdtfeger[1,2], Isabell Zick[1,2], and Katrin Amann-Winkel[1,2] — [1]Institut für Physik, Johannes Gutenberg Universität, Mainz — [2]Max-Planck-Institut für Polymerforschung, Mainz

Water is a fundamental substance whose behavior under supercooled temperatures shows many anomalous properties. Among the many curiosities, water can even form different amorphous states. These amorphous states are hypothesized to be directly related to two different liquid states of water, namely high- and low-density liquid. Understanding the pressure-induced amorphization of aqueous solutions can reveal how solutes alter water's phase diagram and give further insight to the predicted liquid-liquid transition.

While the impact of small molecules is known from previous studies, the role of larger polymers remains unexplored. Here, we discuss experiments on aqueous polyethylene glycol (PEG) solutions with different molar weights, studying their effect on the pressure-induced phase transitions. Our dilatometric measurements show how solutes broaden the transition from hexagonal ice to high-density amorphous ice (HDA), depending on the molar fraction. We also investigate the polyamorphic transition between low- and high-density amorphous ice (LDA-HDA), which for pure water is known to exhibit a strong temperature-dependence. The samples are further characterized by X-Ray diffraction (XRD).

CPP 46.2 Thu 9:30 P5

Phase transition in water-glycerol solutions — •Klara Holl[1,2], Louisa Kraft[1,2], and Katrin Amann-Winkel[1,2] — [1]Institut für Physik, Johannes Gutenberg-Universität, Mainz — [2]Max-Planck-Institut für Polymerforschung, Mainz

Water is omnipresent in our daily lives with many anomalous properties and a unique phase diagram. Studies of supercooled water provides insight into the hypothesis of the coexistence of two liquid states of water and a liquid-liquid transition. This proposes two different types of supercooled liquid water in a high-density and low-density liquid state, that are separated by a first order phase transition at low temperatures and elevated pressure. But how does this hypothesis impact on aqueous solutions?

Water-glycerol mixtures are often used in pharmaceuticals and act as cryoprotectants, common in biomedicine as well as automotive antifreeze. While pure water crystallizes easily, the glass-forming agent glycerol can serve as soft confinement for water. Changing the concentration of the two components alters the liquid's physical and thermodynamic properties, including depression of the crystallisation temperature.

We investigate different water-glycerol solutions at low-temperatures and high-pressure conditions using a diamond anvil cell. This allows in situ optical observation of crystallisation and glass transition. Structural changes are studied by X-ray diffraction and differential scanning calorimetry.

CPP 46.3 Thu 9:30 P5

Photooxidation of vanillic acid at the air-water interface — •Manuel Hofmann[1,2] and Ellen H.G. Backus[1,2] — [1]Institute of Physical Chemistry, Faculty of Chemistry, University of Vienna, Währinger Str. 42, 1090 Vienna, Austria — [2]University of Vienna, Vienna Doctoral School in Chemistry (DoSChem), Währinger Str. 42, 1090 Vienna, Austria

Phenolic compounds like vanillic acid, emitted from biomass burning, can form secondary organic aerosols (SOA) through aqueous phase reactions. Photooxidation of vanillic acid is a potential source of Humic-Like Substances (HULIS), that influence atmospheric chemistry through light absorption.[1]

The air-water interface provides a distinct chemical environment where structural behavior and reactions may differ from those in bulk. To specifically probe this interface, sum-frequency generation (SFG) spectroscopy and surface tension measurements are employed, offering complementary insights into molecular behavior.[2]

This study examines vanillic acid at the air-water interface across different pH values, before and after UV/H2O2-induced photooxidation. Control experiments with vanillic acid alone separate direct photolysis from radical mediated processes. Preliminary SFG spectra reveal pH-dependent vibrational signatures of adsorbed species and significant changes upon photoreaction. The goal is to identify reaction products, structural changes, and how pH affects vanillic acid photoreactivity.

[1]S. Tang et al., ACS Earth Space Chem., 4 (2020) 862-872.[2]C.-M. Saak et al., J. Phys. Chem. Lett., 15 (2024) 4546-4559.

CPP 46.4 Thu 9:30 P5

Biophysical Interaction of Steroid Hormones with Model Lipid Membranes — •Rabia Rabia[1,2,3], Prashant Hitaishi[1,2], Bridget Murphy[1,2], and Julia Herzen[3] — [1]Institute of Experimental and Applied Physics, Kiel University, Leibnizstraße 19, Kiel, 24118, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, Hamburg, 22607, Germany — [3]Technische Universität München

Menopause is characterized by declining 17βestradiol (E2), increased adiposity, reduced insulin sensitivity, and higher type 2 diabetes risk. Vasomotor symptoms, such as hot flushes and night sweats, significantly impair quality of life, and transdermal E2 provides effective relief at lower doses than oral therapy, with potentially fewer systemic risks. Despite its clinical benefits, the molecular mechanisms of E2 remain incompletely understood. While steroid hormones classically act via intracellular receptors to regulate gene transcription, they also interact directly with lipid membranes, influencing packing and elasticity. We studied βestradiol, progesterone, 17αethynylestradiol, and cholesterol in DPPC and POPC monolayers at the air water interface using Langmuir isotherms and surface elasticity measurements. E2 was found to expand molecular area and reduce packing density, increasing membrane elasticity. Planned X-ray measurements will further clarify how steroid-induced reorganization of lipid interfaces modulates downstream cellular signaling.

CPP 46.5 Thu 9:30 P5

The structure and orientation of ice under confinement in Periodic Mesoporous Organosilicas (PMOs) — Niels C. Giesselmann[1], Philip Lenz[2,3], Sophia-Marie Meinert[2], Robert P.C. Bauer[1,4], Nele N. Striker[1], Michael Fröba[2,3], and •Felix Lehmkühler[1,3] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Institute for Inorganic Chemistry, University of Hamburg,Germany — [3]The Hamburg Center for Ultrafast Imaging, Hamburg, Germany — [4]Freiberg Center for Water Research, TU Bergakademie Freiberg, Germany

We studied water in periodic mesoporous organosilicas (PMOs) with pore diameters in the range of 2-5 nm. In these materials, the molecular mobility of water is influenced by the polarity of the organic moiety. We collected and analyzed X-ray scattering data of water and ice under confinement in PMOs with varying degrees of hydrophobicity and pore diameters and at varying temperature. A decrease in the density of the confined water was observed during cooling, which was strongly dependent on the organic moiety, as well as the pore diameter. We furthermore found deviations in the lattice constants of hexagonal ice in these materials compared to bulk water. In most cases, one lattice parameter was more strongly affected. This could be caused by orientational dependencies between the ice crystal and the pore. The orientation between the hexagonal crystallites in relation to the pore axis was therefore investigated using X-ray Cross Correlation Analysis (XCCA), indicating more uniformly oriented crystallites in more hydrophilic pores.

CPP 46.6 Thu 9:30 P5

Impact on snow albedo of soot aggregates inferred from their radiative properties — •Llorenc Cremonesi[1], Luca Teruzzi[1], Valentina Raspagni[2], and Marco Potenza[1] — [1]University of Milan, Milan, Italy — [2]Ca' Foscari University of Venice, Venice, Italy

Despite having a short lifespan in the atmosphere, soot aggregates are abundant and volatile enough to be found in various environments far from their sources. While suspended in the atmosphere, they influence local thermodynamic conditions and interact with water triggering cloud nucleation. These particles are also among the drivers of cryospheric degradation in climate-sensitive areas such as the Arctic and the European Alps.

The effectiveness with which soot aggregates interact with solar radiation is known to be related to their morphology as well as their composition. However, studies of their radiative properties rely on indirect or model-dependent measurements. We use a non-destructive optical technique that enables us to simultaneously measure several optical parameters on a particle-by-particle basis in situ.

Field measurements and laboratory tests show that aggregate particles exhibit exceptional scattering and absorption efficiencies relative to their mass. Directly

assessing these properties obviates the need to characterise their exceptional morphological variability. By quantifying these properties, we evaluate the impact of carbon aggregates on snow, particularly in the uppermost layers.

CPP 46.7 Thu 9:30 P5

Study of nuclear magnetization transfer between water and ice phases in nanoporous solids — •Cristina Abril Gutierrez Ortigoza and Rustem Valiullin — Felix Bloch Institute for Solid State Physics, University of Leipzig, Leipzig, Germany

NMR Cryoporometry is a promising tool for the characterization of nanoporous solids. The technique relies on introducing a probe liquid into the nanopores, where a liquid and frozen phase can coexist at low temperatures. Both phases can be easily identified using NMR due to their vastly different transverse relaxation rates. The magnetization transfer mechanism between these is not well understood, especially its dependence on various parameters such as temperature and pore size. In this contribution, the magnetization transfer between water and ice in porous silica is explored, the pore structure of which is composed of well-ordered spherical nanopores connected by micropores. The measurements are performed by using the Goldman-Shen pulse sequence, which initializes the experiments in a state where all the magnetization is contained in the liquid phase. By studying how the system re-equilibrates, parameters such as the diffusion coefficient in the ice phase and the proton volume fraction in each phase are obtained. Furthermore, the non-frozen layer thickness, which refers to the liquid-like layer that forms between the ice core and the pore wall, can be obtained by exploiting the well-defined geometries of the ice and water phases. The studies were performed at different temperatures to assess the dependence of the results on this parameter. The experimental data are also compared to theoretical models.

CPP 46.8 Thu 9:30 P5

Advanced analysis of NMR cryoporometry data — •Crina Rahause, Georgiy Baroncha, and Rustem Valiullin — Felix Bloch Institute for Solid State Physics, Leipzig University, Leipzig, Germany

NMR cryoporometry is a powerful tool for structural characterisation of multiscale nanoporous materials. It relies on probing the pore size dependent ice-liquid phase transitions of nanoconfined liquid. However, accurate interpretation of the experimental data requires a better description of phase equilibria, as well as a framework that takes into account the network topology and relaxation effects. In this contribution, we perform NMR measurement using water and octamethylcyclotetrasiloxane (OMCTS) as probe liquids inside highly ordered nanoporous alumina membranes with well-defined pore sizes ranging from 25 to 180 nanometres. OMCTS differs from water in terms of relaxation times and the thermodynamic parameters controlling phase transition suppressions; therefore, by comparing the responses of the two liquids in different porous media, we can identify key parameters which are necessary for accurately establishing an advanced cryoporometry methodology, and demonstrating the applicability of this technique to a wide range of materials.

CPP 46.9 Thu 9:30 P5

Comparison of mechanical properties and pore collapse characteristics of hyperuniform disordered anodic aluminium oxide membranes — •Rang Noh[1], Clara Twiehaus[2], Marc Thelen[1], Alexander Sprafke[3], Prerak Dhawan[3], Ralf Wehrspohn[3], Martin Steinhart[2], and Patrick Huber[1,4] — [1]Institute for Materials and X-ray Physics, Hamburg University of Technology, Hamburg, Germany — [2]Institute of Chemistry of New Materials, Osnabrück University, Osnabrück, Germany — [3]Institute of Physics, Martin Luther University of Halle-Wittenberg, Halle (Saale), Germany — [4]Center for X-ray and Nano Science CXNS, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

We investigate how the degree of disorder in hyperuniform Porous Anodic Aluminum Oxide (AAO) membranes influences their mechanical properties and pore-collapse behavior. Elastic moduli of AAO were measured using two different methods; Laser Ultrasonics (LUS) and nanoindentation. The indented points were captured by scanning electron microscopy to observe pore collapse characteristics. The elastic moduli from LUS and nanoindentation agree well; in general, the elastic modulus increases as both porosity and the hyperuniformity index decrease. Even at similar porosity levels, enhanced hyperuniformity results a higher elastic modulus. When the pores are ordered, the pore collapse follows directional grain paths around the indented edge and propagate further in a connected herringbone like pattern. But, in the disordered state, the irregular collapse happens, producing direction-independent crack propagation within the restricted region.

CPP 46.10 Thu 9:30 P5

Microscopic mechanisms of polymer network breakage under mechanical deformation — •Fernando Martín Salamanca[1,2] and Michael Lang[1] — [1]Institute Theory of Polymers, Leibniz-Institut für Polymerforschung Dresden e.V. Kaitzer Strasse, 4 - 01069 (Dresden) — [2]Institute of Polymer Science and Technology, Spanish National Research Council. Juan de la Cierva, 3 - 28006 (Madrid)

The failure of polymer networks arises from a subtle interplay between bond rupture, chain interactions and the underlying topology of the network. In this work, Monte Carlo simulations are used to explore how these factors shape the mechanical response of crosslinked polymers subjected to mechanical stress. The main goal is to evaluate, in a controlled manner, the key elements that modify the mechanical response by computer simulations: the criteria for bond rupture, the mathematical modelling of interactions potentials and force fields, the effect of entanglements and excluded volume. Model networks are evaluated with diverse approaches to quantify the effect of each contribution to elastic modulus. The simulations yield detailed rupture statistics and stress-strain behavior across a broad parameter space, which are compared with predictions from established theoretical descriptions of network elasticity and fracture. Overall, this work provides basic information for understanding network failure and for establishing a first-principles based model for real polymer networks.

CPP 46.11 Thu 9:30 P5

Tuning Foam Kinetics and Structure: The Role of Gas Flowrate in Microgel-Stabilized Foams — •Vera Anna Nina Alina Hesse, Joanne Zimmer, and Regine von Klitzing — Soft Matter at Interfaces, Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 8, D-64289 Darmstadt

The stability and microstructure of foams are critical for their performance in various applications. In this work, aqueous foams are generated by sparging gas (nitrogen) through an aqueous dispersion of PNIPAM microgels, which are used as foam-stabilizers. In specific the effect of the gas flowrate during foam production on the foam structure and kinetics is investigated. In this regard, key parameters such as the foam half lifetime, drainage (liquid content), and bubble size evolution are examined. Our findings reveal a clear dependence: In general, lower flowrates produce smaller initial bubbles, which in turn significantly improve the overall foam stability, as their structural skeleton remains intact for longer periods. On the other hand, a stability optimum is detected, with peak stability occurring at a low flowrate; further reduction however ultimately compromising stability. These findings contribute to a deeper understanding of microgel-stabilized aqueous foams and render the potential for optimizing foam generation processes.

CPP 46.12 Thu 9:30 P5

Shape and inner structure of micelles from tetrablock terpolymers in aqueous solution — •Katarina Döbler[1], Feifei Zheng[1], Pablo A. Alvarez Herrera[1], Joachim Kohlbrecher[3], Anna P. Constantinou[2], Theoni K. Georgiou[2], and Christine M. Papadakis[1] — [1]Technical University of Munich, TUM School of Natural Sciences, Soft Matter Physics Group, Garching, Germany — [2]Imperial College London, U.K — [3]PSI, Villigen, Switzerland

Injectable hydrogels formed by LCST thermoresponsive block terpolymers consisting of thermoresponsive, hydrophilic and hydrophobic blocks are promising materials for tissue engineering by 3D bioprinting. The gel point temperature, gelation mechanism, and physical properties can be tuned by the number, sequence and length of the individual polymer blocks [1,2]. Utilizing small-angle X-ray and neutron scattering in a wide temperature range, we investigate aqueous solutions of thermoresponsive tetrablock terpolymers having different sequences of hydrophilic, hydrophobic and thermoresponsive blocks. By fitting structural models, we gain insight into the shape and size of the micelles as well as their inner structure. Moreover, the gelation mechanism is deduced from the changes of the micellar structure and correlation at the gel point.

[1] A.P. Constantinou et al., Macromolecules 2018, 51, 7019
[2] A.P. Constantinou et al., Macromolecules 2025, 58, 9122

CPP 46.13 Thu 9:30 P5

Interfacial Dilational Rheology of Microgel Layer at the air-water interface — •Jana Sänger, Atieh Razavi, Regine von Klitzing, and Amin Rahimzadeh — Soft Matter at Interfaces, Institute for condensed Matter Physics, Technical University of Darmstadt, Hochschulstraße 8, 64289 Darmstadt, Germany

Interfacial tension and dilational interfacial rheology of Poly (N-Isoprpylacrylamide) (PNIPAM) microgel layer at air-water interfaces are characterized using pendant-drop techniques. Static interfacial tension was first measured with a drop shape analyser by fitting the droplet profile to the Young-Laplace equation. To probe the interfacial elasticity of microgel dispersions, a Profile Analysis Tensiometer (PAT-1) is employed to impose controlled harmonic oscillations on pendant drops with volumes of 10 μL and microgel concentrations between 0.1 wt% and 0.015 wt%. By using a Fourier transformation, the surface dilational modulus is determined, and the elasticity modulus is then identified as the real part of the surface dilational modulus. In order to remain within the linear range of the interfacial dilational elasticity, various amplitude ratios were systematically tested, and a maximum amplitude ratio of 6% was found. Our study shows that the elastic modulus is frequency-dependent. By increasing the frequency, an increasing elastic modulus is determined. Furthermore, we observe a shift of the maximum elasticity modulus towards the lower surface pressure values by increasing the frequency.

CPP 46.14 Thu 9:30 P5

Combined TGA-MS Analysis of Actively Aged Polymers for Assessing Recycling Potential — •Judith Bünte, Inga Ennen, Karsten Rott, and Andreas Hütten — Universität Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany

Thermogravimetric analysis (TGA) combined with mass spectrometry (MS) provides a powerful, complementary approach for characterizing the thermal stability and degradation pathways of polymers subjected to accelerated (active) aging. In this study, aged polymer samples, representing materials encountered in post-consumer recycling streams, are analyzed using simultaneous TGA-MS to monitor mass-loss events and identify evolved gaseous species. These results demonstrate that combined TGA-MS analysis can reveal chemical and structural changes that are not easily evident from bulk mechanical or spectroscopic testing alone. The findings support more accurate assessments of polymer recyclability, highlight indicators of material down-cycling, and inform optimization strategies for sorting, preprocessing, and reprocessing conditions. Ultimately, this work underscores the value of TGA-MS as a diagnostic tool for improving circular-economy approaches.

CPP 46.15 Thu 9:30 P5

Synthese und Reaktivität von Betti-Basen — •Alyona Nikulina — Mikluho-Maklaya Strasse, Moskau 117198

Diese Forschung konzentriert sich auf Naphthoxazine, eine wertvolle Gruppe von Verbindungen, die für ihre biologischen Aktivitäten bekannt sind wie antimikrobielle,antidiabetische und antidepressive Wirkungen sowie für ihr Potenzial in der Entwicklung von duroplastischen Polymeren. Die Synthese dieser Verbindungen beginnt häufig mit Betti-Basen, die Zwischenprodukte für die Bildung von kondensierten 1,3-Oxazinen darstellen.Um die notwendigen Betti-Basen zu erhalten, untersuchten wir zwei Syntheserouten. Eine Strategie war eine einfache Dreikomponenten-Reaktion von β-Naphthol, sekundären cyclischen Aminen und Aldehyden. Der andere Weg umfasste zunächst die Kondensation von 2-Hydroxy-1-naphthaldehyd mit Aminen und anschließend die Reduktion der resultierenden Iminiumsalze mit Natriumborhydrid. Nachfolgende Versuche, diese Basen durch Cyclisierung mit Standardreagenzien wie Silberoxid oder Kupferacetat in die Ziel-Naphthoxazine umzuwandeln, erwiesen sich als ineffizient und ergaben geringe Ausbeuten. Da bekannt ist, dass diese Cyclisierung die Bildung eines Iminiumsalzes beinhaltet, stellten wir die Hypothese auf, dass DIAD als wirksamer Katalysator wirken würde. Das Experiment nahm jedoch eine unerwartete Wendung: DIAD allein führte nicht zu den gewünschten Naphthoxazinen. Der entscheidende Moment kam, als wir ein katalytisches System aus Kupfer(I)-iodid und Cesiumcarbonat zugaben, das eine unvorhergesehene intramolekulare Umlagerung der Betti-Basen auslöste und stattdessen zu Diketon führte.

CPP 46.16 Thu 9:30 P5

Functional ZnPc-Polymer-Magnetic Nanocomposite Systems for Photodynamic Therapy — •Lungu Ion — Laboratory of Organic/Inorganic Materials for Optoelectronics, Institute of Applied Physics Moldova State University, 60 Al. Mateevici St., MD-2009, Chisinau, Republic of Moldova

Hybrid photosensitizing materials combining organic and magnetic components provide a promising route toward multifunctional systems for photodynamic therapy (PDT). In this work, we investigate the photophysical and magnetically induced processes in a series of functional zinc phthalocyanine (ZnPc) derivatives-ZnPc(COOH)4 and ZnPc(COOH)8 and their conjugates with dextran (Dx) and Fe3O4 nanoparticles. The systems were studied in DMSO/H2O (1:1) solutions using steady-state and time-resolved fluorescence and phosphorescence spectroscopy. All ZnPc-based compounds exhibit characteristic Q-band absorption (650-700 nm) and room-temperature phosphorescence with microsecond lifetimes, confirming efficient intersystem crossing (ISC). Dextran conjugation enhances fluorescence efficiency (ΦF = 2.37 %) and reduces aggregation, whereas Fe3O4 incorporation modifies the spin-orbit coupling, promoting magnetically assisted ISC and additional non-radiative channels. The triplet lifetimes vary between 1-9 μs, depending on molecular substitution and interfacial coupling. These results demonstrate that combining photoactive ZnPc cores with natural polymer matrices and magnetic nanoparticles enables control over excited-state dynamics and ROS generation for biomedical applications.

CPP 46.17 Thu 9:30 P5

Biopolymer-Templated Deposition of Hierarchical 3D-Structured Graphene Oxide/Gold Nanoparticle Hybrids for Surface-Enhanced Raman Scattering — •Yingjian Guo[1,2], Guangjiu Pan[2], Yusuf Bulut[1,2], Arno Jeromin[1], Thomas F. Keller[1], Andreas Stierle[1], Gergely Nemeth[3], Ferenc Borondics[3], Benedikt Sochor[1], sarathlal K. Vayali[1], Daniel Söderberg[4], Peter Müller-Buschbaum[2], and Stephan V. Roth[1,4] — [1]DESY, Hamburg — [2]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [3]Synchrotron SOLEIL, Saint-Aubin, France — [4]Department of Fibre and Polymer Technology, KTH, Stockholm, Sweden

Cellulose has emerged as a promising bio-based template for sensors, smart windows, and bioelectronics. Typically, Surface Enhanced Raman Scattering (SERS), an advantageous analytical technique, allows for the rapid detection and structural analysis of chemical compounds through their spectral patterns in nanotechnology. Crucial for SERS is fabricating the substrates with strong enhancements of the Raman signal over large areas. Herein, we present a straightforward approach utilizing the layer-by-layer spray coating method to fabricate films loaded with gold nanoparticles and graphene oxide to serve as SERS substrates. GISAXS combined with nano-FTIR spectroscopy was used to confirm a synergistic Raman enhancement mechanism of localized surface plasmon resonance and interface charge transfer. Our approach provides a reference for facile and scalable production of SERS substrates.

CPP 46.18 Thu 9:30 P5

Regulation of HUVEC Adhesion by Mechanical and Biochemical Tuning of PNIPAM Microgel Coatings — •Leonie Beer, Souraj Mandal, and Regine v. Klitzing — Soft Matter at Interfaces, Department of Physics, TU Darmstadt, Darmstadt 64289, Germany

A bioactive and stable interfacial layer favouring HUVEC cell adhesion is a key factor in artificial vascular network construction. This work investigates the impact of the mechanical and biochemical properties of PNIPAM microgel (MG) coatings on HUVEC cell adhesion and proliferation on 3D printed polymeric surfaces. MG stiffness can be varied based on cross-linking, and bioactivity can be imparted by functionalizing MG with RGD-based peptide mimicking extracellular matrix (ECM) ligands. HUVEC cell culture studies showed significant effects of MG stiffness on cell adhesion and proliferation, with further improvement due to biochemical functionalization. In addition, different spacers were used to enhance cell attachment and growth.

MG adhesion on different substrates was also evaluated, revealing significantly stronger adsorption on 3D-printed polymeric surfaces compared to inorganic substrates. AFM imaging confirmed the presence of firmly adhered MGs beneath the cells, demonstrating long-term coating integrity under biological conditions.

These results demonstrate that PNIPAM MG coatings provide a robust, tunable, and bioactive platform for controlling HUVEC behaviour and represent a promising strategy for endothelialization of 3D-printed vascular structures.

CPP 46.19 Thu 9:30 P5

Crystallization behavior of electron beam modified Polylactide acid (PLA) — •Regine Boldt[1], Elisabeth Hauschild[1], Michael Müller[1], and Markus Stommel[1,2] — [1]Leibniz Institut fuer Polymerforschung Dresden, Germany — [2]Dresden University of Technology, Germany

Polylactic acid (PLA) is a polymer synthesized from renewable raw materials. The properties of PLA are essentially determined by its chemical/physical structure, such as molar mass, molar mass distribution, D-isomer content, and the resulting morphology. The morphology can be influenced by modifying the molecular structure on the one hand, and by the process parameters during processing on the other. Since PLA crystallizes very slowly, high cooling rates, which occur in processing methods such as injection molding, usually result in amorphous components. In this work, we modified PLA using high-energy electrons in order to accelerate its crystallization without adding external additives. The resulting changes in crystallization kinetics were analyzed and correlated with the morphology after irradiation. The spherulite growth rates were determined quantitatively using hot stage experiments on a light microscope. The results show that electron-modified PLA exhibits substantially increased crystal growth rates, enabling significant reductions in cooling time during processing operations such as injection molding.

CPP 46.20 Thu 9:30 P5

Diffusion and stiffness characterization of photocrosslinked hydrogels to replicate biological tissues — •Lena Hilf[1], Dimitris Missirlis[1,2], and Kai Melde[1] — [1]Institute for Molecular Systems Engineering and Advanced Materials, Universität Heidelberg — [2]MPI for Medical Research, Heidelberg

Microphysiological systems (MPS), such as organs-on-a-chip, aiming to replicate the spatial arrangement of biological tissues found in vivo are in need of a reliable and replicable way to recreate the biophysical environment including topography and mechanical properties. One possible route is via selective photocrosslinking of hydrogel scaffolds, which can be performed in situ in microfluidic platforms.

However, we still lack reliable information about key properties of potential hydrogel candidates in these systems, which influence cell adhesion and spreading, as well as the uptake of media components.

In this work, we characterize the stiffness, mesh size and diffusion constant of a range of hydrogels created using photolithpgraphy. We employ both optical and mechanical approaches, taking into account the versatility of hydrogel responses to different measurement methods.

Our results together with cell proliferation assays allow for a more targeted choice of hydrogels to serve as artifical extracellular matrices in MPS.

CPP 46.21 Thu 9:30 P5

Characterization of bimodal PMMA-PDMS suspensions using light scattering — •Katharina Gaus and Joachim Wagner — University of Rostock, Rostock, Germany

Poly-dimethylsiloxane coated PMMA particles index matched in tetraline/decaline mixtures are well defined model systems for hard spheres with tunable particle size. Binary mixtures of these core-shell particles with slightly different sizes artificially increase the polydispersity of colloidal model systems preventing crystallization at large volume fractions and thus enabling the preparation of colloidal glasses. Using a priori knowledge of both species' topology, even in the limited range of wave vectors accessible with light scattering experiments, the reliable structural characterization of mixtures is possible. Hence, such binary mixtures are promising model systems for colloidal glasses.

CPP 46.22 Thu 9:30 P5

Cycles of buckling in gel phase giant unilamellar vesicles — •Azeline Hilaire, Antonio Stocco, Jean Farago, and Fabrice Thalmann — Institut Charles Sadron, Strasbourg, France

Buckling can be observed in giant unilamellar vesicles (GUVs) in gel phase, leading to shape deformations under external stress. Such deformations may offer functional advantages, particularly for inducing motion at low Reynolds numbers.

Recently, lipid-coated microbubbles were shown to exhibit directed motion through deformation cycles, suggesting a broader potential for soft interfaces to generate propulsion. Inspired by this, we investigate whether similar mechanisms can be used in isolated GUVs under cycles of deformation, with the goal of understanding and eventually triggering symmetry-breaking dynamics. We aim to use shape hysteresis for producing directed motion.

Gel-phase GUVs were fabricated via hydration method and characterized by their ability to transition between buckled and unbuckled states. We exposed these vesicles to cyclic fields using three distinct methods: (i) oscillatory shear flows, (ii) osmotic pressure, (iii) On/Off cycles of light applied with optical tweezers. In some of these cases, the membrane exhibited buckling.

Although directed motion has not yet been observed, the buckling response establishes a first result for future efforts to induce propulsion in vesicles. These preliminary results offer a first step towards exploring whether shape hysteresis in membranes could one day be used for active functions.

CPP 46.23 Thu 9:30 P5

Dynamics of trifunctional hybrid nanoparticle assemblies — •Thomas Dartige[1], Yinan Fan[2], Clément Marque[1], Ali Abou-Hassan[2], and Antonio Stocco[1] — [1]Institut Charles Sadron, Strasbourg, France — [2]Phenix Lab, Paris, France

Active colloids are colloidal systems able to consume energy to produce work, such as directed motion. Self-propulsion in micrometric particles can be achieved through surface asymmetries, using diffusiophoresis (via asymmetric catalytic properties) or thermophoresis (via asymmetric light absorption). However, the combining of several active properties into one single colloidal system remains poorly explored. In this work, we present a hybrid system synthesized by combining distinct nanoparticles, and investigate its ability to exhibit diffusiophoresis, thermophoresis, and respond to magnetic field gradients.

CPP 46.24 Thu 9:30 P5

Physics-Informed Neural Inference with Multilayer DWBA Modeling for Quantitative GISAXS — •Özüm Emre Asirim[1,2], Yufeng Zhai[1], Marina Tropmann-Frick[2], and Stephan V. Roth[1,3] — [1]Deutsches Elektronen-Synchrotron DESY FS-SMA Notkestr. 85 22607 Hamburg Germany — [2]HAW Hamburg Berliner Tor 7 20099 Hamburg Germany — [3]KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden

Quantitative GISAXS analysis is often constrained by the complexity of multilayer scattering, film-nanoparticle coupling, and the limited availability of physically interpretable synthetic datasets for training modern inference models. We address these challenges with a physics-informed neural framework that integrates a compact multilayer DWBA formulation with a hybrid CNN-Transformer architecture. The forward model captures essential film and nanoparticle scattering through per-layer incoherent DWBA terms, normalized form factors, structure factors, and DWBA-based field enhancement, yielding a reduced and physically coherent parameter space suitable for inversion. Measurement variability is modeled through noise, detector effects, and the ability to generate time-series data for evolving structures. Leveraging this parameterization, the CNN-Transformer network jointly extracts local scattering motifs and long-range reciprocal-space correlations, enabling accurate recovery of film- and particle-level parameters. Validated through forward reconstruction using the same physics model, the workflow provides a fast, interpretable, and physically grounded solution for high-throughput GISAXS analysis.

CPP 46.25 Thu 9:30 P5

How Polymer Architecture Shapes the Phase Behavior of Polyelectrolyte Complex Coacervates — •Lena Tarrach, David Beyer, and Christian Holm — Institute for Computational Physics, University of Stuttgart, Stuttgart, Germany

Polyelectrolyte (PE) complex coacervation is an associative liquid-liquid phase separation that can occur in mixtures of oppositely charged macromolecules. Although this phenomenon is widely studied, the effects of the polymer architecture on the phase behavior of PE complex coacervates have not been considered so far. To close this gap, in this contribution, coarse-grained molecular dynamics (MD) simulations with the ESPResSo software [1] are applied to calculate the phase diagram of branched PEs with varying numbers of arms but the same overall molecular weight. The slab method is used to establish the coexistence of the coacervate phase and the supernatant solution. The number of arms of the PEs is systematically increased to assess the influence of the PE topology on the phase behavior. The obtained phase diagrams are subsequently compared to theoretical phase diagrams calculated using the random phase approximation.

[1] Florian Weik, Rudolf Weeber, Kai Szuttor, Konrad Breitsprecher, Joost de Graaf, Michael Kuron, Jonas Landsgesell, Henri Menke, David Sean, and Christian Holm. ESPResSo 4.0 - an extensible software package for simulating soft matter systems. The European Physical Journal Special Topics, 227(14):1789-1816, 2019. doi:10.1140/epjst/e2019-800186-9.

CPP 46.26 Thu 9:30 P5

Self-assembled Micelles from Charged Block Copolymers: Insights from Small-Angle X-ray Scattering (SAXS) — •Yijun Zhao[1], Varvara Chrysostomou[2], Athanasios Skandalis[2], Stefano Da Vela[3], Stergios Pispas[2], and Christine M. Papadakis[1] — [1]TUM School of Natural Sciences, Soft Matter Physics Group, Garching, Germany — [2]Theoretical and Physical Chemistry Institute, NHRF, Athens, Greece — [3]EMBL at DESY, Hamburg, Germany

Block copolymer micelles have been widely studied due to their ability to load drugs. Positively charged micelles have been proposed to complex DNA, enabling efficient gene therapy. To achieve highly tunable morphology, self-assembled micelles from the diblock copolymers PDMAEMA-b-PLMA and the triblock terpolymers PDMAEMA-b-PLMA-b-POEGMA are investigated in aqueous solution [1]. Here, PDMAEMA stands for the weak polycation poly(2-(dimethylamino)ethyl methacrylate), PLMA for the hydrophobic, but soft poly(lauryl methacrylate), and POEGMA for the hydrophilic poly(oligo(ethylene glycol) methacrylate). Small-angle X-ray scattering (SAXS) on dilute aqueous solutions revealed that PDMAEMA-b-PLMA forms ellipsoidal core-shell micelles, with their size and inner structure depending on temperature and the pH value. For the triblock terpolymers, the micellar structures depend strongly on the block lengths.

[1] V. Chrysostomou et al., J. Polym. Sci. 63 1684-1694 (2025).

CPP 46.27 Thu 9:30 P5

Pump-probe spectroscopy on the polyelectrolyte donor polymer PTHS for solar cell applications — •Mick Gindorf[1], Anna Köhler[1], Christopher Vogt[2], and Johannes C. Brendel[2] — [1]Chair of Soft Matter Optoelectronics, University of Bayreuth — [2]Chair of Macromolecular Chemistry I, University of Bayreuth

Poly(3-hexylthiophene) (P3HT) is a well-researched donor polymer for application in organic solar cells (OSCs). Side chain modification of P3HT with sulfonate groups yields PTHS, a polyelectrolytic donor polymer with high hole transport mobility [1]. This polyelectrolyte possesses two key advantages: Firstly, exchange of the cationic counter ions enables insolubilization of the donor layer, allowing simple fabrication of donor-acceptor bilayer systems by sequential spin coating with a wide variety of acceptors, including both fullerene and non-fullerene acceptors (NFAs). Secondly, adjusting the counter ion composition enables tuning of the donor energy level and thereby the donor-acceptor energy level offset (E_{off}), which is critical for achieving high open circuit voltages (V_{oc}). These properties make PTHS an ideal model system for the investigation of exciton dissociation in OSCs with spectroscopic techniques, including time-resolved transient absorption spectroscopy. Probing the exciton dissociation dynamics as a function of E_{off} on a picosecond timescale in different donor-acceptor systems yields valuable insights into the energetic and entropic contributions that help overcome the exciton binding energy in OSCs.

1) Brendel, J. et al. Chem. Mater. 2014, 26, 6, 1992-1998

CPP 46.28 Thu 9:30 P5

PEDOT Molecular Imprinting in PEDOT:PSS/PDADMA Layer-by-Layer Films — •Martin Hunger, Muhammad Khurram, and Christiane A. Helm — martin.hunger@uni-greifswald.de

PPEDOT:PSS films are widely used because they offer high conductivity & tunable electro-optical properties. We prepare PEDOT:PSS films with a thickness of up to 150 nm using Layer-by-Layer assembly. We vary the preparation conditions: flow cell, dip coating, PEDOT:PSS concentration in solution, and rinsing steps. Whenever PDADMA is the top layer, UV-vis-IR absorption spectroscopy

shows that there is significantly less PEDOT in the films than when PEDOT:PSS is the top layer. Films prepared using the flow cell have the highest electrical conductivity (approx. 200 kS/m) with PEDOT:PSS. When PEDOT is the top layer, conductivity is reduced by a factor of 100. The conductivity of films prepared with dip coating with PEDOT:PSS as the top layer is one order of magnitude lower or more. When PDADMA is the top layer, conductivity drops by an additional 4 to 5 orders of magnitude. Thus, during assembly, PEDOT can be selectively removed and subsequently rebound to the film, leaving behind well-defined molecular cavities that preserve their shape and enable reconstruction of percolative pathways.

CPP 46.29 Thu 9:30 P5

PDADMA/PSS Multilayer Buildup in NaBr Solution: Vertical PSS Diffusion and Unusual Growth — •Per-Ole Hilken, Issam Assi, and Christiane A. Helm — Institute of Physics, University of Greifswald, Germany

Polyelectrolyte multilayers form by sequential adsorption of oppositely charged polyelectrolytes. The interfaces between the adsorption layers are fuzzy; in the exponential growth regime of PDADMA/PSS (poly(diallyldimethylammonium)/polystyrene sulfonate) multilayers PSS diffuses vertically through the film. We determine its vertical diffusion coefficient D_{PSS} using a quartz crystal microbalance with dissipation (QCM-D). The scaling laws for D_{PSS} in dependence of the NaBr concentration are similar to those found with NaCl in the deposition solution (Sill et al., Macromolecules 2025), however, the diffusion coefficient is one to two orders of magnitude larger. The dependence on PSS molecular weight M_{PSS} is qualitatively the same as with NaCl in the deposition solution: Polymer diffusion dominates multilayer build-up when $M_{PSS} < 76$ kDa.; at larger M_{PSS}, site diffusion dominates; i.e. diffusion of charged repeat units with their counterions. For polyelectrolyte multilayers in the non-exponential growth regimes it is well known and also found with that an increase in the salt concentration leads to thicker multilayers. This is not the case if the NaBr concentration exceeds ≈ 0.6 M; additionally, film stability becomes an issue. To understand the unusual behavior, the dissipation during film build-up is quantified. The surface topography is investigated with AFM.

CPP 46.30 Thu 9:30 P5

Structural influences on nonlinear optical activity in the heterocubane family — •Alexander Kapp and Simone Sanna — alexander.kapp@pysik.uni-giessen.de

Recent progress in the study of molecular clusters with extreme nonlinear optical response has highlighted their potential for coherent broadband light generation. To extend the library of suitable candidate materials, we investigate the linear and nonlinear optical properties of a family of heterocubanes with the general formula $[(RM)_4Pn_4]$, where M = C, Si, Ge, Sn, Pn = N, P, As, Sb, Bi, and R = H, Me, Ph. Using *ab initio* density functional theory, we analyze their structural and electronic characteristics, including optimized geometries, symmetry features, band gaps on different theoretical levels and shape of the HOMO–LUMO orbitals. Both the linear and the nonlinear (SHG) optical responses of all systems are computed using the Yambo code. Clear trends emerge that link the optical activity to the choice of pnictogen, tetrel, and substituent. These findings help identify promising candidates for nonlinear optical applications and contribute to a deeper understanding of structure–property relations in heterocubane materials.

CPP 46.31 Thu 9:30 P5

A micellar solution from thermoresponsive block copolymers during pressure jumps — •Yandong Wang[1], Geethu P. Meledam[1], Leonardo Chiappisi[2], Cristiane Henschel[3], André Laschewsky[3,4], Alfons Schulte[5], and Christine M. Papadakis[1] — [1]TUM School of Natural Sciences, Soft Matter Physics Group, Garching, Germany — [2]ILL, Grenoble, France — [3]Universität Potsdam, Germany — [4]Fraunhofer IAP, Potsdam-Golm, Germany — [5]University of Central Florida, Orlando, U.S.A.

The diblock copolymer PMMA-b-PNIPAM, consisting of a hydrophobic poly(methyl methacrylate) and a thermoresponsive poly(N-isopropylacrylamide) block, forms core-shell micelles in dilute aqueous solution at atmospheric temperature. These micelles aggregate upon heating or applying pressure. Previous studies have shown that the micellar shell remains hydrated in the two-phase region under high pressure, in contrast to the strongly dehydrated micelles observed in the two-phase region at atmospheric pressure [1]. In this work, we analyzed the micellar transition kinetics during rapid pressure jumps using time-resolved small-angle neutron scattering (SANS). The system was driven from the one-phase region into the two-phase region at target pressures in both low- and high-pressure regimes.

[1] P. A. Alvarez Herrera et al., Macromolecules 2024, 57, 10263.

CPP 46.32 Thu 9:30 P5

Photoresponsive Interfacial Behavior of Hybrid Photosensitizer-Surfactant Mixtures — •Phat Tan Pham[1], Julius Gemen[2], Frank Glorius[2], and Björn Braunschweig[1] — [1]Universität Münster, Institut für Physikalische Chemie, Corrensstr. 28/30, 48149 Münster — [2]University of Münster, Organisch-Chemisches Institut, Corrensstraße 40, 48149 Münster

Fluid interfaces that adapt to external triggers such as light or temperature are of great interest for driving changes in soft matter systems like foams and emulsions. Arylazopyrazoles (AAPs), as photo-responsive surfactants, can control surface tension and molecular organization at air-water interfaces through E/Z photoisomerization. However, light-induced switching of AAP derivatives is typically limited to UV and green light. To overcome this, we combined AAP with the water-soluble photosensitizer resazurin (Rez) and achieved pronounced interfacial changes under 625 nm red-light irradiation. By tuning the AAP/Rez molar ratio, we further introduced history-dependent, quasi-adaptive changes in surface tension and molecular structure. The latter was examined in situ with surface tensiometry and vibrational sum-frequency generation (SFG) when the samples where irradiated at 365, 520, or 625 nm. We propose that red-light activation occurs at the interface, through photoexcited Rez moieties at 625 nm and subsequent intersystem crossing to adjacent interfacial AAP molecules. These results demonstrate a new strategy to extend the optical control of photo-responsive surfactants into the red-light region.

CPP 46.33 Thu 9:30 P5

Thermoresponsive Microgel Membrane for applications in an Electrochemical Device — •Aditi Gujare[1], Stefanie Uredat[2], Jonas Runge[2], Domenico Truzzolillo[1], Julian Oberdisse[1], and Thomas Hellweg[2] — [1]Soft Matter Physics Team, Laboratoire Charles Coulomb, University of Montpellier, Montpellier, France — [2]Physical and Biophysical Chemistry, Bielefeld University, Bielefeld, Germany

Microgels based on NIPAM are thermoresponsive with a volume phase transition temperature (VPTT) of 33°C. The VPTT has been observed to shift by copolymerizing these microgels with comonomers such as N-hydroxymethyl acrylamide (HMAM).[1] Different sets of copolymers have been tested, NIPAM-co-HMAM and NIPMAM-co-HMAM. These microgels have been observed to have a VPTT up to 60°C. The copolymer microgels based on the comonomer HMAM has an alcohol group, making it prone to condensation at high temperatures (above 90°C) resulting in formation of a membrane. These thermoresponsive, chemically crosslinked membranes have been prepared by dropcasting and crosslinking at 100°C. Such membranes can be prepared in a range of thickness, of 30-800 μm. The resistance of these membranes of different thickness, comonomer content, and at different temperatures are being tested. Resistance measurements at room temperatures show that thicker membranes are more resistive in a certain concentration of an electrolyte. [1]Gujare,Uredat,Runge,Morgenstern,Truzzolillo,Hellweg,Oberdisse, Langmuir 2025, 41, 45, 30442

CPP 46.34 Thu 9:30 P5

Correlating molecular properties of tetraphenylethylene substituted tetraphenyl heteoadamantanes to nonlinear optical activity — •Eva Westenfelder Gil and Simone Sanna — Institut für Theoretische Physik, Justus-Liebig-Universität Gießen, Germany

Recent studies have demonstrated white light generation from molecular clusters with adamantane-like cores and various substituents [1,2]. Subsequent investigations on isolated molecules revealed correlations of the structural, electronic and optical properties [3]. Building on this foundation, we focus here on further investigating structural, electronic, and (nonlinear) optical properties from first principles for isolated molecules with modified cores. In this contribution, we report on $[(PhSn)_3(TPESi)S_6]$ and $[(PhSn)_3(TPESi)Se_6]$ clusters, which are modeled within density functional theory. Distinct changes in the spectral signatures can be observed. The presented results expand on theoretical foundations for the design of tailored nonlinear optical sources.

[1] N. W. Rosemann *et al*, Science 2016, 352, 1301
[2] N. W. Rosemann *et al*, J. Am. Chem. Soc. 2016, 138, 50, 16224-16227
[3] F. Ziese *et al*, 2024. J. Phys. Chem. A 128, 8360-8372

CPP 46.35 Thu 9:30 P5

Modeling Structural and Electronic Properties of Functional Organic Molecules — •Linda Düren and Simone Sanna — Institut für Theoretische Physik, Justus-Liebig-Universität Gießen, Germany

In this work, various organic molecules with the general composition $[(RT)_4E_6]$ are investigated using density functional theory (DFT) to model their structural, electronic, and optical properties. Ground-state geometries and energies, as well as the frequency-dependent optical parameters, are calculated for the isolated clusters. The study includes *tetraphenyladamantane* and its halogenated derivatives, as well as other heteroadamantanes with a heterogeneous ligand field of the type $(MeC)(CH_2)_3(PhSn)E_3$ with E = S, Se, Te, CH_2.

The theoretical results provide insights into the relationship between molecular structure and optical behavior, building on previous studies of nonlinear optical responses in organotetrel and (hetero)adamantane-type clusters [1] and amorphous molecular materials for directed supercontinuum generation [2]. The results are compared with experimental data where available and demonstrate the potential of these classes of molecules for applications in optics.

[1] Ziese et al., *J. Phys. Chem. A* **128**, 8360 (2024)
[2] Dehnen et al., *ChemPhotoChem* **5**, 1032 (2021)

CPP 46.36 Thu 9:30 P5

Tuning PNIPAM Phase Transition and Interfacial Structures — •Zugeng Cong, Michael Hardt, and Björn Braunschweig — University of Münster, Institute of Physical Chemistry, Münster, Germany

In this work, we aim to introduce the concept of a self-regulating negative-feedback system in which an exothermic photochemical process would be coupled to the thermo-responsive polymer PNIPAM. In such a scheme, reaction-generated heat would raise the solution temperature, trigger PNIPAM collapse, increase turbidity, and thereby limit light penetration—providing an intrinsic mechanism to suppress further heat generation. For that, we characterize the PNIPAM phase transition through temperature-dependent turbidity measurements while varying SDS and NaCl concentrations as well as the water-ethanol co-solvent composition. To elucidate interfacial contributions, surface-specific sum-frequency generation (SFG) spectroscopy is used to probe adsorption layers at the air-water interface, taken as a model for micellar environments. These measurements reveal how surfactant loading, solvent composition, and electrolyte concentration reorganize interfacial structures below and above the PNIPAM phase-transition temperature. This provides the physicochemical basis required for designing a feedback-controlled photochemical soft matter system.

CPP 46.37 Thu 9:30 P5

Quasi-elastic neutron scattering of perdeuterated poly(N-isopropylacrylamide) and hydration changes across the demixing transition — •Alfons Schulte[1], Eric Rende[1], Marcell Wolf[2], Thomas Müller[3], Dirk Schanzenbach[4], Andre Laschewsky[4,5], and Christine M. Papadakis[6] — [1]Department of Physics and College of Optics and Photonics, University of Central Florida, Orlando, U.S.A. — [2]Heinz Maier-Leibnitz Zentrum (MLZ), TUM, Garching, Germany — [3]FZ Jülich, JCNS at MLZ, Garching, Germany — [4]Institut für Chemie, Universität Potsdam, Potsdam-Golm, Germany — [5]Fraunhofer-Institut für Angewandte Polymerforschung, Potsdam-Golm, Germany — [6]TUM School of Natural Sciences, Soft Matter Physics Group, Garching, Germany

We investigate the hydration dynamics of perdeuterated poly(N- isopropylacrylamide) (PNIPAM-d10) to elucidate the molecular mechanism of its demixing transition. Quasi-elastic neutron scattering (QENS) and Raman spectroscopy were measured in a 25 wt% PNIPAM-d10 aqueous solution over the temperature range from 298 to 325 K. There is a significant upward shift in the cloud point by about 4 degrees. Deuteration suppresses incoherent scattering from the polymer, allowing a clear view of hydration water dynamics. The dynamic susceptibilities reveal the relaxation processes for bulk and bound water, with the bound fraction decreasing sharply near the transition. The relaxation times of hydration water are consistently lower than in the protiated polymer, indicating faster local dynamics. Raman spectra show abrupt C-D band frequency shifts at the transition, reflecting side-group dehydration.

CPP 46.38 Thu 9:30 P5

Thermoresponsive Microgels with hydrophilic Monomers — •Stefanie Uredat[1], Aditi Gujare[2], Jonas Runge[1], Domenico Truzzolillo[2], Julian Oberdisse[2], and Thomas Hellweg[1] — [1]Physical and Biophysical Chemistry, University Bielefeld, Bielefeld, Germany — [2]Laboratoire Charles Coulomb (L2C), University of Montpellier, CNRS, Montpellier, France.

To develop fully smart membranes for use in low-temperature fuel cells operating at around 80-90 °C it is essential to achieve a high volume phase transition temperature (VPTT) within this range. To reach these high VPTTs, new monomers are required for microgel synthesis. The most common and researched monomers have a VPTT around the human body temperature [1]. To rise the VPTT we increased the hydrophilicity of the monomers by adding a hydroxy group to the well-known NIPAM and got HIPAM (N-(2-hydroxyisopropyl)acrylamide).

To tune the VPTT to higher Temperatures a series of microgels with two different main monomers (NIPAM and NIPMAM) with different contents of HIPAM as comonomer were synthesised. The microgels were observed by Dynamic Light Scattering and AFM. With higher HIPAM content the VPTT of the microgels increases and widens. We also observe a jump in size with increasing hydrophilic monomer content. We also investigated a second hydrophilic monomer N-(hydroxymethyl)acrylamide (HMAM). [2]

[1] Uredat, Runge, Gujare, PCCP, 2024, 2732. [2] Gujare, Uredat, LANGMUIR 2025, 41, 45, 30442 [3] The authors acknowledge funding from the DFG (505656154) and ANR (ANR-22-CE92-0052-01)

CPP 46.39 Thu 9:30 P5

The phase transition of perdeuterated thermoresponsive polymers — •Chenrui Ding[1], Kuno Schwärzer[2], Alfons Schulte[3], and Christine M. Papadakis[1] — [1]TUM School of Natural Sciences, Soft Matter Physics Group, Garching, Germany — [2]JCNS-1, FZ Jülich GmbH, Germany — [3]University of Central Florida, Department of Physics and College of Optics and Photonics, Orlando, U.S.A.

The interaction of thermoresponsive polymers with water has been amply studied with respect to the cloud point temperature and the latent heat at the transition, using, among others, turbidimetry and differential scanning calorimetry (DSC) [1]. New information on the polymer-water interaction can be gained using perdeuterated polymers. We present results on poly(N-isopropyl acrylamide) (PNIPAM) and poly(N-isopropyl methacrylamide) (PNIPMAM) and their perdeuterated versions in aqueous solution as a function of polymer concentration and establish the transition behavior.

1. C.-H. Ko, C. M. Papadakis et al., Macromolecules 53, 6816 (2020)

CPP 46.40 Thu 9:30 P5

Steel Mesh-Supported SNW-1/CsPbBr3 Nanocomposite: Photocatalyst for Sustainable Ammonia Production — •Negin Khosroshahi and Vahid Safarifard — Iran University of Science and Technology, Tehran 16846-13114, Iran

The conversion of solar energy into chemical energy through photocatalysis is an important field of interest in green energy generation and environmental improvement [1]. Nevertheless, its effectiveness currently falls short of expectations, primarily due to the issue of charge recombination. To address this challenge, the photocatalytic effect has become an optimistic approach for enhancing processes [2]. In this research, we have developed a Steel Mesh-Supported SNW-1/CsPbBr3 nanocomposite by combining covalent-organic frameworks with metal halide perovskite. To gauge their effectiveness, the heterostructure was assessed by employing multiple characterization methods including XRD, IR, FESEM, DRS, EDX, VSM, PL, EIS, Zeta, and BET. After the composite's preparation and characterization, we examined its photocatalytic activity in nitrogen reduction. The SNW-1/MHP/Steel mesh nanocomposite exhibited exceptional performance in ammonia generation. These findings suggest that the SNW-1/MHP/Steel mesh nanocomposite holds promise as an environmentally friendly and cost-effective photocatalyst, capable of addressing the challenges of sustainable ammonia production. This study presents a promising method for identifying effective photocatalytic materials using mesh substrates to address environmental concerns.

CPP 46.41 Thu 9:30 P5

Engineering MOF@MOF Heterojunction for Photocatalytic N2 Reduction to NH3 — •Maedeh Atoufi Kashani, Negin Khosroshahi, and Vahid Safarifard — Iran university of science and technology, Tehran, Iran

Photocatalytic nitrogen fixation is a promising green alternative to the Haber-Bosch process, but cobalt-based MOFs typically suffer from poor stability in water. Here, two Co-terephthalate frameworks were synthesized via solvothermal routes: MOF-71 from Co(NO3)3.6H2O and ultrathin Co-BDC nanosheets from CoCl2.6H2O in the presence of triethylamine, water, and ethanol. Both materials showed high phase purity and strong visible-light absorption. To improve the limited stability of Co-BDC, a Ce-based MOF overlayer was constructed on Co-BDC and MOF-71, forming a Ce-Co MOF-on-MOF composite. The Ce shell enhanced water stability, facilitated charge separation, and promoted N2 activation at the heterointerface. As a result, the Ce-Co-BDC composite delivered markedly higher ammonia production and durability than pristine Co-BDC. This work highlights the critical roles of precursor chemistry and Ce-Co interfacial engineering in developing robust MOF photocatalysts for solar-driven nitrogen fixation. [1] S. Nabi, M.M. Bhat, A. Hamid, A.Y. Bhat, A.U. Bashir, Q. Jan, P.P. Ingole, M. Bayati, M.A.J.A.S.S. Bhat, (2025) e00112. [2] G. Song, Y. Shi, B. Yang, Y. Yang, H.J.I.C. Pang, 64 (2025) 6265-6274.

CPP 46.42 Thu 9:30 P5

Structural Insights into Supported Ionic Liquid Phases — •Yufei Wu[1], Julius Schlüter[2], Chandan K. Das[3], Zhuo Chen[1], Alexis Bordet[1], Maria Fyta[3], and Thomas Wiegand[1,2] — [1]Max Planck Institute for Chemical Energy Conversion, Mulheim an der Ruhr, Germany — [2]Institute of Technical and Macromolecular Chemistry, RWTH Aachen University, Aachen, Germany — [3]Computational Biotechnology, RWTH Aachen University, Aachen, Germany

Metal nanoparticles supported on molecularly modified surfaces (MMSs) offer significant potential for the development of advanced materials chemistry, particularly in catalysis. In this work, we focus on supported ionic liquid phases (SILPs) as a representative class of MMS materials. The SILP material was synthesized by functionalizing an amorphous silica surface with a layer of phosphonium-based ionic liquid (IL) covalently bound to the silica. The structural features of the SILP, specifically the conformation of the phosphonium IL cations, were characterized using magic-angle spinning (MAS) solid-state NMR spectroscopy. To complement the experimental findings, all-atom molecular dynamics (MD) simulations were performed on IL-modified silica surfaces. These simulations provided atomic-level insights into the structural organization and conformational dynamics of the IL molecules in the SILP materials. This combined approach paves the groundwork for future studies aimed at realizing SILP materials as efficient catalytic templates.

CPP 46.43 Thu 9:30 P5

Towards stable passivation layers on III-V-semiconductor nanowires for photoelectrochemical water splitting applications — •Chris Yannic Bohlemann, Pavithira Manoharan, Sahar Shekarabi, Peter Kleinschmidt, Thomas Hannappel, and Juliane Koch — Technische Universität Ilmenau, Fundermentals of Energy Materials, Ilmenau, Germany

The production of green hydrogen is expected to play a crucial role in achieving a sustainable, climate-neutral economy. Although III-V semiconductors offer record solar-to-hydrogen conversion efficiencies, the large-scale deployment is limited by the scarcity of the required materials. III-V nanowires (NWs) are a promising approach, as they require less material than planar films, and exhibit an enhanced optical absorption, as well as benefit from a high surface-to-volume ratio [1].

However, the instability of III-V materials in aqueous electrolytes leads to rapid corrosion and short lifetimes of photoelectrodes. To address this limitation, we investigated the growth behavior, electrical properties, and corrosion stability of GaAsP NWs and subsequently passivated with GaP(N) shells grown via metal-organic vapor-phase epitaxy. Scanning electron microscopy was used to examine the growth quality, crystal orientation, defect structures, and degradation before and after extended operation under water splitting conditions. Our results demonstrate that the application of a GaP(N) passivation layer significantly enhances the structural integrity and durability of the NWs during continuous photoelectrochemical water splitting.

[1] J. Koch et al., Adv. Energ. Sust. Res. e202500156, 2025.

CPP 46.44 Thu 9:30 P5

A Bottom-Up Coarse-Grained Model of Nanoparticles Decorated with Oppositely Solvent-Responsive Diblock Copolymers for Reversible Self-Assembly — •Daniel Otschkowski and Arash Nikoubashman — Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany

Polymer-grafted nanoparticles (PGNPs) combine the optical, magnetic, or electronic functionality of inorganic cores with the elasticity and responsiveness of polymer chains. This hybrid character offers multiple, orthogonal design parameters for controlling the structure and properties of PGNP-based materials. In this work, we study spherical NPs grafted with amphiphilic diblock copolymers composed of two blocks with opposing solvent affinities, enabling reversible transitions between assembly and disassembly states. In the assembly state, the inner polymer block is solvophilic while the outer block is solvophobic, thus collapsing into attractive patches; in the disassembly state, the inner block forms a dense polymer shell which is surrounded by a stabilizing hydrophilic polymer corona. To access device-relevant time and length scales, we develop a bottom-up coarse-grained (CG) model, where we describe the PGNPs in the assembly state as particles with flexible, spring-tethered patches. Smoothly varying the effective interactions allow the CG model to reproduce the continuous transition between both states. This approach enables efficient simulation of large PGNP systems and provides insight into their reversible, stimuli-responsive behavior.

CPP 46.45 Thu 9:30 P5

Organic cathodes based on polyaniline and cellulose for aqueous Zn-ion batteries — •Ramsha Wasi Khan[1], Meriem Boudjenane[1], Gilles Wittmann[1], Xaver Brehms[2], Simon Schraad[3], Xinyu Jiang[3], Stephan V. Roth[3], and Lucas P. Kreuzer[1] — [1]Heinz Maier Leibnitz Zentrum (MLZ), TUM, Garching, Germany — [2]CEA, Grenoble, France — [3]DESY, Hamburg, Germany

Aqueous zinc-ion batteries are promising candidates for a non-toxic and safer alternative to lithium-ion batteries, where organic cathodes provide distinct advantages of sustainability, tunability and mechanical flexibility. In this work, we investigate the role of polyaniline (PANI) as an organic cathode material, motivated by its high theoretical capacity, reversible redox chemistry, and intrinsic electrical conductivity. To enhance stability against humidity-induced degradation, cellulose derivatives are employed as green binders, enabling regulation of water uptake and improved mechanical stability. Comprehensive multiscale characterization is conducted to optimize the electrochemical performance and structural integrity of PANI-based cathodes, as well as understand the morphological changes and nanoscale water dynamics under humidity. Advanced techniques such as cyclic voltammetry, scanning electron microscopy (SEM), and quasi-elastic neutron scattering (QENS) are used to support this analysis. It was observed that the use of composite cellulose films as a binder with an optimized composition effectively triples the current density and improves peak reproducibility as well as the water uptake behaviour of the film.

CPP 46.46 Thu 9:30 P5

Integration of Ag_2S nanocrystals into flexible polymer matrices — •Dolores García de Viedma Guerra, Peijiang Wang, and Beatriz Hernández Juárez — Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Madrid E-28049, Spain

A broad range of modern optical technologies, for instance flexible photonics, require luminophores to be embedded within mechanically versatile host materials [1]. Usually, transferring nanocrystals from colloidal dispersions into polymer networks alters their physicochemical environment, which promotes surface traps and can thus signify a loss in photoluminescence [2].

In this work we investigate Ag_2S nanocrystals integrated into flexible polymer matrices with the goal of preserving their NIR response. We assess nanocrystal dispersion and spatial homogeneity, and probe their optical performance under 808 nm laser excitation via photoluminescence measurements and infrared spectroscopy, while NIR imaging maps emission uniformity. The results yield bright, uniform nanocrystal-polymer composites suitable for optoelectronic integration.

[1] Gordillo, H. et al. "Polymer/QDs Nanocomposites for Waveguiding Applications".*Journal of Nanomaterials* 2012, 960201, 2012.

[2] Marcus Jones et al. "Signatures of Exciton Dynamics and Carrier Trapping in the Time-Resolved Photoluminescence of Colloidal CdSe Nanocrystals". *The Journal of Physical Chemistry* C 2009, 113 (43), 18632-18642.

CPP 46.47 Thu 9:30 P5

Exploring the length limit for freestanding electrodeposited Ni nanowires — •Anneliese Wirth and Karin Leistner — Chemnitz University of Technology, Chemnitz 09107, Germany

Magnetic nanowire arrays are of interest from a fundamental and application point of view due to the shape anisotropy and high surface-to-volume ratio. This can be advantageous for 3D memory devices, micro-hard magnets and catalysis. The goal of this project is to obtain freestanding Ni nanowire arrays in order to functionalize their surface and possibly apply electrolytic gating strategies for 3D magneto-ionic materials in the future.[1] The Ni nanowire synthesis is performed by electrodepositing Ni into aluminum oxide membranes that serve as templates. Afterwards, the template is removed via dissolution of the aluminum oxide to achieve freestanding nanowires. For nanowires with high aspect ratio, this step usually leads to the collapse of the wires into agglomerated bundles.[2] This causes the loss of the nanowires' perpendicular alignment to the substrate. We show an optimized synthesis that avoids the collapse of nanowires with high aspect ratio in a large-scale array with a total size of around 0.5 cm^2. The deposition time during the electrodeposition is varied to obtain nanowires reaching up to more than 10 μm length while the diameter is fixed to 200 nm. Scanning electron microscopy indicates that the freestanding nature is related to irregularities of the nanowires which are introduced by the specific template geometry and lead to the stabilization of the array. [1] M. Nichterwitz et. al, ACS Mater. Au 2024, 4, 55. [2] N. Winkler et. al, J. Mater. Chem. 2012, 22, 16627.

CPP 46.48 Thu 9:30 P5

Structure and Morphology Investigations of Perovskite Nanocrystal Film — •Azam Davoodabadifarahani[1,2], Thomas Baier[1], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]University of Applied Sciences, Munich, Germany

In recent years, perovskite quantum dot solar cells with the ABX3 structure have shown great promise due to their high power conversion efficiency (PCE), high photoluminescence quantum yield (PLQY) and narrow photoluminescence (PL) peak. Within the presented work, the active layer consists of PQD thin films based on CsPbI3 and FAPbI3, which exhibit high photoelectric performance. However, CsPbI3 has a challenge with phase instability and FAPbI3 suffers from weak structural stability. To balance the performance and stability of the active layer, FAxCs1-xPbI3 PQDs are employed as the light-absorbing layer. The samples are evaluated using various optical and structural characterization techniques, such as PL spectroscopy, scanning electron microscopy (SEM), X-ray diffraction (XRD) and grazing incidence x-ray scattering (GIXS) to observe the influence of the synthesis process, temperature, and deposition techniques on the crystal size, orientation, phase, and stability, all of which determine the external quantum efficiency and optical performance.

CPP 46.49 Thu 9:30 P5

Surface-induced morphology and in-plane order in thin films of polydiketopyrrolopyrroles — •Anton Sinner and Oleksandr Dolynchuk — Martin Luther University Halle-Wittenberg, Germany

Board-like conjugated polymers are of particular interest in the context of surface-induced ordering because they often exhibit a preferred out-of-plane molecular orientation in thin films. Recent studies of ordering in conjugated polymer films have found that the free surface induces the formation of sanidic liquid crystalline (LC) mesophases with out-of-plane, smectic-like positional order between polymer chains. However, the question of whether the surface influences the in-plane order between polymer chains during ordering remained open. Here, we use atomic force microscopy to investigate the surface morphology and nanoscale structure formed on the surface of polydiketopyrrolopyrrole (PDPP) films after slow cooling and ordering from the melt. We find that the surface morphology consists of disc-like crystallites with diameters roughly equivalent to the polymer contour length and heights equivalent to several out-of-plane polymer layers. Thus, the observed LC morphology is consistent with the earlier study of out-of-plane molecular order. On a larger scale, multiple LC discs arrange into string-like morphologies, suggesting the existence of orientational order among them. Quantitative analysis of the surface morphology allows for calculating a distance-dependent orientation correlation function for six-fold symmetry, which indicates the presence of quasi-long-range order on the surface of PDPP films.

CPP 46.50 Thu 9:30 P5

Investigation of structure and transport properties in redox-active polymers — •Laura Hölzer[1] and Diddo Diddens[2] — [1]Institut für Physikalische Chemie, Universität Münster, 48149 Münster, Germany — [2]Helmholtz Institute Münster, Forschungszentrum Jülich GmbH, 48149 Münster, Germany

Organic radical batteries are seen as an alternative to traditional lithium-ion batteries. Their advantages include fast charge and discharge processes, and mechanical flexibility. However, high power densities are required for their application in the Internet of Things. To achieve this, good charge transport is essential. This transport mechanism is guided by two factors: the movement of electrons along the polymer, which is dictated by its structure, and the compensation of charge by counterions, which affects their mobility. The focus here is on a cathode material consisting of a redox-active polymer such as poly(2,2,6,6-tetramethylpiperidinyloxy-4-ylmethacrylate) (PTMA), which is in contact with a solvent. Classical molecular dynamics simulations of a PTMA cathode model are carried out. These provide insights into the structural properties and dynamics of charge transport. An outlook on the behaviour at interfaces around the cathode is given.

CPP 46.51 Thu 9:30 P5

Ex-Situ Investigation of Latex Deformation — •Simon Schraad[1,2], Shuxian Xiong[1,2], Helder Marques Salvador[3], Benedikt Sochor[1], Sarathlal Koyiloth Vayalil[1,4], Peter Müller-Buschbaum[2], and Stephan V. Roth[1,5] — [1]DESY, Hamburg, Germany — [2]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [3]CPP, Venlo/Poing, Netherlands/Germany — [4]UPES, India — [5]KTH, Department of Fibre and Polymer Technology, Stockholm, Sweden

Colloidal polymer latexes are used in ink-jet printing to form a pigment stabilizing layer on top of the cellulose layer. The latex film formation (LFF) is influenced by humidity, temperature, minimum film formation temperature (MFFT), and glass transition temperature (T_g). Exceeding MFFT polymer colloids begin to deform and further heating above the T_g polymers interdiffuse and coalesce into a homogeneous coating layer. Here we investigate cellulose nanofibrils (CNF) thin films coated with polystyrene colloids (diameters ranging from 100 to 500 nm) and commercially available polymeric colloids with different MFFT (Neocryl A639 and A1127). The samples were prepared by spray coating at temperatures below and above their T_g. Scanning electron microscopy revealed the size and shape of the colloids. Grazing incidence small angle scattering data shows contributions of spherical form factors from the colloids with respective diameters, which changes upon heating. We present a design of an experimental spray chamber to allow in-situ GISAXS and the spectral reflectance during spray deposition of latex inks to be used at synchrotron facilities.

CPP 46.52 Thu 9:30 P5

A DFTB Pseudoatom-Based Fragmentation Strategy — •Kevin Mächtel — Karlsruher Institut für Technologie, Institut für Physikalische Chemie, Karlsruhe, Germany

Theoretical investigations of charge transport mechanisms in large molecular systems often rely on efficient fragmentation strategies, to reduce computational costs. In conventional approaches, link atom fragmentation has been used for this purpose, but pseudoatom approaches offer a more versatile alternative. They enable more efficient molecular fragmentation, simplifying the overall fragmentation process. In this study, we develop a novel density functional tight-binding pseudoatom fragmentation scheme for complex molecular systems. We tested our approach on 9,10-di(quinolin-6-yl)phenanthrene and demonstrated strong agreement with the established link atom method.

CPP 46.53 Thu 9:30 P5

Benchmarking the Transferability of Machine Learning Interatomic Potentials for Polymers — •Mirko Fischer and Andreas Heuer — Institute for Physical Chemistry, University of Münster, Corrensstraße 28/30, 48149 Münster

Machine Learning Interatomic Potentials (MLIPs) enable molecular dynamics (MD) simulations with nearly quantum-chemical (QM) accuracy and have been successfully applied to various molecular systems. However, their systematic application to polymer systems has not yet been explored. A key challenge arises from the large molecular size, which makes QM reference calculations for the training data computationally demanding. Moreover, relaxation processes and diffusive behavior in polymers require long simulation times, making a direct comparison between MLIP-based and *ab initio* MD simulations infeasible.

In this study, we first train Atomic Cluster Expansion (ACE) potentials for small oligomers on MD reference data, thereby circumventing the need for expensive QM reference simulations and enabling long, cost-efficient MD trajectories. We then benchmark the transferability of the trained ACE potentials to longer polymer chains with respect to density, structural, and dynamic properties. The insights gained allow us to identify an optimal oligomer chain length that balances training cost and transferability. Based on this, we can efficiently train a QM-accurate potential for polymers on QM reference data in a second step.

CPP 46.54 Thu 9:30 P5

Fourth-Generation High-Dimensional Neural Network Potentials for Molecular Chemistry in Solution — •Djamil A. A. Maouene[1,2], Moritz R. Schäffer[1,2], Moritz Gubler[3], Stefan Goedecker[3], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany — [3]Department Physik, Universität Basel, Switzerland

Machine learning potentials have become essential tools in chemistry and materials science, offering accurate, efficient representations of high-dimensional potential energy surfaces for atomistic simulations. Here we compare two generations of high-dimensional neural network potentials (HDNNPs) 2G-HDNNPs and 4G-HDNNPs in their ability to model organic molecules in aqueous solution. 2G-HDNNPs perform well for systems dominated by local interactions because they rely on descriptors of the immediate atomic environment. However, in cases of long-range charge transfer 4G-HDNNPs provide a more reliable description by explicitly accounting for charge redistribution in the system as a function of its global structure. We illustrate these differences for organic molecules in water.

CPP 46.55 Thu 9:30 P5

Controlling porosity in supraparticles: A simulation study using spherical and rod-shaped particles — •Kritika Kritika[1,2], Mayukh Kundu[3], Michael Howard[3], and Arash Nikoubashman[1,2] — [1]Leibniz Institute of Polymer Research Dresden, Germany — [2]Institute of Theoretical Physics, TU Dresden, Germany — [3]Department of Chemical Engineering, Auburn University, Auburn, USA

Supraparticles (SPs) are large assemblies of smaller colloidal particles, whose properties can be tuned by modifying, e.g., the chemistry, shape, and size of the individual constituent particles and their arrangement within the SP. SPs can be formed through droplet drying, a process commonly observed in both everyday life and industrial applications, such as spray drying and printing. Porous SPs are of particular interest, since their high surface area and tunable pore size distribution make them ideal materials for catalysis, photonics, and adsorption applications. In this computational study, we explore the drying-induced formation of SPs made from spherical and rod-shaped particles. After drying, we selectively remove one of the particle components, leaving behind a highly porous SP. The initial volume fraction between spherical and rod-shaped particles plays a key role in shaping the porosity within the SP, while increasing the aspect ratio of the rods further amplifies the porosity of the SPs. Additionally, we observed that slower drying leads to a distinct increase in average pore size.

CPP 46.56 Thu 9:30 P5

Demystifying the decoupling of conformation and phase behavior in PNIPAM cononsolvency — •Ved Mahajan and Nico F. A. van der Vegt — Department of Chemistry, Technical University of Darmstadt

Cononsolvency describes the situation in which a polymer becomes insoluble in a mixture of two individually good solvents. PNIPAM, a widely studied thermoresponsive polymer, exhibits a strong coupling between its temperature-driven coil-globule transition and its phase behavior at low methanol concentrations; however, these two responses decouple as the methanol content increases. In this work, we use a minimal physical model, a hydrophobic polymer in water-methanol mixtures, that reproduces these key experimental observations. Despite its simplicity, the model captures both the emergence of cononsolvency and the crossover from coupled to decoupled thermal responses. At low methanol concentration, the polymer conformation remains temperature dependent, whereas at high methanol concentration, it becomes insensitive to temperature. In contrast, hydrophobic aggregation consistently strengthens with increasing temperature. Together, these results reveal a simple mechanism for the observed decoupling: the differing temperature sensitivities of polymer collapse and hydrophobic aggregation, both rooted in the hydrophobic effect.

CPP 46.57 Thu 9:30 P5

Molecular insights into the anion-dependence of the double-layer capacitance — •Richard Schömig[1], Xuqiang Xu[2], Jana Zaumseil[2], and Alexander Schlaich[1] — [1]Institute for Physics of Functional Materials, Hamburg Technical University, Hamburg — [2]Institute for Physical Chemistry, Heidelberg Universiy, Heidelberg

Mixed ionic-electronic conductors are promising candidates for organic electrochemical transistors (OECTs). Single-walled carbon nanotubes (SWCNTs), a key example, show transconductance and capacitance responses that are strongly influenced by the properties of the surrounding electrolyte [1]. To uncover the mechanisms governing this behavior, we perform molecular dynamics simulations of aqueous electrolytes containing ions of different sizes and concentrations under varying applied potentials. As a simplified model for the more complex SWCNT electronic structure, we here use graphene as the electrode material. Employing atomistic constant-potential simulations, we investigate how these electrolyte characteristics shape the interfacial structure and differential capacitance. Analysis of the hydrogen-bond network and associated free-energy

changes highlights the central role of ion size in determining interfacial behavior.

[1] Xu, X.; Fresta, E.; Lindenthal, S.; Michel, E.; Zaumseil, J. ACS Appl. Mater. Interfaces 2025, 17(25), 37002-37011.

CPP 46.58 Thu 9:30 P5

Computing static and dynamic structure in colloidal models for solutions of globular proteins — •Sven Köbler — Institute of Applied Physics, University of Tübingen, Tübingen, Germany

Crowded solutions of globular proteins are commonly probed using neutron and X-ray scattering to obtain static and dynamic structure factors across a broad range of concentrations. Complementary insight can be gained from Brownian dynamics simulations based on coarse-grained colloidal models; however, extracting meaningful scattering observables particularly dynamic structure factors which requires fast and scalable trajectory analysis tools. We present an efficient computational framework for calculating both static structure factors $S(q)$ and intermediate scattering functions $F(q,t)$ directly from simulation trajectories. Our tools are highly optimized and build with CUDA compatibility to exploit computing speeds of GPUs. Its performance is demonstrated using binary colloidal models designed to mimic mixtures of bovine serum albumin (BSA) and ferritin. The resulting simulated scattering functions are compared with experimental X-ray photon correlation spectroscopy data.

CPP 46.59 Thu 9:30 P5

Dynamic properties of telechelic polyisobutylene with sticker ends: atomistic vs. coarse-grained molecular dynamics simulation — •Anastasiia Pivovarova and Viktor Ivanov — Martin-Luther-University Halle-Wittenberg, Halle (Saale), Germany

Modeling associating polymer networks, such as telechelic polyisobutylene (PIB) with barbiturate stickers, requires not only constructing accurate coarse-grained (CG) interaction potentials but also resolving the inherent problem of accelerated dynamics. This challenge becomes evident when comparing Green-Kubo viscosity calculations across different levels of resolution. Atomistic simulations of PIB with barbiturate end groups reproduce the expected rheological behavior of associating systems, yielding a viscosity of about 3.32 Pa*s. In contrast, CG simulations performed for pure PIB used as an initial step toward a full CG description of the telechelic system show a pronounced reduction in viscosity, reflecting substantially faster dynamics intrinsic to coarse-graining. These observations illustrate how dynamical acceleration can dominate the predicted viscoelastic properties even when structural features are reproduced, underscoring the need for systematic strategies to recover realistic dynamical behavior in CG models of associating polymer networks.

CPP 46.60 Thu 9:30 P5

Density of states in monodisperse and polydisperse hard disks: Concentration dependent SAMC estimation — •Viktor Ivanov, Joram Heimbold, Malte Kautzsch, and Timur Shakirov — Martin-Luther-University Halle-Wittenberg, Halle (Saale), Germany

We propose a new variant of flat-histogram Monte Carlo, where the density of particles is the control parameter for the density of states and the visiting histogram. We simulate a system of point particles with zero diameter. The square of the minimal interparticle distance, r^2_{min}, is used as the control parameter for a macrostate. The density of states and the visiting histogram depend on r^2_{min} and are updated at each step of the algorithm according to the usual SAMC rules. For a microstate (particilar configuration of particles) with a given value of the minimal distance between particles r_{min} one can replace the points with the hard disks of the diameter r_{min} or smaller, which corresponds to a system with a specific particle density. We apply this algorithm to 2d systems of monodisperse and polydisperse hard disks (with diameter distributions $1/d^2$) and study the density driven crystallization transition. For monodisperse hard disks the transition from the liquid to the hexatic phase proceeds via a first-order like pseudo-phase transition, whereas the transition from the hexatic to the crystalline phase is continuous. With increasing polydispersity, crystallization is significantly suppressed, such that no transition to the crystalline phase is observed for a 10% variation in particle radii.

CPP 46.61 Thu 9:30 P5

Benchmarking bond dissociation energies with plane-wave pseudopotential and Gaussian all-electron methods — •Yue Pan[1], Jochen Heil[2], Ali Karimi[2], and Arash Mostofi[1] — [1]Imperial College London, South Kensington Campus, London, SW7 2AZ, UK — [2]Continental Reifen Deutschland GmbH, Hanover, Germany

Accurate homolytic bond dissociation energies (BDE) are important for understanding bond breaking processes in molecules. They are also frequently used to benchmark the accuracy of different method for electronic-structure calculations. Most calculations of BDE focus on datasets of small gas-phase molecules and, accordingly, are carried out with localised-orbital methods, while systematic comparisons to periodic plane-wave DFT remain scarce. This is relevant for modelling interfacial failure processes in hybrid systems such as polymer nanocomposites, in which molecules are attached to inorganic surfaces, and it becomes less clear which method is more suitable from the perspective of accuracy and efficiency.

In this work, we benchmark the performance of two widely used approaches for DFT calculations, namely the plane-wave basis pseudopotential methods and Gaussian all-electron methods. We use C*C bond dissociation in gas phase hydrocarbons and surface-anchored molecules. We then compare our calculated BDEs with theoretical results obtained from highly accurate quantum chemistry methods and experimental values. Our work represents a step towards a better understanding of bond breaking and interfacial failure in materials.

CPP 46.62 Thu 9:30 P5

Continuum Modeling of Light-Matter Interaction in Polymer-Based Hollow-Core Optical Fibers with Different Geometrical Configurations — •Zehra Gizem Mutlay and Mustafa Ordu — UNAM - National Nanotechnology Research Center and Institute of Materials Science and Nanotechnology, Bilkent University, Ankara 06800, Türkiye

Recent studies have demonstrated that nested hollow-core optical fibers (HCFs) can achieve attenuation below 0.1 dB/km while maintaining broad transmission bandwidths. This performance demonstrates the promise of air-guided waveguides as alternatives to conventional solid-core optical fibers. In this work, we perform continuum modeling based on the finite-element method to investigate light interaction with polymer in HCFs by implementing three- and four-tube cladding structures. The analysis involves designs with and without nested elements and supporting bars. Our comparative investigation includes silica- and polymer-based structures to identify how intrinsic material properties and geometrical parameters influence mode confinement, optical loss, and transmission behavior. The findings show that even minor changes in geometry or material composition significantly influence light propagation, which underlines the sensitivity of optical guidance to light-material interaction. This study establishes a continuum-based framework for analyzing electromagnetic behavior in polymer systems and lays the groundwork for developing 3D-printed polymer-based hollow-core fibers with reduced attenuation for future applications in optical and materials physics.

CPP 46.63 Thu 9:30 P5

General Polarization Dependent Dynamic Light Scattering Using the Dynamic Mueller Matrix — •Reinhard Sigel — Independent Scientist, Markdorf, Germany

The Mueller Matrix for a general description of the polarization transfer of an optical system is combined with Dynamic Light Scattering (DLS) [1]. Azzam's procedure [2] based on two rotated quarter wave plates is combined with photo correlation measurements to detect the Dynamic Mueller Matrix, which contains all possible polarization dependent correlation functions. The related Siegert relation is derived. Applications are dynamic ellipsometric light scattering [3] experiments on soft colloidal particles and 3D correlation ellipsometry [4] experiments on soft interfaces [5].

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CPP 46.64 Thu 9:30 P5

Versatile X-Ray Reflector Extension Setup for Grazing-Incidence Experiments for Liquid Surface Study at the Beamline P03/PETRA III — •Jan Rubeck, Andrei Chumakov, and Matthias Schwartzkopf — DESY, Notkestr. 85, 22607 Hamburg, Germany

Existing beamlines for in situ GISAXS on liquids are either limited in angular range or incompatible with the large sample-detector distance required for submicron resolution. We present a low-cost, easily assembled beam-tilting extension for synchrotron-based ultra-small-angle X-ray scattering (USAXS) facilities, enabling grazing-incidence (GI-) and transmitted scattering (GIUSAXS, GTUSAXS) studies on liquid surfaces. The setup is compatible with standard USAXS beamlines and requires only 0.5 m of space at the sample stage. It allows X-ray beam incidence angles of up to 0.6° at the liquid surface, equal to twice the angle of incidence on a reflector and below its critical angle of reflector materials, and provides access to a q-range of approximately 0.003-0.5 nm^{-1}. The system was tested at P03 beamline (DESY) using polystyrene nanoparticles, self-assembled at the air/water interface. The proposed scheme enables selective depth profiling and expands the research capabilities of existing SAXS synchrotron facilities for in situ studying submicron nanostructured objects at liquid surfaces under GI-geometry, combined also with GIWAXS and TXRF techniques. https://doi.org/10.1107/S1600577525003431

CPP 46.65 Thu 9:30 P5

Hybrid field coupling in nanoscale infrared spectroscopic imaging of nanostructured soft matter — •Sharon Xavi[1], Mashiat Huq[1], Matthias Zeissberger[2], Daniela Täuber[1,2], and Christin David[1,3] — [1]Friedrich Schiller University Jena, 07743 Jena — [2]Leibniz Institute of Photonic Technology, 07745 Jena — [3]University of Applied Sciences, 84036 Landshut, Germany

Anisotropic intensity distributions are frequently observed on nanostructured surfaces in the emerging field of nanoscale infrared (IR) spectroscopic imaging methods, including mid-IR scattering scanning optical nearfield microscopy (IR-sSNOM) and methods combining mid-IR illumination with mechanical detection using atomic force microscopy (AFM-IR). Such methods bridge the gap between high-resolution structural imaging in electron and atomic force microscopy and chemical imaging in conventional far-field IR spectroscopy by overcoming the limitations of optical diffraction in far-field IR spectroscopic imaging. In the mid-IR spectral region, the hybrid field coupling of the incident field with a polymer nanosphere and a metallic AFM probe is nearly as strong as the plasmonic coupling in case of a gold nanosphere [Anindo et al., J. Phys. Chem. C, 2025, 129, 4517]. We modeled this hybrid field coupling on varied nanostructured surfaces to enhance the understanding of the observed anisotropies and contribute to the development of advanced applications of these methods [Ali et al. Anal. Chem., 2025, 97, 23914].

CPP 46.66 Thu 9:30 P5

Learn how to switch off: In-silico Modelling of Thermal Ring-closing Process in Spiropyran Derivatives — •Bowen Cheng, Robert Strothmann, Hendrik Heenen, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin, Germany

Spiropyran (SP) and its derivatives undergo a ring-opening reaction via UV radiation and a ring-closing reaction in thermal conditions, making them excellent candidates for photoswitches. One key aspect that governs the sensitivity of such photoswitches is the rate of the thermal ring-closing process. A main challenge in modelling this process is the existence of various thermally accessible conformers, leading to a complex reaction network.

In this study, we highlight a combined workflow using machine-learned interatomic potential (MLIP) and a microkinetics model (MKM) to address this. With a fine-tuned MACE-OFF24 foundation model, we predict different transition state energies within the reaction network using the nudge elastic band method, and correlate these energies to experimental observations using the MKM.

Our workflow can be migrated between different SP derivatives to reveal the effect of functional group decorations. Our findings demonstrate the potential of using MLIPs to predict transition states and enable larger-scale studies of complex reaction networks. We also aim to condense our workflow as a new descriptor for *in-silico* screening in future spiropyran photoswitch design.

CPP 47: Focus Session: Controlling Microparticles and Biological Cells by Ultrasound (joint session BP/CPP/DY)

Recently ultrasound has emerged as a very promising physical modality to control the behavior of microparticles and even of biological cells, which can be moved and stimulated by sound waves. For biological cells, one can further control the effect of sound through gene expression (sonogenetics), similar to the control by light (optogenetics). However, because the wavelength of sound is much larger than the one of light, one of the challenges is to localize the effect of sound waves, e.g. by using gas bubbles. Here, we bring together experimental and theoretical researchers who currently explore the potential of ultrasound to control active and passive microsystems and to develop new applications ranging from biomedicine to soft robotics.

Organized by Peer Fischer and Ulrich S. Schwarz (Heidelberg)

Time: Thursday 10:15–12:45 Location: BAR/0106

Invited Talk CPP 47.1 Thu 10:15 BAR/0106

Mechanogenetics for Cell ImmunoTherapy — •Yingxiao Wang — 1002 childs way, Los Angeles, CA 90089

Cell-based cancer immunotherapy is a promising therapeutic intervention for cancer treatment. However, non-specific toxicity against healthy tissues (e.g. off-tumor toxicity) is a major hurdle for solid tumor treatment. We have developed controllable on-switch gene cassettes in which a specific antigen production on the target cancer cell can be remotely and mechanically induced by an external focused ultrasound (FUS). FUS was applied to stimulate the production of the synthetic and clinically validated antigen on tumor cell surface orthogonal to the endogenous proteins. SynNotch was further engineered into primary human T cells (SynNotch-CAR T) to recognize the synthetic antigen expressed on the ultrasound-induced tumor cells and activate the production of CAR, which can lead to the recognition of a native tumor specific antigen (TSA) universally expressed on the whole population of tumor cells for immunotherapy. We applied this system to treat prostate cancer cells whose locally metastasized tumors are confined in space but intermingled with vessels and nerves. Our results showed that FUS can mechanically induce the synthetic antigen production in prostate cancer cells, which results in the engagement and activation of SynNotch CAR T cells for the tumor eradication. This local activation of engineered tumor cells by FUS should allow a high precision and safety in eradicating tumors. Hence, this approach for immunotherapy should open new opportunities to integrate engineering mechanics with genetic medicine for successful translation.

CPP 47.2 Thu 10:45 BAR/0106

Shaping sound to tickle cells — •Dimitris Missirlis[1,2], Athanasios Athanassiadis[1,2], Rom Lerner[1,2], and Peer Fischer[1,2] — [1]Institute for Molecular Systems Engineering and Advanced Materials, Im Neuenheimer Feld 225, 69120 Heidelberg, Germany — [2]Max Planck Institute for Medical Research, Jahnstr. 29, 69120, Heidelberg, Germany

The ability to shape ultrasonic waves precisely is finding growing relevance in biomedical applications, where ultrasound is increasingly used to noninvasively stimulate biological tissues for therapeutic purposes. However, it remains an unsolved question how high-frequency ultrasound can interact with cells to excite biological responses. Our recent work on shaping and controlling ultrasound waves has provided us with a new tool to address the fundamental question how ultrasound interacts with and influences cells. To this end we have developed adaptable setups where we can control relevant ultrasound parameters in vitro as well as in vivo. By systematically examining the critical parameters, we discuss the role of different ultrasonic effects, including thermal effects, radiation forces, and sound-induced shear flows. Further, we discuss both physical and sonogenetic methods that can be used to enhance the coupling of ultrasound to cells.

CPP 47.3 Thu 11:00 BAR/0106

A Theoretical Model for Ultrasound-Induced Intracellular Streaming — •Niels Gieseler[1,2,3], Falko Ziebert[1,2], and Ulrich S. Schwarz[1,2] — [1]Institute for Theoretical Physics, Heidelberg University, Philosophenweg 19, Heidelberg 69120 Germany — [2]BioQuant, Heidelberg University, im Neuenheimer Feld 267, Heidelberg 69120 Germany — [3]Max Planck Institute for Medical Research, Jahnstrasse 29, Heidelberg 69120, Germany

Ultrasound is not only the basis of an essential imaging method for biomedicine, recently it has also become a promising avenue to control biological systems, for example, in sonogenetics or ultrasound neuromodulation. However, the underlying physical effects are not well understood, and a complete theoretical description is missing. In fact, many different physical effects compete, including radiation forces, streaming, cavitation, and local heating. Here, we focus on intracellular streaming, which might induce organelle movement or alter gene expression, as the steady second-order rotational flow generated by an acoustic source. As a model for the viscoelastic nature of cells and their surroundings, we use Oldroyd-B fluids. Building on existing work, we calculate the streaming flows inside and outside of a sphere sonicated with a plane wave. The streaming is treated as a second-order perturbation expansion of the Navier-Stokes equations, which is solved separately for both media and combined using suitable boundary conditions. Our work shows under which conditions intracellular streaming can be induced in biological cells.

15 min. break

Invited Talk CPP 47.4 Thu 11:30 BAR/0106

Recent theoretical progress on sound-propelled microsystems — •Raphael Wittkowski — Department of Physics, RWTH Aachen University, 52074 Aachen, Germany — DWI – Leibniz Institute for Interactive Materials, 52074 Aachen, Germany

The research area of sound-propelled microsystems is growing fast and has a great potential for various future applications in engineering, medicine, and other fields. The progress in this area is accelerated by theoretical methods, as analytical modeling and computer simulations can provide new insights that cannot be obtained by experiments.

In this talk, I will address the theoretical investigation of sound-propelled microsystems and present examples from the recent research progress in this area. The talk will cover different types of sound-propelled microsystems including microrobots, micromachines, artificial muscles, and soft robots.

Funded by the Deutsche Forschungsgemeinschaft (DFG) – 535275785.

CPP 47.5 Thu 12:00 BAR/0106

Rarefaction wave amplification from non-resonant deforming bubbles — Yuzhe Fan, Saber Izak Ghasemian, and •Claus-Dieter Ohl — Otto-von-Guericke University, Magdeburg, Germany

Gas bubbles in liquids or soft matter exposed to acoustic waves behave as oscillators, with maximum response at their resonance frequency. When driven below resonance at sufficient pressure amplitudes, bubbles can collapse with strong energy focusing and even emit light; when driven near resonance, surface instabilities and fast jet flow develop during oscillation. Like other oscillators, bubbles cease to respond when driven far above resonance. Although their oscillations are minimal, bubbles in this regime act as pressure-release interfaces, can reflect high peak pressure shock into rarefaction wave, and may therefore seed cavitation when interacting with high-power therapeutic ultrasound. Yet, here we show that even diagnostic ultrasound with peak positive pressures as low as ~10 MPa can nucleate cavitation in microseconds. This is caused through the non-resonant deformation of the bubble into a concave shape that refocuses scattered waves, amplifying the tension leading to microcavitation. Our findings reveal that cavitation can be triggered by high-frequency positive pressure over a much wider amplitude range than previously recognized, offering a new perspective for current safety guidelines for ultrasound bioeffects and applications in medical ultrasound.

CPP 47.6 Thu 12:15 BAR/0106

Optimizing acoustically propelled microrobots using genetic algorithms — •Lennart Gevers[1,2,3] and Raphael Wittkowski[1,2,3] — [1]Department of Physics, RWTH Aachen University, Aachen, Germany — [2]DWI – Leibniz Institute for Interactive Materials, Aachen, Germany — [3]Institute of Theoretical Physics, Center for Soft Nanoscience, University of Münster, Münster, Germany

The promising potential applications of acoustically propelled microparticles demand methods to create particle designs that allow for targeted autonomous motion. Current methods remain largely based on experiments due to the intricate nature of the underlying dynamics. Large-scale computational studies, specifically when combined with optimization algorithms, are impeded by the cost of traditional acoustofluidic simulations.

In this talk, we present the implementation of an analytical framework describing non-Brownian motion of colloidal molecules driven by acoustic streaming. The analytical framework is combined with vectorized, GPU-accelerated, and distributed computation. This enables fast, large-scale simulations, where 10^5 trajectories over 10 s real time can be simulated on a normal personal computer within one minute. Coupling this approach with genetic algorithms reveals particle geometries, control parameters, and underlying principles for acoustically propelled particles that exhibit controllable and stable behavior over long times.

Funded by the Deutsche Forschungsgemeinschaft (DFG) – 535275785.

CPP 47.7 Thu 12:30 BAR/0106

Equations of motion for arbitrarily shaped acoustically propelled rigid microparticles — •Justus Schnermann[1,2,3] and Raphael Wittkowski[1,2,3] — [1]Department of Physics, RWTH Aachen University, Aachen, Germany — [2]DWI – Leibniz Institute for Interactive Materials, Aachen, Germany — [3]Institute of Theoretical Physics, Center for Soft Nanoscience, University of Münster, Münster, Germany

Much experimental research concerns the acoustic propulsion of microparticles, but theoretically, only axisymmetric particles with a stable orientation have been studied thus far. In this talk, we present an analytical derivation of the ordinary differential equation of motion for an arbitrarily shaped acoustically propelled rigid microparticle. This equation governs the time evolution of the orientation and position of the particle. Its parameters depend only on the particle's leading-order oscillation velocity field. Based on this equation, we classify qualitatively the possible long-term trajectories of arbitrary particles in unidirectional ultrasound.

Funded by the Deutsche Forschungsgemeinschaft (DFG) – 535275785.

CPP 48: Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics VI

Time: Thursday 11:30–12:45 Location: ZEU/LICH

CPP 48.1 Thu 11:30 ZEU/LICH

Simulating Light Induced Phase Separation in Mixed Halide Perovskites — •Sebastian Schwartzkopff, Ivan Zaluzhnyy, Ekatarina Kneschaurek, Paul Zimmermann, Dmitry Lapkin, Hans Mauser, Alexander Hinderhofer, and Frank Schreiber — University of Tübingen

By varying the halide composition in mixed organic-inorganic perovskites such as $MAPbBr_{1.8}I_{1.2}$ (MA-methylammonium), one can precisely tune the band gap. This is a desirable property for solar cell design, as it allows for the production of high efficiency solar cells. However, illumination with visible light drives these materials to phase-separate into Br-rich and I-rich domains, thereby degrading the tuned bandgap. To better understand and potentially control this behavior, we employ phenomenological approaches such as Cahn-Hilliard and Monte Carlo models. While Cahn-Hilliard methods were initially explored, they proved challenging in reproducing experimentally observed dynamics. On the other hand, Monte Carlo methods have shown themselves to enable a systematic exploration of how factors such as halide ratio, charge-carrier density, temperature, and illumination intensity influence light-induced phase separation. Overall, we found that Monte Carlo simulations, with appropriately chosen parameters, can successfully reproduce key features observed in experimental diffraction measurements.

CPP 48.2 Thu 11:45 ZEU/LICH

Reorientation-driven degradation in oriented perovskite films: shifting facet engineering to thermodynamic stability — •Xiaojing Ci[1], Xiongzhuo Jiang[1], Guangjiu Pan[1], Kun Sun[1], Altantulga Buyan-Arivjikh[1], Zerui Li[1], Lixing Li[1], Thomas Baier[1], Matthias Schwartzkopf[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]DESY, Hamburg

Hybrid perovskite solar cells suffer from underexplored links between crystallographic orientation and thermal stability. We fabricate highly oriented mixed Sn-Pb perovskite films via an additive-free two-step method. Accelerated aging studies under high temperature reveal that high orientation paradoxically compromises stability and PSCs built from highly oriented perovskite films retain only 73% of their initial PCE versus 89% in less-oriented devices. Operando GIWAXS of the PSCs shows that thermal stress induces significant reorientation and lattice distortion in the oriented crystallites. Structural analyses confirm progressive crystallographic transitions, including grain reconfiguration, shifts toward isotropy, and systematic diffraction migrations. Critically, we demonstrate that metastability is an intrinsic consequence of high crystallographic order, which is why the very high alignment strategies that enhance performance induce thermodynamic vulnerability. This necessitates redesigning crystal engineering priorities where suppressing instability requires engineering thermodynamic equilibrium states over maximizing alignment for stable perovskite photovoltaics.

CPP 48.3 Thu 12:00 ZEU/LICH

Understanding the molecular origins of giant surface potential: a case study of TPBi — •Mauricio Sevilla[1], Naomi Kinaret[1], Muhammad Nawaz Qaisrani[1,2], Albin Cakaj[4], Alexander Hofmann[4], Falk May[3], Wolfgang Brütting[1], and Denis Andrienko[4] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Technische Universität Ilmenau, Ilmenau, Germany — [3]Merck Electronics KGaA, Darmstadt, Germany — [4]University of Augsburg, Augsburg, Germany

In the context of organic light-emitting diodes, the molecular orientation in thin layers of organic materials plays a crucial role in charge injection, light outcoupling, and the formation of internal electrostatic fields due to the alignment of molecular dipoles. This latter phenomenon is referred to as the giant surface potential (GSP). Predicting GSP soleley from the chemical structure is challenging, as it is highly sensitive to processing conditions such as temperature and deposition rate during the physical vapor deposition process. Using both all-atom and coarse-grained simulations, we develop and test a framework capable of predicting the molecular ordering of organic materials under varying substrate temperatures and deposition rates. The framework's accuracy is validated by comparing the predicted GSP and birefringence of thin films to experimentally measured values, for a series of TPBi isomers.

CPP 48.4 Thu 12:15 ZEU/LICH

Additives to enhance efficiency and stability of PPDT2FBT:PC60BM organic solar cells — •Hassan Ismail[1,2], Jose Prince Madalaimuthu[1,2], Ulrich Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstrasse 10, 07743 Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany

The development of organic solar cells (OSCs) requires simultaneous optimization of photovoltaic performance and long-term thermal stability, often mediated by processing solvents and additives. This study investigates the role of small amphiphilic molecules (AMs) as surfactants in stabilizing the bulk heterojunction morphology of PPDT2FBT:PCBM-based OSCs. Our research goal is to understand how the chemical nature of AMs and their interface engineering within the device affect stability and efficiency. We demonstrate that the AM's polar headgroup chemistry is a critical determinant for operational stability, and by strategically applying interface engineering across all major interfaces, we identify optimal scenarios for enhancing both efficiency and device durability. Interface engineering not only improves charge transport and mitigates degradation but also supports large-area fabrication and practical device reliability, addressing prominent challenges for commercialization. These findings guide future molecular design and interface engineering strategies, contributing to the realization of more robust and reliable organic solar cells.

CPP 48.5 Thu 12:30 ZEU/LICH

Controlling singlet fission in diketopyrrolopyrole diner through solvent choices — •Sruthy Asa Rajan[1,2], Isaac M. Etchells[3], Jegadesan Subbiah[2], Sergey Bagnich[1], Paul E. Shaw[3], David Jones[2], and Anna Köhler[1] — [1]Universität Bayreuth — [2]University of Melbourne — [3]University of queensland

The efficiency of conventional solar cells is constrained by the Shockley-Queisser limit, which is arises from thermalisation loss. Singlet fission (SF) offers a promising pathway to surpass this efficiency limit. However, a key challenge lies in identifying SF molecules with triplet energy levels that align with the silicon band gap, enabling the efficient formation of correlated triplet pairs, 1(TT), and their separation. PDPP is a molecule with a comparable triplet energy to the silicon bandgap. But monomer molecules are not SF active in solution. We prepared PDPP-dimers with a pyrene bridge. We investigate the influence of solvent properties on the optical behaviour of these N-alkylated pyrene-bridged PDPPs. We employ temperature-dependent steady-state and time-resolved photoluminescence studies on N-alkylated pyrene-bridged PDPPs in protic polar and aprotic polar solvents to study the optical properties of the evolution of different species. At an intermediate temperature, we observed an intermediate emission, which then, on further decreasing the temperature (less than 100K), is replaced by 1(TT) emission. We also measured TA on different solvents which showed different pathway. In protic polar solvent, our molecule showed intermolecular SF whereas in aprotic polar solvent it showed intermolecular

CPP 49: Gels, Polymer Networks and Elastomers I

Time: Thursday 11:30–12:45 Location: ZEU/0255

CPP 49.1 Thu 11:30 ZEU/0255

Nanoparticle–Polymer Coupling in Magnetic Gels Studied by Means of Computer Simulations and Experiments — •Rebecca Stephan[1], Surojit Ranoo[2,4], Patrick Kreissl[1], Chinmay Pabshettiwar[1], Jessica Kubis[2], Christian Holm[1], Annette M. Schmidt[2], Regine von Klitzing[3], and Rudolf Weeber[1] — [1]Institute for Computational Physics (ICP), Universität Stuttgart — [2]Institute of Physical Chemistry, Department of Chemistry, University of Cologne — [3]Institute for Condensed Matter Physics, Technical University of Darmstadt — [4]Laboratoire Colloïdes et Matériaux Divisés, ESPCI Paris

Magnetic gels - soft hydrogels with embedded magnetic nanoparticles (MNPs) - combine the viscoelastic properties of a gel with the magnetic behavior of the MNPs. Their response to an external magnetic field enables tunable mechanical and dynamic properties such as shape, stiffness, and swelling. The microscopic coupling mechanisms between the MNPs and the surrounding polymer matrix are crucial for the material's stimuli-responsive properties. However, these mechanisms are not yet fully understood.

In this work, we juxtapose results for PAAm hydrogels with embedded cobalt ferrite nanoparticles with coarse-grained molecular dynamics simulations coupled to lattice-Boltzmann hydrodynamics. In both cases, we probe the coupling using magnetic AC susceptibility spectra. Our findings demonstrate that the local polymer environment and the surface heterogeneity of the magnetic particles - chemical or topographical - play an important role in MNP-polymer coupling.

CPP 49.2 Thu 11:45 ZEU/0255

Strain-stiffening critical exponents of fibre networks under uni-axial deformation — •Atharva Pandit[1] and Abhinav Sharma[1,2] — [1]Institut für Physik, Universität Augsburg, 86159 Augsburg, Deutschland — [2]Bereich Theorie der Polymere, Leibniz-Institut für Polymerforschung, 01069 Dresden, Deutschland

Disordered fibre networks exhibit a floppy to rigid mechanical phase transition as a function of connectivity. Sub-isostatically connected networks can undergo this transition via straining. Critical exponents governing this transition have been estimated theoretically and by numerical simulations of various types of networks. We present improved results, achieved through a combination of refined numerical simulations, larger system sizes and incorporation of theoretical predictions for better post-simulation analysis. A linear evolution of the critical strain and critical exponents is observed as the network is sheared while being subjected to non-volume-preserving uni-axial deformations.

CPP 49.3 Thu 12:00 ZEU/0255

Probing Mechanical Properties of Magnetic Gels Using Computer Simulations — •Yashas Tejaskumar Gandhi, Christian Holm, and Rudolf Weeber — Institute For Computational Physics, University of Stuttgart, Germany

Magnetic gels are liquid swollen polymer networks embedded with magnetic nanoparticles (MNPs). Their motion, shape and mechanical properties can be governed by an external magnetic field. The mechanical properties of a magnetic gel depend on both the polymer network and the embedded MNPs. They can also be heated by applying an AC magnetic field due to viscous and hysteresis losses.

There are two ways to probe the mechanical properties of magnetic gels: at the nanoscopic level using AC susceptometry, and at the macroscopic level by measuring stress under deformation. While macroscopic measurements are relatively straightforward, they are computationally demanding. The Gemant-DiMarzio-Bishop theory provides a framework for connecting magnetic AC susceptibility data to nanoscale mechanical properties. Our objective is to test this theory in computer simulations by comparing nanoscale measurements with macroscale measurements.

The polymer network is modelled as a coarse-grained bead-spring system. We also incorporate a solvent model for hydrodynamic interactions in the system. Shear deformation is applied using periodic Lees-Edwards boundary conditions. Our simulations use the 'Extensible Simulation Package for Research on Soft Matter Systems (ESPResSo)' simulation package.

CPP 49.4 Thu 12:15 ZEU/0255

Dynamic control of rigidity via geometric frustration — •Santiago Gomez Melo[1,2], Falko Ziebert[1,2], and Ulrich S. Schwarz[1,2] — [1]ITP, Philosophenweg 19, Heidelberg — [2]BioQuant, Im Neuenheimer Feld 267, Heidelberg

Recent advances in materials design and 4D-printing now allow one to realize programmable metamaterials that upon receiving a suitable stimulus dynamically change their unconventional macroscopic properties. For mechanical metamaterial, these tunable features have so far been restricted to geometric quantities, such as the Poisson ratio and the strain-to-twist ratio, but the effective elastic moduli have not been addressed yet. Here we combine central force network theory and responsive hyperelasticity to show that it is also possible to dynamically control the elastic moduli, and more specifically the shear modulus, by programming geometric frustration into a stimuli-responsive structure. This phenomenon, known as geometric incompatibility, produces a rigidity phase transition in which the elastic modulus changes by several orders of magnitude. It results from inducing a state of self-stress that eliminates the floppy modes of the system by producing second-order rigidity. The underlying physical principle seems to be also at work in biological systems, most prominently in epithelial monolayers, but here it is predicted for entirely synthetic materials, like temperature-sensitive hydrogels and nematic elastomers, opening up the perspective of designing a new class of dynamic metamaterials.

CPP 49.5 Thu 12:30 ZEU/0255

Aqueous Foams stabilized by PNIPAM Microgels: Effect of Cross-linker and Concentration — •Joanne Zimmer, Kevin Gräff, Luca Mirau, and Regine von Klitzing — Soft Matter at Interfaces, Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 8, D-64289 Darmstadt

Aqueous foams are abundant in everyday life, important for industrial applications and interesting from a fundamental point of view. In this work, aqueous foams are generated by sparging gas (nitrogen) through an aqueous dispersion of PNIPAM microgels, which are used as foam stabilizers. The microgel cross-linker content as well as the microgel concentration are varied and prove to significantly influence the foam formation properties (foamability) and the foam stability. A lower cross-linker content as well as a higher microgel concentration elevate the foamability, generate foams with higher liquid content and smaller

bubbles and increase the foam stability. These observations are correlated with the microgel behaviour at the single air-water interface, i.e. pendant drop measurements and Langmuir trough. Our findings highlight good agreement across both length scales: an increase in foamability correlates with a faster decrease in surface tension, and a higher foam stability with a higher surface elastic modulus of a microgel-covered single air-water interface. The ability of the microgels to form a collective polymer network seems to dominate these processes.

CPP 50: Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates II (joint session CPP/BP)

Time: Thursday 11:30–12:45 Location: ZEU/0260

CPP 50.1 Thu 11:30 ZEU/0260

Exponential Size Control in Biomolecular Condensates via Universal Scaling of Power-Law Distributions — •Yifan Huang[1], Chuan Tang[1], Haoyu Song[2], Bing Miao[3], and Qiyun Tang[1,4] — [1]Key Laboratory of Quantum Materials and Devices of Ministry of Education, School of Physics, Southeast University, Nanjng 211189, China — [2]School of Physics, Zhejiang University, Hangzhou 310058, China — [3]Center of Materials Science and Optoelectronics Engineering, College of Materials Science and Opto-Electronic Technology, University of Chinese Academy of Sciences, Beijing 100049, China — [4]Jiangsu Physical Science Research Center, Nanjing 210093, China

Power-law distributions are ubiquitous phenomena in diverse systems, whereas concomitant scale invariance hinders the exploration of precise size control for biocondensates in recent experiments. Using massive computer simulations and the kinetic theory of coalescence, we demonstrate that the cutoff volume can collapse all power-law distributions of biocondensates in different parameters onto one master curve. Remarkably, the cutoff size can increase exponentially by increasing monomer concentrations $R \sim e^{\phi}$, of which nanometer condensates in simulations can be extrapolated to micrometer droplets in experiments. The findings provide a new mechanism to rapidly tailor the biocondensates to appropriate sizes through power-law distributions, which can stimulate explorations in biological and other nonequilibrium systems

CPP 50.2 Thu 11:45 ZEU/0260

Droplet-assisted folding of long regulatory RNAs — Simon Doll[1], Lukas Pekarek[1], Fathima Ferosh[1], Jovana Vasiljević[1], Marcus Jahnel[1], and •Tyler Harmon[2] — [1]BIOTEC, Dresden, Germany — [2]IPF, Dresden Germany

Long regulatory RNA regions orchestrate complex cellular processes, including gene expression and epigenetic modifications. How these RNAs dynamically fold and refold in response to cellular signals remains poorly understood. Given that RNAs interact with ubiquitous RNA-binding proteins (RBPs) prone to form biomolecular condensates, we explore how protein droplets interacting along an RNA impact its folding process. Attached droplets prevent premature folding by competing with RNA:RNA interactions. When droplets dissolve due to cellular signals, capillary effects cause the RNA to collapse while refolding. We test this process of condensate-guided RNA folding by adapting established RNA secondary structure predictors to mimic various folding pathways and supplement this with coarse-grained simulations. We find that interactions with transient droplets robustly leads to the formation of long-range RNA contacts, which are otherwise hard to achieve. Our results compare favorably with available experimental data. We propose that this strategy, which we call droplet-assisted RNA folding, represents a previously unexplored mechanism for shaping RNA structures. Given the widespread propensity of RBPs to form condensates, this process could play a fundamental role in the structural organization, conditional reshaping, and functional regulation of long regulatory RNAs.

CPP 50.3 Thu 12:00 ZEU/0260

Simulation Insights into the Assembly of Polyplexes for RNA Delivery — •Jonas Hans Lehnen[1], Jorge Moreno Herrero[3], Heinrich Haas[3], Friederike Schmid[1], and Giovanni Settanni[1,2] — [1]Department of Physics, Johannes-Gutenberg University Mainz — [2]Faculty of Physics and Astronomy, Ruhr University Bochum — [3]BioNTech SE, Mainz

RNA-based pharmaceuticals proved successful with the COVID-19 vaccines and are now undergoing clinical trials for a broad range of therapeutic indications. Lipid-based nanoparticles (LNPs) have been used so far as delivery systems, although alternatives are still needed to meet efficacy and safety requirements across a broader range of applications. Polyplexes, formed by the self-assembly of cationic polymers with the anionic nucleic acids, constitute a valuable substitute, especially if precise control of the number and shape of the encapsulated RNA chains is possible. Here[1], we use molecular dynamics simulations of a coarse-grained polyplex model to show that the most important factors controlling it are the charge ratio between polyelectrolytes and RNA and their concentration during assembly. Close to the isoelectric point, the polyplexes are large, whereas in large excess of cationic polymer, their size decreases, allowing one RNA copy per nanoparticle. Our results are consistent with recent experimental work on polyethylenimine polyplexes.

[1] Simulation Insights into the Assembly of Polyplexes for RNA Delivery, Lehnen et al., Biomacromolecules (2025), DOI: 10.1021/acs.biomac.5c01219

CPP 50.4 Thu 12:15 ZEU/0260

Polymer-assisted condensation as key to chromatin localization — •Arghya Majee[1] and Jens-Uwe Sommer[1,2,3] — [1]Leibniz Institute of Polymer Research Dresden, Germany — [2]Institute for Theoretical Physics, TU Dresden, Germany — [3]Cluster of Excellence Physics of Life, TU Dresden, Germany

We put forward a novel mechanism [1] to account for the experimentally observed [2] positional shifts of chromosomes within the cell nucleus, which appear to be driven by compositional alterations in the nuclear lamina. By considering chromatin as a biomolecular condensate we demonstrate that the adsorption of the chromatin-binding proteins at the lamina leads to a wetting of the condensate while spreading of the chromatin on the lamina is avoided. This leads to the non-monotonous density profile of the polymer with respect to the surface which can be explained by the competition between the tendency of the protein component to wet the surface and the conformational restrictions of the polymer near the impenetrable surface. A change in the composition of the the lamina can lead to repositioning of chromatin towards the center of the nucleus. Our theory not only offers an explanation for specific chromatin conformation experiments, but also contributes to the broader understanding of wetting onto responsive surfaces in multi-component systems.

References:
[1] A. Majee and J.-U. Sommer, bioRxiv 2025.06.11.658974 (submitted).
[2] Amiad-Pavlov *et al.*, Sci. Adv. **7**, eabf6251 (2021).

CPP 50.5 Thu 12:30 ZEU/0260

Bridging Scales to Understand the Role of Ubiquitylation and Sumoylation in Protein Phase Separation — •Supriyo Naskar, Kurt Kremer, and Oleksandra Kukharenko — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

The post-translational modifiers, such as mono- and poly-ubiquitins and SUMOs, are known for their ability to modulate protein-protein interactions by becoming covalently attached to other target proteins. Despite the high similarity in the tertiary structure and sequence, they differentially influence the target protein properties. In this work, we employed a multiscale simulation approach that encompasses atomistic to different levels of coarse-grained modeling techniques, combined with data-driven methods, to explore the structural differences and multidimensional energy landscapes of ubiquitin, SUMO, and their conjugates. We finally investigate the influence of distinct features of the targets and modifiers on protein phase separation and aggregation, providing molecular-level insight into the corresponding in vitro measurements and informing further experiments through the adjustment of relevant parameters.

CPP 51: Focus Session: 75 Years Polymer Physics Division: From Curiosity to Smart Materials (joint session CPP/BP)

Polymer materials are ubiquitous in modern society. In recent years, the focus has been on the development of functional, tunable or responsive materials, oftentimes inspired by biological materials. At this, a number of fundamental problems arise, e.g. regarding the interaction of polymers with water, biomolecules or inorganic nanoparticles and the resulting self-assembled morphologies as well as the underlying dynamics and the kinetics of morphological changes upon a stimulus. These problems are nowadays addressed in an interdisciplinary way by experimental methods, computer simulations and theory, often in close collaboration with polymer chemists. In five talks by renowned speakers, the focus session aims at highlighting few of these aspects that are currently under investigation worldwide. The fact that the Polymer Physics Division of the German Physical Society was founded in 1951 and hence, 2026 is the 75th anniversary, seems to be a good occasion to bring modern polymer physics into the focus.

Organized by Christine M. Papadakis, Christian Holm, Tayebeh Ameri and Kristian Franze.

Time: Thursday 15:15–17:45 Location: ZEU/LICH

Topical Talk CPP 51.1 Thu 15:15 ZEU/LICH

The Loops of Life — Brian Chan and •Michael Rubinstein — Duke University, Durham, NC, USA

In mammalian cells, the cohesin protein complex is believed to regulate chromatin during interphase through active loop extrusion, in which dynamic loops are formed by cohesin translocating along chromatin. We developed a theoretical model that quantifies how key parameters, including cohesin residence time on chromatin, extrusion velocity, and the number density of chromatin-bound cohesins, regulate genomic contacts. The model describes chromatin contact probabilities and predicts that loop formation probability is a nonmonotonic function of loop length. Our theory demonstrates that active loop extrusion causes the apparent fractal dimension of chromatin to cross over between two and four at contour lengths on the order of 30 kilobase pairs. This work provides a theoretical basis for the compact organization of interphase chromatin, explaining the physical reason for the segregation of topologically associated domains and suppression of chromatin entanglements by up to a factor of 50, which contributes to efficient gene regulation by distal elements such as enhancers or silencers.

Topical Talk CPP 51.2 Thu 15:45 ZEU/LICH

Polyelectrolytes and Biological Systems: A Charged Relationship — •Matthias Ballauff — Chemie und Biochemie, Freie Universitaet Berlin

If charges are appended to linear or crosslinked polymers, a polyelectrolyte results. Polyelectrolytes are ubiquitous and play a major role in biophysics. Important natural polyelectrolytes as e.g. DNA or Heparin are central in biology, and a thorough understanding of these systems and of charge-charge interaction is one of the main tasks of biophysics. In my lecture, I will discuss our recent research done on -Interaction of linear polyelectrolytes with proteins. This problem is also relevant for the formation of biocondensates by the interaction of cationic and anionic proteins; -Charged polymer networks and their interaction with proteins; -Role of polyelectrolytes in virus infections. In all cases, a quantitative understanding of the systems in terms of analytical models can be achieved, which may pave the way for future pharmaceutical applications.

Topical Talk CPP 51.3 Thu 16:15 ZEU/LICH

From block copolymer morphologies to functional polymer membranes — •Volker Abetz — Helmholtz-Zentrum Hereon, Institute of Membrane Research, Max-Planck-Str. 1, 21502 Geesthacht, Germany — University of Hamburg, Institute of Physical Chemistry, Martin-Luther-King-Platz 6, 20146 Hamburg, Germany

Depending on solvent selectivity and the time of evaporation different structures can be obtained in cast block copolymers, showing that there is an interplay between kinetics and thermodynamic driving forces during the self-assembly before the sample is dry. When preparing membranes from block copolymer solutions, besides molecular weight, composition of the block copolymer and its concentration, also the choice of solvent, and the casting conditions play an important influence on the obtained morphology of the finally obtained membrane. This is especially important when membranes are prepared via the so-called non-solvent induced phase separation process after initial self-assembly by partial evaporation of solvent. The obtained membranes, when prepared successfully, display a rather isoporous top layer and can be subsequently post functionalized, in order to tune pore size and pore surface property. Different examples of the separation properties will be shown and also the potential use as a membrane reactor will be discussed.

Topical Talk CPP 51.4 Thu 16:45 ZEU/LICH

Molecular electronic materials and devices for solar energy conversion — •Jenny Nelson — Imperial College London

To maximize the potential of solar power, new materials will be needed to harvest and convert solar energy alongside existing photovoltaic technologies. Molecular electronic materials, such as conjugated polymers and molecules, can achieve photovoltaic conversion through a process of photon absorption, charge separation at a heterojunction, and charge collection. Through a remarkable series of advances in materials design, the efficiency of photovoltaic energy conversion in molecular materials has risen from 1% to over 20% within two decades. We will discuss the factors that control the function of molecular solar cells including the nature of the charge separating heterojunction, and the impact of chemical and physical structure on phase behaviour, energy and charge transport, light harvesting, and loss pathways, comparing experimental measurements with a computational model of the generation and evolution of excited states and charges in such systems. We identify key molecular parameters that are likely to assist charge generation and consider the extent to which these parameters are optimised in the best performing materials. Finally, we will address the limits to conversion efficiency in such systems.

Topical Talk CPP 51.5 Thu 17:15 ZEU/LICH

Control of cell and tissue stiffness by biopolymer networks and particle inclusions — •Paul Janmey — University of Pennsylvania, Philadelphia, PA, USA

Filamentous networks of semiflexible polymers are ubiquitous in biology. Collagen fibers form much of the extracellular matrix, the cytoskeleton controls cell mechanics, and chromatin fibers span the volume of the nucleus. The mechanical properties of the biopolymer fibers, the way in which the fibers link into networks, and the types of cells within the network all affect the way in which tissues respond to mechanical stress.

CPP 52: Members' Assembly

Time: Thursday 18:00–19:00 Location: ZEU/LICH

All members of the Chemical and Polymer Physics Division are invited to participate.

CPP 53: Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics VII

Time: Friday 9:30–11:15 Location: ZEU/LICH

Invited Talk CPP 53.1 Fri 9:30 ZEU/LICH

Limits and Prospects of Organic Solar Cells — •Dieter Neher — Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str 24-25, 14476 Potsdam

Since the advent of low bandgap non-fullerene acceptors (NFAs), the performance of organic solar cells (OSCs) has improved significantly, with record efficiencies that now safely exceed 20 %. A critical parameter is the offset between the relevant frontier orbitals at the DA heterojunction, which in most NFA-based blends is the difference in HOMO energies. Here we combine a wide range of methods, from femtosecond transient absorption to steady state photoluminescence and electroluminescence, spectroscopy to study the mechanisms and efficiency of free charge generation and recombination. For a wide series of NFA-based OSCs, we find that the singlet exciton decay is the main competing pathway for free charge generation while reformation of singlet excitons from reformed CT states dominates the radiative recombination in EL. To explain our data as function of the HOMO offset, we set up a 5-state model which includes singlet and triplet excitons. Our results show that state-of-the-art OSCs already exhibit an optimum HOMO-HOMO-offset. Future work should, therefore, focus on optimizing photon harvesting and reducing bimolecular recombination in order to push the device efficiency well beyond 20 %.

CPP 53.2 Fri 10:00 ZEU/LICH

Temperature Degradation of Slot-Die Printed Organic Solar Cells — •Christoph G. Lindenmeir[1], Simon A. Wegener[1], Christopher R. Everett[1], Julian E. Heger[1], Sigrid Bernstroff[2], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]Elettra-Sincrotrone Trieste S.C.p.A., Basovizza, Trieste, Italy

Organic solar cells (OSCs) have emerged as promising candidates for next-generation photovoltaics due to their rapid efficiency improvements, low toxicity, and compatibility with low-cost, solution-based fabrication methods such as slot-die printing. Their high optical absorption, combined with their lightweight and flexible design, makes them particularly attractive for space applications. Offering a superior power-to-weight ratio compared to conventionally used III-V multijunction cells, OSCs can significantly reduce manufacturing and launch costs. While short-term demonstrations have confirmed their functionality in space, their long-term stability under extreme temperatures, high vacuum, and ionizing radiation still needs to be investigated. Therefore, this study compares the influence of constant-temperature conditions on active-layer morphology and electrical performance with that of temperature cycling. To investigate the degradation process, we employed operando grazing-incidence small-angle X-ray scattering (GISAXS), a nondestructive technique for probing thin-film morphology. Simultaneously, we monitored the electrical performance of the devices under vacuum to simulate space conditions.

CPP 53.3 Fri 10:15 ZEU/LICH

Electronic coarse-graining for accurate and scalable modeling of organic semiconductors — •Andriy Zhugayevych[1], Denis Andrienko[1], and Sergei Tretiak[2] — [1]Max Planck Institute for Polymer Research — [2]Los Alamos National Laboratory, USA

Modeling the electronic properties of organic semiconductors remains challenging due to their complex multiscale structure, which limits the applicability of methods developed for small-molecule solids and inorganic crystals. Fragmentation techniques designed for biomolecular systems are unsuitable for π-conjugated materials because of wavefunction delocalization. We present an electronic coarse-graining methodology that enables accurate and scalable electronic-structure calculations for organic semiconductors composed of monomers with closed-shell π-systems, allowing complete fragmentation along σ-bonds. The approach is demonstrated for crystalline polymers, highlighting how side-group modifications influence the electronic properties of thiophene-based systems such as polythiophene, P3HT, and PEDOT [1]. We further analyze errors introduced by oversimplified electronic models using examples of large flexible molecules, including non-fullerene acceptors for solar cells [2] and OLED materials. The approach can be applied - albeit in less automated way - to broader class of semiconductors, including metal-organic polymers [3], frameworks, and some inorganic semiconductors [4].

[1] Preprint at https://cmsos.github.io/escp; [2] J. Chem. Phys. 159, 024107 (2023); [3] Chem. Sci. 13, 8161 (2022); [4] J. Phys. Chem. Lett. 12, 4674 (2021).

CPP 53.4 Fri 10:30 ZEU/LICH

Facile Correction Method for DFT Band Structures Towards Hybrid Density Functional Level for 2D-Covalent Organic Frameworks — •Laura Fuchs, Maximilian F. X. Dorfner, Matthias Knechtges, Johann Olbrich, and Frank Ortmann — Department of Chemistry, TUM School of Natural Sciences, and Atomistic Modeling Center, Munich Data Science Institute, Technical University of Munich, Germany

Density functional theory (DFT) is the method of choice for predicting the majority of structural, and electronic properties of organic and inorganic materials. Generalized gradient approximations, such as the semi-local PBE functional, are widely used in the community but have one major drawback: the band gap problem. The fundamental band gap is typically underestimated by up to a factor of two by these approaches, which is critical since this electronic property is of utmost importance for assessing the applicability of the investigated material for (opto-)electronic purposes.

Here, we establish a robust linear correlation between the semi-local PBE band gaps and the more accurate, but more expensive, hybrid HSE06 band gaps by analyzing organic molecules as well as extended crystals such as covalent organic frameworks (COFs). By eliminating the need for costly hybrid functional calculations, our approach achieves up to a 54-fold speedup compared to conventional HSE06 computations. We compare various implementation strategies and evaluate each method's advantages and limitations, with particular focus on their implications for predicting electronic transport properties.

CPP 53.5 Fri 10:45 ZEU/LICH

The influence of vibrations on charge and energy transfer dynamics in a singlet fission donor-acceptor complex — •Karin S. Thalmann[1], Johan E. Runeson[1], Pedro B. Coto[2], and Michael Thoss[1] — [1]Institute of Physics, University of Freiburg, Germany — [2]Spanish National Research Council (CSIC), Madrid, Spain

Singlet fission is a photophysical process in molecular materials transforming a singlet excited electronic state to two triplet states [1], effectively doubling the number of charge carriers. This makes molecules exhibiting singlet fission possible candidates to increase the efficiency of solar cells beyond the Shockley-Queisser limit. To investigate this possibility, we analyse the charge and energy transfer dynamics in a donor-acceptor complex consisting of a bis(diazadiborine)-based chromophore [2] and tetracyanoquinodimethane. Using a combined approach of *ab initio* multireference perturbation theory calculations and quantum dynamical simulations based on a harmonic vibronic coupling Hamiltonian [3], we reveal competing charge and energy transfer mechanisms, such as singlet fission-based transfer and energy decay channels. Further, we expand our model Hamiltonian to include all vibrational degrees of freedom and the anharmonicity in the vibrational modes of the chromophore. The use of mixed quantum-classical approaches allows us to analyse the influence of these vibrational modes on the dynamics as well as the charge and energy transfer mechanisms.

[1] M. B. Smith *et al.*, *Chem. Rev.* **110**, 6891-6936 (2010).
[2] T. Zeng, *J. Phys. Chem. Lett.* **7**, 4405-4412 (2016).
[3] S. R. Reddy *et al.*, *J. Chem. Phys.* **151**, 044307 (2019).

CPP 53.6 Fri 11:00 ZEU/LICH

Tracking the degradation of non-fullerene organic solar cells in fluctuating environments — •Lixing Li, Thomas Baier, Xiaojing Ci, Zhaonan Jin, and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, 85748 Garching, Germany

The long-term operational stability of non-fullerene organic solar cells (OSCs) remains a critical challenge that limits practical applications. While substantial efforts have been devoted to understanding the degradation mechanisms of OSCs under extreme conditions such as high or low temperatures, far less attention has been paid to their potential recovery behaviour. In real-world environments, organic solar cells are not exposed to constant stress; instead, environmental factors such as temperature, humidity, and illumination fluctuate continuously over time. These dynamic variations may induce partial or even reversible changes in device performance and morphology. It is essential to explore not only how OSCs degrade under stress but also how they recover once the stress is relieved or altered. In this study, we investigate the recovery processes of BTP-4F non-fullerene organic solar cells subjected to multiple environmental parameters. Advanced characterisation techniques, including grazing-incidence X-ray scattering (GIXS) and atomic force microscopy (AFM), are employed to track both in-situ and ex-situ structural evolution within the active layer. These analyses provide new insights into the mechanisms governing the recovery and structural reorganisation of OSCs under dynamic environmental conditions.

CPP 54: Gels, Polymer Networks and Elastomers II

Time: Friday 9:30–11:15 Location: ZEU/0255

Invited Talk CPP 54.1 Fri 9:30 ZEU/0255

NMR-based molecular rheology and structural characterization of model gels — •Kay Saalwächter and Bidit Lamsal — Institut für Physik - NMR, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany

Low-resolution proton NMR holds great potential for the routine assessment of the relation between the NMR-detected monomer-level mobility and the relevant physical properties of polymer-based materials. In elastomers and gels, multiple-quantum (MQ) NMR allows for the precise measurement of residual dipolar couplings (RDCs) among the monomer protons, which reflects the conformational space of the highly mobile network chains. In this way, not only the average network chain length but also structural inhomogeneities become accessible. In model networks made by end-linking of star polymers, we can go as far as quantifying connectivity motifs in gels made by heterocomplementary [1,2] and homocomplementary coupling reactions [3], either in one-component [1,3] or amphiphilic co-networks [2].

While the measured RDC is consistently found to be proportional to the gels' elasticity modulus [3], the absolute-level interpretation of the measured average RDC to predict the modulus remains a challenge. We here report on recent experiments performed on a variety of PEO-based model gels to elucidate the effects of solvent on local conformational fluctuations, thermodynamic aspects (solvent quality) and the inhomogeneity of the gels.

[1] Macromolecules 44, 9666 (2011); [2] Macromolecules 55, 6573 (2022); [3] Macromolecules 57, 3058 (2024)

CPP 54.2 Fri 10:00 ZEU/0255

Characterization of the deformation and fracture of tough double-network hydrogels — •Eric Euchler[1], Sitao Wang[2], Konrad Schneider[1], and Sven Wiessner[1,3] — [1]Leibniz-Insititut für Polymerforschung Dresden, Dresden, Germany — [2]Leibniz-Insititut für Polymerforschung Dresden, Dresden, Germany — [3]TUD Dresden University of Technology, Dresden, Germany

Double-network hydrogels (DNHs) feature two interpenetrating networks: a stiff, densely crosslinked first network that carries the load at low strain, and a flexible, loosely crosslinked second network that remains deformable under high strain, offering mechanical properties comparable to elastomers and soft load-bearing biological tissues. Additionally, a yielding phenomenon accompanied by necking of the sample can be observed. This necking zone forms under uniaxial tension and grows with continued loading, which is associated with the fracture of the first network. In this contribution, new insights into the mechanical deformation and damage behavior are given by advanced characterization approaches.

CPP 54.3 Fri 10:15 ZEU/0255

The Role of Connectivity Defects in Governing the Rheology and Microstructure of tPEG Networks — •Sayam Bandyopadhyay[1,2], Sebastian Seiffert[3], and Arash Nikoubashman[1,2] — [1]Leibniz-Institut für Polymerforschung Dresden e.V., Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, Germany — [3]Institut für Physikalische Chemie, Johannes Gutenberg-Universität, Germany

We utilized coarse-grained molecular simulations to examine how connectivity defects influence tetra-PEG (tPEG) polymer networks. Both homoleptic and heteroleptic systems were studied, with noncovalent end-group bonds modeled by an inverted Gaussian potential to control valency. Defects were introduced either by deactivating functional end groups or by deviating from ideal stoichiometry in heteroleptic mixtures. Post-gelation structure was quantified using structure factors, radial distribution functions of attractive beads, and internal loop statistics. Network dynamics and molecular mobility were assessed through mean-square displacements of individual tPEG molecules and through bond lifetimes. Our results show that defects enhance loop formation and substantially increase star-polymer mobility. As a consequence, networks with higher defect concentrations exhibit lower viscosity and faster stress relaxation. We also discuss the system's shear response simulated using a mesoscale solvent with hydrodynamic interactions to probe loop and link interconversion kinetics. These findings provide a molecular level understanding of how defects control the structure, dynamics, and mechanical properties of tPEG networks.

CPP 54.4 Fri 10:30 ZEU/0255

Assembling a true Olympic gel from >16,000 combinatorial DNA rings — Sarah K. Speed[1,2], Yu-Hsuan Peng[1,2], Azra Atabay[1,2], Krishna Gupta[1,2], Toni Müller[3,4], Carolin Fischer[5], Ilka Hermes[6], Jens-Uwe Sommer[3,4,7], Michael Lang[3], and •Elisha Krieg[1,2] — [1]Division of Polymer Biomaterials Science, Leibniz Institute of Polymer Research Dresden, Germany — [2]Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, Germany — [3]Division of the Theory of Polymers, Leibniz Institute of Polymer Research Dresden, Germany — [4]Institute for Theoretical Physics, Technische Universität Dresden, Germany — [5]B CUBE - Center for Molecular Bioengineering, Technische Universität Dresden, Germany — [6]Division of Physical Chemistry and Physics of Polymers, Leibniz Institute of Polymer Research Dresden, Germany — [7]Cluster of Excellence Physics of Life, Technische Universität Dresden, Germany

Olympic gels consist of a three-dimensional network of mechanically interlocked cyclic molecules providing unique mechanical properties. We report the successful assembly of a true Olympic gel from a library of DNA rings comprising more than 16,000 distinct molecules. Each of these rings contains a unique sequence domain that can be enzymatically activated to produce reactive termini that favor intramolecular cyclization. Results are shown on the genetic, mechanical, and structural characteristics of the material by next-generation sequencing, oscillatory rheology, large-scale computational simulations, atomic force microscopy, and cryogenic electron microscopy.

CPP 54.5 Fri 10:45 ZEU/0255

On the symmetry breaking between gelation and network degradation — •Michael Lang — Division of the Theory of Polymers, Leibniz Institute of Polymer Research Dresden, Germany

Recent experiments indicate that there is a possible symmetry breaking between gelation and network degradation processes in contrast to the predictions of percolation models and classical mean field models. We analyze this problem by large scale computer simulations and mean field modeling in order to avoid possible problems of the experimental setup. The modeling is generalized to capture the main effects of cyclization and composition fluctuations on the gelation process. Both our modeling and the simulation data confirm the existence of the symmetry breaking already for systems above the overlap threshold. This indicates some general problems of the percolation approach for modeling polymer networks.

CPP 54.6 Fri 11:00 ZEU/0255

Crosslinking Mechanisms of Alginate-based Graft Copolymers with Thermoresponsive Side Chains — •Wenqi Xu[1], Sofia-Falia Saravanou[2], Yefan Song[1], Yandong Wang[1], Joachim Kohlbrecher[3], Constantinos Tsitsilianis[2], and Christine M. Papadakis[1] — [1]TUM School of Natural Sciences, Soft Matter Physics Group, Garching, Germany — [2]University of Patras, Greece — [3]PSI, Villigen, Switzerland

Alginates are naturally occurring, non-toxic polysaccharides which have seen extensive use in biomedicine. Here, we investigate an alginate-based graft copolymer, namely alginate-*g*-P(NIPAM$_{94}$-*co*-N*t*BAM$_6$), where a random copolymer of *N*-isopropylacrylamide (NIPAM) and *N*-*tert*-butyl acrylamide (N*t*BAM) is grafted onto a sodium alginate backbone [1]. While introducing thermoresponsive PNIPAM enables temperature-induced gelation, the hydrophobic comonomer N*t*BAM regulates the transition temperature and the mechanical properties of the hydrogel. The structure and the gelation mechanisms of the copolymers are studied in aqueous solutions using small-angle neutron scattering (SANS). At this, contrast matching of the backbone and the side chains was used to obtain selective information. The SANS data show strong forward scattering above the transition temperature of PNIPAM, which is attributed to the collapse of the side chains, resulting in hydrophobic globules which act as nodes of the hydrogel network.

[1] K. Safakas, C. Tsitsilianis. *Int. J. Mol. Sci.* **2021**, 22(8), 3824.

CPP 55: Focus Session: Theoretical Modeling and Simulation of Biomolecular Condensates III (joint session CPP/BP)

Time: Friday 9:30–11:15 Location: ZEU/0260

Topical Talk CPP 55.1 Fri 9:30 ZEU/0260

Data-driven modelling of phase-separating intrinsically disordered regions — •Giulio Tesei[1,2], Fatima Kamal Zaidi[3], Shanlong Li[4], Julian O. Streit[1], Jianhan Chen[4], Tanja Mittag[3], and Kresten Lindorff-Larsen[1] — [1]Department of Biology, University of Copenhagen, Copenhagen, Denmark — [2]Department of Biomedical Science, Malmö University, Malmö, Sweden — [3]Department of Structural Biology, St. Jude Children's Research Hospital, Memphis, U.S.A. — [4]Department of Chemistry, University of Massachusetts, Amherst, U.S.A.

Intrinsically disordered regions (IDRs) constitute about one third of the human proteome and play important roles in biological processes. While lacking well-defined 3D structures, IDRs adopt heterogeneous ensembles influenced by multivalent interactions; these same interactions can promote phase separation and contribute to the formation of biomolecular condensates. I will first present CALVADOS, an efficient one-bead-per-residue model optimized on experimental data reporting on IDR conformational properties and extensively validated on both single-chain and phase behavior across diverse sequences. I will then describe how we used large sets of CALVADOS simulations to train machine-learning models that accurately predict single-chain compaction and homotypic phase-separation propensity directly from sequence. Finally, I will introduce a hybrid-resolution model with an atomistic backbone representation that matches the accuracy of CALVADOS for global dimensions and phase separation while also capturing local structure and backbone hydrogen bonding.

CPP 55.2 Fri 10:00 ZEU/0260

Born to Condense: Polysomes Drive Co-Translational Condensation of Biomolecular Condensate Proteins — •Zhouyi He, Jens-Uwe Sommer, and Tyler Harmon — Leibniz Institute of Polymer Research, 01069, Dresden, Germany

Biomolecular condensates formed by protein LLPS are ubiquitous and crucial in cells. While the physics and functions of LLPS are well studied, its interplay with protein synthesis, translation, remains largely unexplored. Here we propose Co-Translational Condensation (CTC), a mechanism in which nascent protein chains of polysomes, multiple ribosomes on one mRNA, interact with condensates, localizing translation to condensate surfaces. Using coarse-grained simulations, we show that protein domain architecture dictates the extend of CTC, consistent with a Langmuir adsorption model. Bioinformatic analysis reveals that most condensate-associated proteins have architectures favoring CTC, with strong interaction regions of nascent chains exposed on polysomes. Dynamically, simulation and reaction-diffusion modeling reveal that CTC is kinetically feasible within typical polysome lifetimes, either through large polysomes nucleating new condensates or via diffusion to pre-existing condensates. As a case study, we demonstrate that CTC enhances post-translational modifications by minimizing unmodified intermediates. More broadly, we anticipate CTC may also influence protein folding, misfolding, and signal-integration latency. Together, our results establish CTC as a general mechanism coupling translation with phase separation, with broad implications for protein evolution, cellular organization, and synthetic biology.

CPP 55.3 Fri 10:15 ZEU/0260

Local RNA/protein stoichiometry tunes the electrostatic microenvironment inside reconstituted multicomponent condensates — •Patrick M. McCall — Leibniz Institute for Polymer Research Dresden, Dresden, DE

Biomolecular condensates are demixed phases of biopolymers and, in living cells, commonly form through the associative phase separation of strongly-charged nucleic acids together with protein polyampholytes carrying a weak net charge. While condensates are proposed to offer distinct aqueous environments for the organization of cellular biochemistry, it remains unclear which physical aspects of the microenvironment are relevant and how widely they can vary between condensates. Motivated by the large asymmetry in structural charge between typical condensate components such as RNAs and RNA-binding proteins, we explore here the implications of electroneutrality on the electrostatic environment within model multicomponent condensates. Combining classical Donnan theory with recent measurements of the macromolecular composition of condensates reconstituted from full-length FUS protein and a homopolymeric RNA [McCall et al Nat Chem 2025], we compute the partitioning of salt ions as well as the Donnan potential across the phase boundary. We find that RNA/FUS stoichiometry tunes both co-ion exclusions over a wide range and is coupled to a pH jump across droplet interface. We also find that co-ion exclusion is suppressed by counter-ion condensation and enhanced by non-ideality of un-bound ions. These results provide insight into the range of ionic conditions accessible to a prominent class of biomolecular condensate.

CPP 55.4 Fri 10:30 ZEU/0260

Coarse-grained model to study the effects of electric fields on protein interactions — •Agaya Johnson[1], Debes Ray[2,4], Mahnoush Madani[3], Jan Dhont[2,3], Florian Platten[2,3], Kyongok Kang[2], and Sofia Kantorovich[1] — [1]University of Vienna, Kolingasse 14-16, 1090, Vienna, Austria. — [2]nstitute of Biological Information Processing IBI-4, Forschungszentrum Jülich, 52428 Jülich, Germany. — [3]Faculty of Mathematics and Natural Sciences, Heinrich Heine University Düsseldorf, 40225 Düsseldorf, Germany. — [4]Solid State Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai 400085, India.

Proteins can undergo transition between a wide range of organisational states, from soluble monomers to disordered phases and ordered structures. Experiments have shown that lysozyme in sodium thiocyanate solution can form homogeneous, crystalline, or liquid phases depending on the salt and protein concentrations, and that these phase boundaries can be shifted by applying an electric field. We present a coarse-grained model of lysozyme in sodium thiocyanate solution, representing the protein as an ellipsoid decorated with charged and adhesive surface patches. Counterions and monovalent salt are treated explicitly via excluded-volume repulsion and Coulombic interactions. We investigate (i) how patch size and salt*patch interactions influence ion distributions around a single protein, with and without an external electric field, and (ii) the resulting effective interactions between two proteins as functions of patch properties, salt concentration, and applied electric field.

CPP 55.5 Fri 10:45 ZEU/0260

Entropic Clustering of Stickers Induces Aging in Biocondensates — •Hugo Le Roy[1] and Paolo De Los Rios[2] — [1]Department of Civil, Chemical and Environmental Engineering, University of Genoa, Genoa, Italy — [2]Institute of Physics, Ecole Polytechnique Fédérale de Lausanne

Neurodegenerative conditions, such as Parkinson's disease, results from the aggregation of synaptic proteins such as alpha-synuclein. In a healthy presynaptic neuron, effective neurotransmission relies on the spatial organization of synaptic vesicles within phase-separated droplets. These vesicles release neurotransmitters into the synaptic cleft to activate ion-gated channels on the postsynaptic neuron.

In this work, we investigate how this transmission process is impaired during neurodegeneration. Specifically, we focus on the solidification of these phase-separated droplets, a phenomenon described as aging, leading to protein aggregation and associated with the emergence of pathology. We explore the connection between the mechanical properties of the condensates and their microscopic structure using a minimal physical model that treats complex molecules as stickers and spacers. We show that entropy maximization of spacers leads to an effective attractive force between stickers. As a result, our system displays a surprisingly slow relaxation toward equilibrium, reminiscent of glassy systems and consistent with the liquid-to-solid transition observed in aging droplets. By analyzing the clustering dynamics of stickers, we successfully explain the microscopic origin of this glassy relaxation.

CPP 55.6 Fri 11:00 ZEU/0260

Biomolecular condensates with a Twist: From Assembly to Arrest — •Mahesh Yadav[1,2] and Lukas Stelzl[2] — [1]Institute of Physics, Johannes Gutenberg University, Mainz — [2]Institute of Molecular Physiology, Johannes Gutenberg University, Mainz

In this work, we investigate the phase behavior of RNA-binding protein Fused in Sarcoma (FUS), whose multivalent and intrinsically disordered regions drive the formation of biomolecular condensates through liquid-liquid phase separation. FUS is a multi-domain protein with arginine-glycine-rich segments (RG-rich domains) that participate in essential cellular proceses. We examine how characteristic sequence motifs such as RGG.. mediate homotypic and nucleic acid binding, and how targeted point mutations (e.g., RtoK, RtoA) disrupt these motifs and impair condensate formation. Using the thermodynamics phase diagram as a benchmark we highlighted the shift in phase separation propensity of the FUS and its variants. Furthermore, we identify the role of key interactions such as electrostatics, π-π and cation-π in nucleic acid binding at atomistic scale. We further characterized the emergent viscoelastic behavior of FUS condensates at multiple scales. We observe that upon mutations the overall dynamics slows down which reflects the gel-like state. Within the condensate interior, protein chains exhibit sub-diffusive dynamics arising from intermittent binding and viscoelastic resistance, mobility at the interface is further suppressed due to anisotropic interactions and interfacial confinement. To quantify these behaviors across relevant scales, we employ multi-resolution simulation models.

CPP 56: Molecular and Polymer Dynamics, Friction and Rheology I

Time: Friday 10:45–12:00 Location: HÜL/S386

Invited Talk CPP 56.1 Fri 10:45 HÜL/S386

Liquid Dynamics at Interfaces — •Michael Vogel — Institut für Physik kondensierter Materie, TU Darmstadt, Hochschulstraße 6, 64289 Darmstadt

Liquids at interfaces are of great importance in nature and technology, for instance, in biological cells, clay minerals, and energy materials. Typically, the dynamics of liquids at interfaces significantly differ from those in the bulk. We combine nuclear magnetic resonance and broadband dielectric spectroscopy with molecular dynamics simulutations to determine the magnitude and range of these interface effects in broad frequency and temperature ranges. It is shown that the free energy landscape imposed by an interface on an adjoining liquid enables a basic understanding of the altered dynamical behavior [1]. It will be discussed that a knowledge of interface effects allows one not only to obtain valuable insights into the properties of confined water and, when avoiding crystallization, the anomalies and vitrification of bulk water [2-4], but also to steer ion transport in electrolyte-host systems for improved lithium-ion battery and proton-exchange membrane materials [5-7].

[1] S. Hefner et al., Phys. Rev. Lett. 133, 106201 (2024)
[2] V. Schiller and M. Vogel, Phys. Rev. Lett. 132, 016201 (2024)
[3] J. H. Melillo et al., PNAS 121, e2407030121 (2024)
[4] E. Steinrücken et al., J. Phys. Chem. Lett. 14, 4104 (2023)
[5] M. Stevenson et al., Adv. Funct. Mater. e15706 (2025)
[6] S. F. Winterstein et al., J. Am. Chem. Soc. 145, 27563 (2023)
[7] A. F. Privalov et al., J. Phys. Chem. Lett. 14, 9335 (2023)

CPP 56.2 Fri 11:15 HÜL/S386

The analytical and numerical investigation of star-shaped copolymers with three arms in confined geometries — •Zoriana Danel[1], Joanna Halun[2], and Paweł Karbowniczek[1] — [1]Cracow University of Technology, Poland — [2]Institute of Nuclear Physics, Poland

The influence of star copolymer topology on the depletion interaction potentials, the depletion forces, the radius of gyration and the monomer density profiles is investigated analytically and numerically. The method of analytical calculation of the dimensionless depletion interaction potentials and the dimensionless depletion forces for a dilute solution of ideal star-shaped copolymers with three legs in combination f=2-1 in a Θ-solvent confined in a slit geometry of two parallel walls with repulsive surfaces and for the case of one repulsive and the other inert surface is proposed. Besides, molecular dynamic simulations of a dilute solution of star-shaped copolymers in a good solvent with three number of legs with N=801 monomers (300+300+200+1) for combination f=2-1 and N=701 monomers (300+200+200+1) for combination f=1-2 confined in a slit with different boundary conditions are performed and the results of the monomer density profiles for the above mentioned cases are obtained for the narrow and wide slit region. Furthermore, the numerical calculations of the radius of gyration for star-shaper copolymers in combination f=2-1 and f=1-2 are performed. The obtained results are interesting from scientific and practical point of view, because of their potential application in materials engineering, nano-technology, biotechnology and medicine.

CPP 56.3 Fri 11:30 HÜL/S386

Polymer melt dynamics in the light of viscoelastic hydrodynamic interaction — •Hendrik Meyer — Institut Charles Sadron, Université de Strasbourg, CNRS UPR22, 67034 Strasbourg, France

Our group has shown that anomalous center-of-mass (CM) diffusion occurring on intermediate time scales in polymer melts can be explained by the interplay of viscoelastic and hydrodynamic interactions (VHI). The theory has been solved for unentangled melts in 3D [1] and 2D [2] and excellent agreement between theory and molecular dynamics simulation is found. The theory was developed for momentum conserving dynamics as well as Langevin dynamics. The physical mechanism considers that hydrodynamic interactions are time dependent because of increasing viscosity before the terminal relaxation time. We show that this mechanism is generally active and relevant in melts including entangled systems, rings or stars.

[1] PRL 107, 178301 (2011); PRE 85, 051807 (2012). [2] PRL 109, 248304 (2012); Soft Matter 9, 4249 (2013).

CPP 56.4 Fri 11:45 HÜL/S386

Knots in Polymers under Shear Flow — •Maurice P. Schmitt[1], Andrey Milchev[2], and Peter Virnau[1] — [1]Institut für Physik, Johannes Gutenberg-Universität, Mainz, Germany — [2]Institute of Physical Chemistry, Bulgarian Academy of Sciences, Sofia, Bulgaria

Knots in polymers and biological macromolecules, such as DNA and proteins, are crucial to their structure and function. However, the effect of external forces on knots in polymers is still insufficiently understood. Here, we investigate the impact of shear and Poiseuille flow on knotted flexible polymers using Molecular Dynamics (MD) and Multi-Particle Collision Dynamics (MPCD) simulations. We find that under simple shear (Couette flow), initially loose knots in polymer coils tighten beyond a critical shear rate. Further increase of the shear rate leads to tumbling motions of the chains in flow and fluctuating knot sizes. In contrast, knotted polymer globules subjected to shear unfold into pearl-necklace-like conformations, whereby knots spread across multiple sub-globules and undergo dynamic topological transitions. In Poiseuille flow, knots also tighten under increasing flow strength, with fluctuations in knot size emerging at high shear rates. Unexpectedly, the slit thickness significantly influences the tightening process even at constant mean shear rate. These findings reveal that both Couette and Poiseuille flow induce major structural and topological transformations in knotted polymers, offering insight into the behavior of knots under hydrodynamic forces in confined and driven environments.

CPP 57: Hybrid, Organic and Perovskite Optoelectronics and Photovoltaics VIII

Time: Friday 11:30–13:00 Location: ZEU/LICH

CPP 57.1 Fri 11:30 ZEU/LICH

Novel n-Dopants for Improving Organic Solar Cells — •Yahya Asl Soleimani[1], Nora Engelmann[1], Stephanie Buchholtz[1], Jörn Vahland[2], Adrian Kishonti[2], Steffen Woltering[2], Karl Leo[1], and Johannes Benduhn[1] — [1]Institute of Applied Physics, Technische Universität Dresden, Nöthnitzer Straße 61, 01187 Dresden, Germany — [2]CREDOXYS GmbH, Liebigstraße 26, 01187, Dresden, Germany

Doping is a crucial concept in semiconductor technology, and it is no different for organic semiconductors. It increases conductivity and facilitates carrier injection and extraction. While substantial success has been achieved for organic molecular p-dopants, the same cannot be said for n-dopants. They suffer from an inherent disadvantage: the highest occupied molecular orbital (HOMO) of the n-dopant must be lower than the lowest unoccupied molecular orbital (LUMO) of the host, rendering them typically unstable under ambient conditions. Here, we report a new and efficient molecular n-dopant that can dope C_{60} to a conductivity of 20 S/cm. We investigate the origin of its efficacy and explore the doping mechanism using ultraviolet electron spectroscopy (UPS). Moreover, we incorporate the new n-dopant into organic solar cells, demonstrating its effectiveness by improving the power conversion efficiency of the reference devices.

CPP 57.2 Fri 11:45 ZEU/LICH

Computational Study of Electronic Trapping in TADF Host-Guest Systems — •Naomi Kinaret[1], Andrei Stankevych[2,3], Andriy Zugayevych[1], Rishabh Saxena[1], Alexander Vakhnin[3], Kun-Han Lin[1,4], Denis Andrienko[1], Heinz Bässler[2], Anna Köhler[2], and Andrey Kadashchuk[2,3] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]University of Bayreuth, Bayreuth, Germany — [3]National Academy of Sciences of Ukraine, Kyiv, Ukraine — [4]National Tsing Hua University, Hsinchu, Taiwan

Extrinsic traps created by dopants or impurities are ubiquitous in organic semiconductors and can critically influence charge transport [1]. Here we report a computational study of the trapping of charge carriers in amorphous host-guest systems of the thermally activated delayed fluorescence (TADF) emitter DMAC-TRZ in two different hosts, validated by low-temperature thermally- stimulated luminescence (TSL). In both hosts we find that DMAC-TRZ forms an additional Gaussian density of states (DOS), offset from the host DOS by a trap depth ϵ_t. In both systems trap depths and DOS widths, σ_{DOS}, agree with experimentally observed values over a range of compositions, showing that the nominal trap depth is concentration independent. In the case of deep traps, $\epsilon_t > 3\sigma_{DOS}$, we observe concurrent charge detrapping via guest-to-host and guest-to-guest pathways, with the latter dominating for $c_t > 5\%$. Guest-guest transfers are observed already at the low guest concentration of $c_t = 1\%$, attributed to local guest clustering and superexchange- mediated inter-cluster transfers.

[1] Kotadiya, N.B., et al., Nat. Mater. (2019).

CPP 57.3 Fri 12:00 ZEU/LICH

Interface Engineering toward High-Performance Subphthalocyanine-based Single-Component Organic Photodetectors — •Anncharlott Kusber[1], Ying Sun[2], Jakob Wolanksy[1,3], Fred Kretschmer[1], Conrad Winkler[1,3], Anna-Lena Hofmann[1], Ji-Seon Kim[2], Karl Leo[1], and Johannes Benduhn[1,3] — [1]Institute of Applied Physics, Technische Universität, Dresden, Germany — [2]Imperial College London, United Kingdom — [3]German Centre of Astrophysics, Görlitz, Germany

Organic photodetectors (OPDs) have attracted considerable attention due to their capability to convert light into electrical signals and enable high-quality imaging, while simultaneously offering the intrinsic benefits of organic materials. Single-component (SC) OPDs, using a single photoactive organic semiconductor material, have several advantages over the commonly used bulk heterojunction OPDs such as its simplified structure. The influence of several organic electron transport layers (ETLs) on energetic landscape at the immediate interface with organic layers has not yet been systematically reported. This is necessary to gain a deeper understanding of physics of organic interfaces, thereby enabling the further optimization of OPD performance. Sensitive measurement techniques were used to analyse the influence of different organic interfaces on the OPD performance.

These investigations lead to SubNc SC OPD devices, which achieves an EQE of 56 % at 0 V, an ultra-low J_D of $2.5 \cdot 10^{-11}$ A $\cdot$ cm^{-2} at -0.5 V and D* of $3.8 \cdot 10^{14}$ Jones at 0 V (based on calculated shot noise).

CPP 57.4 Fri 12:15 ZEU/LICH

Impact of additive on the morphology and electronic states of PPDT2FBT:PCBM organic solar cells — Md Moidul Islam[1,2], Hassan Ismail[1,2], Saib Qazi[1,2], Ulrich S. Schubert[1,2], and •Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Humboldtstrasse 10, 07743 Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich Schiller University Jena, Philosophenweg 7a, 07743 Jena, Germany

Among organic solar cells using PCBM as an acceptor, the donor PPDT2FBT yields one of the highest power conversion efficiencies (PCE) of nearly 10%. It has been demonstrated that the processing additive diphenyl ether (DPE) contributes to that success essentially. However, the exact mechanism responsible for the performance improvement has so far not been revealed. Therefore, we undertook a systematic study for comparing PPDT2FBT:PCBM solar cells, under variation of annealing temperatures and use of DPE. A combination of optical, electrochemical, microscopic, and further characterization methods enabled the decoding of the impact of DPE on the blend morphology. In addition, the limitation in device stability by extended morphological degradation has been revealed and strategies to overcome those are being discussed.

CPP 57.5 Fri 12:30 ZEU/LICH

Photo-physics of symmetric and asymmetric ITIC-2F non-fullerene acceptors in organic solar cells — •Shahidul Alam[1,2], Nisreen Alshehri[2], Michael Bulgakov[3], Zerui Li[4], Khawla Alkhezaim[2], Maryam Alqurashi[2], Oleksandr Matiash[2], Vojtech Nadazdy[5], Martin Hager[6], Ulrich S Schubert[6], Vladimir Dyakonov[3], Harald Hoppe[6], Peter Müller-Buschbaum[4], Andreas Sperlich[3], and Frédéric Laquai[1,2] — [1]LMU Munich — [2]KAUST, Saudi Arabia — [3]University of Wurzburg — [4]TU Munich — [5]Slovak Academy of Sciences, Slovak Republic — [6]FSU Jena

Fluorination is an effective strategy to tune the electronic and structural properties of organic semiconductors by lowering frontier orbital energies, enhancing intermolecular interactions, and improving stability. We investigated ITIC and its fluorinated derivatives, sITIC-2F and aITIC-2F, in blends with PBDB-T and its halogenated analogue PM6 to elucidate the effects of fluorination on molecular packing and energetics. Optically detected magnetic resonance reveals triplet excitons in all pristine materials and blends, with their donor-acceptor distribution governed by fluorination. These results demonstrate that fluorination effectively modulates molecular organization and excited-state dynamics, leading to improved structure-property-performance relationships in organic solar cells.

CPP 57.6 Fri 12:45 ZEU/LICH

Single-Component Vacuum-Deposited Organic Photodetectors Achieving NIR Detection — •Jakob Wolansky[1,4], Jacob Hille[1], Cedric Hoffmann[2], Michel Panhans[3], Frank Ortmann[3], Natalie Banerji[2], Karl Leo[1], and Johannes Benduhn[1,4] — [1]IAPP, TU Dresden, Germany — [2]DCBP, University Bern, Switzerland — [3]NAT-School, TU Munich, Germany — [4]DZA, Görlitz, Germany

Efficient charge separation in organic semiconductor devices typically relies on an energetic offset at the donor-acceptor interface to dissociate photogenerated electron-hole pairs. While such an offset facilitates charge generation, it can limit the maximum open-circuit voltage. Additionally, interfacial traps generate charge carriers in the dark. To address these limitations, significant research is exploring single-component (SC) architectures that minimize interfacial losses.

In this work, we investigate SC organic photodetectors in which a newly developed small molecule serves as the active layer. By chemically tuning the molecular structure, extended near-infrared absorption up to 900nm is achieved, while maintaining devices with a large linear dynamic range of 160dB, a -3dB cut-off frequency of 50kHz, and an external quantum efficiency of 20% at zero bias. Comparison with the widely studied small molecule DCV2-5T allows the extraction of structure-property relationships that serve as a basis for future molecular design. Furthermore, an in-depth analysis of the charge generation process in DCV2-5T provides new insights into the pathways governing efficient photogeneration in SC organic systems.

CPP 58: Gels, Polymer Networks and Elastomers III

Time: Friday 11:30–13:00 Location: ZEU/0255

CPP 58.1 Fri 11:30 ZEU/0255

X-ray induced structural changes in supramolecular polymer networks — •Niels C. Giesselmann[1,2], Yasothaa Thavayogarajah[3], Mostafa Ahmadi[3], Sebastian Seiffert[3], and Katrin Amann-Winkel[1,2] — [1]Institute of Physics, Johannes Gutenberg University, Mainz, Germany — [2]Max Planck Institute for Polymer Research, Mainz, Germany — [3]Institute of Chemistry, Johannes Gutenberg University, Mainz, Germany

Supramolecular polymer networks consist of non-covalently cross-linked macromolecules. Such transient links can be established through functionalized polymer building blocks. An interesting property of this group of materials is their ability to self-heal mechanical damage. We observed polymer networks made of star-shaped four-arm PEG building blocks with metal-complexing end groups. Due to their transient binding, the building blocks diffuse through the polymer network in a process that is not yet understood in detail. In this study, we employed both X-ray scattering in order to probe the structure of the network on the molecular as well as the macromolecular level. This way, we hope to better understand the mechanical and self-healing properties of these polymer networks. We report the emergence of structural changes in dependence of the X-ray flux that futhermore persist when measuring far away from the initially illuminated area. This effect can be explained by the affected molecules spreading throughout the sample by means of the transient binding dynamics mentioned above.

CPP 58.2 Fri 11:45 ZEU/0255

Deciphering the photopolymerization-induced nanostructure and interface formation for submicron additive manufacturing — •Shouzheng Chen[1,2,3], Yufeng Zhia[2], Lixing Li[1], Sarathlal Koyiloth Vayalil[2], Rolf A.T.M. van Benthem[4], Johan F.G.A Janssen[5], Mats K. G. Johansson[6], Peter Müller-Buschbaum[1], and Stephan V. Roth[2,6] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]DESY, Hamburg — [3]MLZ, TUM, Garching, Germany — [4]TU/e, Eindhoven, the Netherlands — [5]Covestro (Netherlands) B.V., Geleen, the Netherlands — [6]Department of Fibre and Polymer Technology, KTH, Stockholm, Sweden

UV-curing is widely used in additive manufacturing due to its controllable spatiotemporal characteristics. In submicron additive manufacturing, the involvement of solvents and limitations on film thickness complicate the precise regulation of nanostructures and interlayer interface. By using grazing incidence small angle X-ray scattering (GISAXS) and employing the oligomer (urethane dimethacrylate, UDMA)/monomer (2-ethylhexyl acrylate, 2-EHA) based resin system, we quantify the heterogeneous distribution of UDMA- and 2-EHA-rich nanodomains (around 23 nm and 13 nm in radii, respectively) in the cured system. Combining Bornagain, we reveal the buried "frozen" nano-wrinkles at interlayer interfaces(cones with radius of 70 nm, slope angle of 18°) induced by solvent and constraint stress synergistically. Our findings offer deeper insights for high precision submicron additive manufacturing.

CPP 58.3 Fri 12:00 ZEU/0255

From real polymers to random graphs: percolation thresholds in associative polymer solutions — •Xinxiang Chen, Lennart Hebestreit, and Friederike Schmid — Johannes Gutenberg-University Mainz, Mainz, Germany

Multivalent reversible crosslinking is ubiquitous in soft matter and biomolecular condensates, yet their sol-gel transitions often deviate from the classical Flory-Stockmayer picture due to chain conformations, intrachain binding, and loop formation. Here, we develop a unified framework combining molecular dynamics simulations with random-graph and random-geometric-graph approaches to quantitatively link real polymer architectures to abstract network models. For single- and two-component reversible polymers with one-to-one specific bind-

ing, we determine gel points from topological connectivity and find percolation thresholds substantially higher than Flory-Stockmayer predictions. By comparing spatially unconstrained random graphs with spatially correlated random geometric graphs, we show that intrachain binding and loops markedly reduce the effective interchain bonding needed to form an infinite cluster. Meanwhile, the theoretical results of the generating function and the Lagrange inversion further yield cluster size distributions and giant cluster fractions. Our work demonstrates how spatial correlations and polymer conformations fundamentally reshape reversible network formation, offering a unified topological and physical perspective on reversible gels and biomolecular condensates.

CPP 58.4 Fri 12:15 ZEU/0255

From Champagne Fizzling to Confined Polymer: Natural and Artificial Bubble Nucleation — •Carlos Arauz-Moreno[1,2], Keyvan Piroird[2], and Elise Lorenceau[1] — [1]Université Grenoble Alpes, CNRS, LIPhy, F-38000 Grenoble, France — [2]Saint-Gobain Research Paris, F-93360 Aubervilliers, France

Bubbles dazzle the senses when pouring a Champagne glass. However, there is a hidden trick to this elegant experience: natural nucleation sites, such as tartrate crystals from washing or cellulose fibers from drying, or artificial sites, like crenels in the flute, are used to trigger bubble nucleation by lowering the energy barrier required to grow a bubble; otherwise, Champagne wouldn't bubble at all. By using a model system of viscoelastic polyvinyl butyral (PVB), we show that the concepts of natural and artificial nucleation from Champagne equally apply to confined viscoelastic polymers. Our experimental results show that water vapor, which tends to aggregate inside the PVB matrix in the form of clusters, escapes in copious amounts from the polymer bulk when the latter is heated and decompressed (e.g., at 140°C, dP=1bar). However, bubbles may only form at naturally trapped fibers, dust speckles, or in artificial crenels on the glass surface. The number of natural nuclei is apparently and counterintuitively inversely proportional to the applied temperature. Moreover, bubbles can take on different shapes and sizes because coalescence does not occur. Finally, we investigated how the growth rate of bubbles is impacted by whether nucleation is natural or artificial, revealing a clear distinction between the two: the growth rate in the former is global while in the latter is local.

CPP 58.5 Fri 12:30 ZEU/0255

Steric Origins of Microgel Thermoresponsiveness Revealed by All-Atom Polymer Simulations — •Jannis Krüger[1], Letizia Tavagnacco[2], Emanuela Zaccarelli[2], and Thomas Hellweg[1] — [1]Physical and Biophysical Chemistry, Bielefeld University, Germany — [2]Department of Physics, Sapienza University of Rome, Italy

Microgels based on N-isopropylacrylamide (NIPAM) are well established in soft matter science due to their thermoresponsive swelling behavior. Dynamic light scattering (DLS) reveals a sharp decrease in the hydrodynamic radius at a characteristic volume phase transition temperature (VPTT), which occurs around 34°C. In our previous work[1] we observed that by adding a non-thermoresponsive comonomer such as N-tert-butylacrylamide (NtBAM), this transition broadens in temperature until it disappears at high molar contents. The VPT is typically interpreted in terms of hydrophilicity or hydrophobicity; however, the steric demand of chemical substituents is often overlooked. In this work, we compare DLS measurements with all-atom molecular dynamics simulations of NIPAM and NtBAM polymer chains in water, to show how subtle differences, like replacing an isopropyl with a tert-butyl group, substantially affects the coil-globule transition of polymers in water, thereby providing deeper insights into the molecular origin of the broadening and lowering of the VPTT in real microgels.

[1] J. Krüger, S. Kakorin, and T. Hellweg, Colloid Polym. Sci. 303, 1815 (2024).

CPP 58.6 Fri 12:45 ZEU/0255

Photo-responsive microgels as model systems with tunable crosslinking density — •Dominik Wöll and Christian Metzen — Institute of Physical Chemistry, RWTH Aachen University

Functional microgels have powerful applications due to their specific structure, which can quickly respond to external stimuli such as temperature, pH, ionic strength, solvent composition, and light. We synthesized double-responsive poly(N-isopropylacrylamide) (PNIPAM) microgels that react to both light and temperature. The light responsiveness is achieved by the addition of photoswitchable trans-azobenzene (Azo) units that crosslink with the corresponding β-cyclodextrin (β-CD) units copolymerized into the microgel. Irradiation with light causes switching from trans-Azo to cis-Azo and thus opening of the crosslink. With the wavelength of light, and the corresponding photostationary state, the crosslinking density in these microgels can be precisely controlled with light. This model system allows us to investigate the influence of crosslinking density on the structure and properties of microgels.

CPP 59: Crystallization

Time: Friday 11:30–13:00 Location: ZEU/0260

CPP 59.1 Fri 11:30 ZEU/0260

Structure formation in Polyamide 6 under process-relevant conditions: In situ SAXS/WAXS study using a modular FlowCell setup — •Anna Katharina Sambale[1], Eric Euchler[1], Moritz Kurkowski[1], Enno Henn[1], Regine Boldt[1], Matthias Schwartzkopf[2], Sarathlal Koyiloth Vayalil[2,3], and Markus Stommel[1,4] — [1]Leibniz-Institut fuer Polymerforschung Dresden e.V., Dresden, Germany — [2]Deutsches Elektronen Synchrotron DESY, Hamburg, Germany — [3]Applied Science Cluster, UPES, Dehradun, India — [4]TUD Dresden University of Technology, Dresden, Germany

The microstructural evolution of semi-crystalline thermoplastics during melt processing is governed by local thermo-rheological conditions, which strongly influence crystallization kinetics and consequently, the final material properties. To analyze these interdependencies under process-relevant conditions, a modular FlowCell setup was developed for time-resolved in situ SAXS/WAXS experiments at the synchrotron beamline P03 at DESY, Hamburg. The setup combines a commercial single-screw extruder with customized temperature-controlled slit capillary that enables measurements during controlled cooling from the melt to solid state, with synchronized acquisition of IR-thermography data and, in extended configurations, Raman spectroscopy. Recent experiments on polyamide 6 demonstrate the impact of different cooling strategies and nucleation conditions on the resulting structure. The results highlight the relevance of spatially and temporally resolved analysis techniques for understanding structure formation towards industrial polymer processing.

CPP 59.2 Fri 11:45 ZEU/0260

Influence of Composition on Sanidic Liquid Crystalline Mesophases in Statistical Copolythiophenes — •Alexander Much[1], Jakob Danziger[1], Qian Wang[2], Michael Sommer[2], and Oleksandr Dolynchuk[1] — [1]Martin-Luther-Universität Halle-Wittenberg — [2]Technische Universität Chemnitz

Liquid-crystalline (LC) materials exhibit a variety of structural forms depending on the degree of order, allowing for the novel combination of their anisotropic properties. Board-like conjugated polymers with stiff backbones and short side chains, such as poly-(3-hexylthiophene) (P3HT), are of particular interest because they exhibit weakly explored sanidic LC mesophases.

Here, we study the influence of chemical side-chain modification on the LC phase transitions in statistical copolymers poly-(3-hexylthiophene)-stat-poly-[3-(6-cyanohexyl)thiophene] using differential scanning calorimetry (DSC) and temperature-resolved wide angle X-ray scattering. We find that the copolythiophenes go trough a cascade of sanidic LC mesophases during heating, similar to those in P3HT. Remarkably, the temperature range where sanidic mesophases exists follows the melting range from DSC as a function of comonomer composition and increases towards the intermediate composition with an apparent minimum in values of melting temperature and enthalpy. This suggest that energetic contributions reduce the thermal stability of sanidic LC phases in copolythiophenes, and that LC transition temperatures can be tuned through statistical copolymerization without negating their existence.

CPP 59.3 Fri 12:00 ZEU/0260

In-situ structure and morphology investigations of slot-die coated perovskite nanocrystal films — •Thomas Baier[1], Altantulga Buyan-Arivjikh[1], Lixing Li[1], Xiaojing Ci[1], Markus Döblinger[2], Matthias Schwartzkopf[3], Thomas Bein[2], Sarathlal Koyiloth Vayalil[3,4], and Peter Müller-Buschbaum[1] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]Department of Chemistry, LMU, Munich — [3]DESY, Hamburg — [4]UPES, Dehradun

Colloidal perovskite nanocrystals (PNCs) are promising in contributing to next-generation optoelectronic and energy conversion technologies. In this work, mixed-cation cesium-formamidinium lead-iodide (Cs(1-x)FAxPbI3) PNCs were synthesized via a colloidal hot-injection route and subsequently processed into thin-film active layers using slot-die coating for scalable manufacturing. The evolution of structural order during deposition was probed in-situ using grazing-incidence small- and wide-angle X-ray scattering (GISAXS and GIWAXS), providing direct insights into nanocrystal packing, ordering, and defect formation. Simultaneous optical characterization via photoluminescence (PL) provided complementary information on the evolution of optical properties during deposition, while transmission electron microscopy (TEM) en-

abled correlation with nanoscale information. By combining colloidal synthesis, in-situ structural probes, and optical characterization, this work directly links nanoscale assembly, defect states, and the optoelectronic performance of perovskite nanocrystal thin films.

CPP 59.4 Fri 12:15 ZEU/0260

Interplay of heterogeneous nucleation and prefreezing in PBS droplets on graphene — •Marthinus van Niekerk, Moritz Hartelt, and Oleksandr Dolynchuk — Experimental Polymer Physics, Martin-Luther-University Halle-Wittenberg, Germany

The dominant crystallization mechanism depends on the kinetics of formation and crystal growth. Heterogeneous nucleation, leading to spherulitic morphology, and prefreezing, leading to epitaxial morphology, are two mechanisms of interface-induced crystallization in polymers. However, research on prefreezing is in a seminal phase, and its possible competition with nucleation during cooling remains unexplored. Here, we study the crystallization behavior of dewetted poly(butylene succinate) (PBS) droplets on graphene, a known prefreezing substrate for PE and PCL, during cooling from the melt at different rates using optical- and atomic force microscopy and wide-angle X-ray scattering. Across a large range of cooling rates, nucleation was found to be dominant, resulting in spherulitic morphology in large droplets. However, indications of prefreezing were observed in very small droplets exhibiting epitaxial morphology. Subsequent annealing close to T_m resulted in significant reordering and enhancement of out-of-plane orientation, causing a change in morphology from spherulitic to epitaxial for all droplets up to several hundred nanometers. Theoretical analysis revealed a significant lattice mismatch between graphene and PBS, suggesting it is a plausible reason for the absence of rapid prefrozen layer growth during initial cooling from the melt.

CPP 59.5 Fri 12:30 ZEU/0260

Crystallization of polymer networks in the constant-strain and constant-stress ensembles — Atmika Bhardwaj[1], Huzaifa Shabbir[1], Jens-Uwe Sommer[1,2], and •Marco Werner[1] — [1]Bereich Theorie der Polymere, Leibniz-Institut für Polymerforschung Dresden e.V., Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, Germany

We investigate how deformation and cross-links affect the crystallization of polymer networks using molecular dynamics simulations. A cooling- and heating cycle are simulated both under constant-strain and constant-stress conditions, monitoring specific volume, crystallinity, and orientational order as functions of temperature. In both ensembles, deformation induces chain pre-alignment along the loading direction, driving crystallization at higher transition temperatures. Under constant stress, the pre-alignment promotes crystal growth along the mechanically induced director resulting in a substantial increase of deformation in favor of that direction. These results show how mechanical ensemble, deformation, and cross-linking can be combined to tailor the shape response of polymer networks upon phase transition.

CPP 59.6 Fri 12:45 ZEU/0260

Surface-induced ordering and continuous breaking of translational symmetry in conjugated polymers — Anton Sinner, Alexander Much, and •Oleksandr Dolynchuk — Martin Luther University Halle-Wittenberg, Germany

Surface-induced liquid crystalline (LC) phase transitions elicit fundamental interest and hold potential for leveraging the accompanying anisotropic order at the surface. Board-like conjugated polymers are of particular interest due to the novel sanidic LC phases they exhibit, which have remained largely unexplored. Specifically, although preferential molecular orientation near the free surface has been observed in films of conjugated polymers, the mechanism of its formation is not yet fully understood. In this study, grazing-incidence X-ray scattering is employed to monitor the formation and breaking of positional order in situ in thin films of two conjugated polymers representative of two classes: polythiophenes and polydiketopyrrolopyrroles. Our findings demonstrate that the surface induces positional order in films of both conjugated polymers via the formation of a highly oriented, sanidic disordered LC phase. The ordering process continues upon cooling and undergoes multiple LC transitions into more ordered phases, both at the surface and in the bulk, which can compete with each other. The positional smectic-like order parameter displays continuous temperature dependence in the vicinity of the transition, signifying a continuous breaking of translational symmetry by the surface. Theoretical analysis enables accurate description of the order parameter when critical behavior is considered.

CPP 60: Molecular and Polymer Dynamics, Friction and Rheology II

Time: Friday 12:15–13:00 Location: HÜL/S386

CPP 60.1 Fri 12:15 HÜL/S386

Fouling in Emulsion Polymerization of Different Copolymers investigated in-situ with the Quartz Crystal Microbalance (QCM) — •Kevin Marvin Hoffmann and Diethelm Johannsmann — Clausthal University of Technology, Institute of Physical Chemistry, Arnold-Sommerfeld-Straße 4, 38678 Clausthal-Zellerfeld, Germany

In emulsion polymerization, reaction and particulate fouling leads to clogging, product contamination, and reduced heat transfer efficiency. Common techniques for in-line monitoring of fouling are based on the heat transfer efficiency across the surface and the pressure drop in pipes or tubes. These techniques show fouling layers at thicknesses of a few tens of micrometers, at least. They are not sensitive enough to study the initial stages of a fouling.

A quartz crystal microbalance with dissipation monitoring (QCM-D) was used to study fouling in-situ. The QCM infers changes in mass on its surface to changes of its resonance frequency. It is sensitive down to the nanometer range. In addition to an estimate of the layer thickness, the QCM-D provides for additional information, derived from the comparison between the shifts in frequency and half-bandwidth as well as the comparison between different overtones.

It was found that polyacrylates behaved characteristically differently from polyvinyl acetates. The polyacrylates formed compact and stiff fouling layers. The polyvinyl acetates formed softer and more porous, extended layers. We assume that the stabilizing agent has a major impact on the fouling layer's nature.

CPP 60.2 Fri 12:30 HÜL/S386

Cluster growth dynamics of nickel particles in viscoelastic matrices — •Konstantin Gerstenberger und Günter K. Auernhammer — Leibniz Institute of Polymer Research Dresden, Hohe Str. 6, 01069 Dresden, Germany

Magnetic elastomers can dynamically modify their mechanical properties in response to a magnetic field giving them the potential for new applications as soft actuators. A common method of producing these materials involves embedding magnetic particles in an elastomer matrix. In the presence of an applied magnetic field, the particles tend to arrange themselves into chain-like clusters which react to external stimuli, even if the matrix is crosslinked.

As part of the research unit FOR 5599 on structured magnetic elastomers we investigate the formation process of these materials, paying particular attention to the interaction between particle cluster formation and simultaneous crosslinking of the surrounding matrix. We use particle tracking velocimetry techniques to observe the cluster development over time and investigate how this process depends on various parameters. Therefore, it can be concluded that the development of chains is influenced by not only the particle concentration and matrix viscosity, but also the rotation of the applied magnetic field. This rotation can be used to adjust the mean length of the chains to a specific value.

Further investigation of larger sample sizes will be possible due to a new kind of Hallbach array that is currently under construction. This presentation will also cover the general idea of this machine.

CPP 60.3 Fri 12:45 HÜL/S386

Maps of High Viscoelastic Properties Generated with an Instrument Combining a Quartz Crystal Microbalance (QCM) with an AFM — •Cedric Jünemann, Diethelm Johannsmann, and Arne Langhoff — Clausthal University of Technology, Instutite of Physical Chemistry, Arnold-Sommerfeld-Straße 4, 38678 Clausthal-Zellerfeld

We present an instrument, which images the high-frequency viscoelastic properties of various samples. The instrument combines an atomic force microscope (AFM) with a quartz crystal microbalance with dissipation monitoring (QCM-D). Imaging becomes possible by a fast measurement of a resonator's frequency and bandwidth, achieved with a multi-frequency lockin amplifier (MLA). The MLA tracks multiple overtones simultaneously. To improve contrast and to facilitate quantitative interpretation, the colloidal force probe configuration was used. The cantilever was modified by gluing a glass sphere with a diameter of 50 μm to the tip, thereby increasing the contact radius to a few hundred nanometers. The sphere is heavy enough to clamped in place by inertia, which simplifies the analysis. A quantitative interpretation can rely on ratios between the different QCM signals, which eliminates the unknown contact area from the analysis. Printed drops and a biofilm composed of yeast were chosen for demonstration. This approach provides for a flexible method to investigate viscoelastic properties on the nanoscale at high frequencies.

CPP 61: Closing Talk (joint session CPP/BP/DY)

Time: Friday 13:15–14:00 Location: HSZ/0002

Invited Talk CPP 61.1 Fri 13:15 HSZ/0002

Biomolecular Condensates: Challenges for Polymer Physics — •Jens-Uwe Sommer — Leibniz-Insitut für Polymerforschung Dresden, Bereich Theorie der Polymere,Hohe Straße 6, 01069 Dresden, Germany — TU Dresden, Insitut für Theoretische Physik, Zellescher Weg 17, D-01069 Dresden, Germany

Biomolecular condensates (BMCs) constitute an emerging paradigm in the understanding of biological functions. They shift the focus from individual biochemical processes toward the collective behavior of biopolymers, in which phase-separation mechanisms and intrinsically disordered proteins lacking canonical enzymatic roles play central and often decisive functions. Consequently, universal principles of complex (bio)polymer solutions gain relevance, and several classical questions in the physics of living matter can now be revisited from this polymer-physics perspective. In this talk, I will discuss theoretical approaches and concepts that are based on universal principles, with a particular emphasis on current challenges in the field.

Thin Films Division
Fachverband Dünne Schichten (DS)

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Technische Universität Ilmenau
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Overview of Invited Talks and Sessions

(Lecture halls REC/B214 and REC/C213; Poster P2)

Invited Talks

DS 6.1	Tue	9:30–10:00	REC/C213	**Soft X-ray Microscopy of Ferroic Thin Films** — •Tim A. Butcher, Simone Finizio, Michael Schneider, Jörg Raabe, Stefan Eisebitt, Bastian Pfau
DS 6.6	Tue	11:15–11:45	REC/C213	**Charge transfer at interfaces of free-standing oxide membranes and heterostructures** — Kapil Nayak, Lee-Kang Huang, Anton Kaus, Marcus Wohlgemuth, Alexandros Sarantopoulos, Christoph Baeumer, Regina Dittmann, •Felix Gunkel
DS 13.1	Wed	15:00–15:30	REC/B214	**Tailored thermal treatments for multi-layer, multi-material polymer devices** — •Katherina Haase, Shaoling Bai, Mike Hambsch, Vojtech Millek, Stefan C. B. Mannsfeld
DS 18.8	Thu	17:00–17:30	REC/C213	**Insights from Quantum Dynamics Simulations: From Molecules to Organic-Material Interfaces** — •Frank Ortmann

Invited Talks of the joint Symposium SKM Dissertation Prize 2026 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	HSZ/0002	**Stochastic-Calculus Approach to Non-equilibrium Statistical Physics** — •Cai Dieball
SYSD 1.2	Mon	10:00–10:30	HSZ/0002	**Nonuniform magnetic spin textures for sensing, storage and computing applications** — •Sabri Koraltan
SYSD 1.3	Mon	10:30–11:00	HSZ/0002	**Anomalous Quantum Oscillations beyond Onsager's Fermi Surface Paradigm** — •Valentin Leeb
SYSD 1.4	Mon	11:00–11:30	HSZ/0002	**Coherent Control Schemes for Semiconductor Quantum Systems** — •Eva Schöll
SYSD 1.5	Mon	11:30–12:00	HSZ/0002	**On stochastic thermodynamics under incomplete information: Thermodynamic inference from Markovian events** — •Jann van der Meer

Invited Talks of the joint Symposium The Sustainability Challenge: A Decade of Transformation (SYSC)

See SYSC for the full program of the symposium.

SYSC 1.1	Mon	15:00–15:30	HSZ/AUDI	**Open-Endedness and Community-Based Approaches to Sustainability Challenges** — •Hiroki Sayama
SYSC 1.2	Mon	15:30–16:00	HSZ/AUDI	**Education as a Social Tipping Element: Evidence from Climate and Physics Education Research** — •Thomas Schubatzky
SYSC 1.3	Mon	16:00–16:30	HSZ/AUDI	**Mechanistic and Material Perspectives on Enzymatic Hydrolysis of Semicrystalline Polyesters** — •Birte Höcker
SYSC 1.4	Mon	16:45–17:15	HSZ/AUDI	**Decarbonization Options for Industry** — •Uwe Riedel
SYSC 1.5	Mon	17:15–17:45	HSZ/AUDI	**Impacts of Cosmic Dust and Space Debris in the Terrestrial Atmosphere** — •John Plane

Invited Talks of the joint Symposium Tipping Points in Social and Climate Systems (SYTP)

See SYTP for the full program of the symposium.

SYTP 1.1	Thu	15:00–15:30	HSZ/AUDI	**Social Tipping in Heterogeneous and Polarized Populations** — •Sara Constantino, Sonke Ehret, Elke Weber, Sonja Vogt, Charles Efferson
SYTP 1.2	Thu	15:30–16:00	HSZ/AUDI	**Tipping points and regime shifts in coupled social-climate systems** — •Chris Bauch
SYTP 1.3	Thu	16:00–16:30	HSZ/AUDI	**How to tune Earth system models toward tipping?** — •Sebastian Bathiany, Niklas Boers
SYTP 1.4	Thu	16:45–17:15	HSZ/AUDI	**Algorithmic amplification and contextual sensitivity in political information exposure** — Iris Damião, Ana Vranic, Paulo Almeida, Lília Perfeito, •Joana Gonçalves de Sá
SYTP 1.5	Thu	17:15–17:45	HSZ/AUDI	**The complex interplay between democracy and platform power** — •Philipp Lorenz-Spreen

Invited Talks of the joint Symposium Interacting Degrees of Freedom in Ultrathin Quantum Films (SYQF)

See SYQF for the full program of the symposium.

SYQF 1.1	Fri	9:30–10:00	HSZ/AUDI	**Exciton dressing by extreme nonlinear magnons in a layered semiconductor** — •Geoffrey M. Diederich
SYQF 1.2	Fri	10:00–10:30	HSZ/AUDI	**A tale of demons and decay in two-dimensional (alter)magnets** — •Alexander Mook
SYQF 1.3	Fri	10:30–11:00	HSZ/AUDI	**Magnetism, light and matter - Role of excitons in two-dimensional magnets** — •Florian Dirnberger
SYQF 1.4	Fri	11:15–11:45	HSZ/AUDI	**Advantages and challanges of resonance Raman scattering with infrared excitation energy** — •Leonetta Baldassarre
SYQF 1.5	Fri	11:45–12:15	HSZ/AUDI	**Shining light on 2D antiferromagnets** — •Dmytro Afanasiev

Sessions

DS 1.1–1.3	Mon	9:30–10:15	REC/C213	**Organic Thin Films**
DS 2.1–2.7	Mon	15:00–18:15	HSZ/0003	**Focus Session: Tunable Correlations in van der Waals Quantum Materials I (joint session TT/DS/HL)**
DS 3.1–3.4	Mon	15:00–16:00	REC/C213	**Thin Film Properties I: Methods**
DS 4.1–4.6	Mon	16:30–18:15	REC/C213	**Thin Film Properties II**
DS 5.1–5.4	Tue	9:30–10:45	HSZ/0105	**Focus Session: Tunable Correlations in van der Waals Quantum Materials II (joint session TT/DS/HL)**
DS 6.1–6.6	Tue	9:30–11:45	REC/C213	**Thin Oxides and Oxide Layers**
DS 7.1–7.5	Tue	10:00–11:30	REC/B214	**Thermoelectric and Phase Change Materials**
DS 8.1–8.5	Tue	14:00–15:30	REC/B214	**Transport Properties**
DS 9.1–9.5	Tue	14:00–15:15	REC/C213	**Thin Film Properties III: Oxides**
DS 10.1–10.7	Wed	9:30–12:45	HSZ/0003	**Focus Session: Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects I (joint session TT/DS/MA)**
DS 11.1–11.8	Wed	9:30–11:45	REC/B214	**Layer Deposition**
DS 12.1–12.9	Wed	9:30–12:00	REC/C213	**2D Materials I**
DS 13.1–13.4	Wed	15:00–16:15	REC/B214	**Layer Properties**
DS 14.1–14.9	Wed	15:00–17:30	REC/C213	**2D Materials II (joint session DS/HL)**
DS 15.1–15.11	Thu	9:30–12:30	HSZ/0003	**Focus Session: Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects II (joint session TT/DS/MA)**
DS 16.1–16.10	Thu	9:30–12:30	REC/C213	**Thin Film Application**
DS 17.1–17.9	Thu	15:00–18:45	HSZ/0003	**Focus Session: High-Temperature Superconductivity in Hydride Materials at High Pressures (joint session TT/DS)**
DS 18.1–18.8	Thu	15:00–17:30	REC/C213	**Spins in Molecular Systems**
DS 19	Thu	17:45–18:30	REC/C213	**Members' Assembly**
DS 20.1–20.52	Thu	18:30–20:30	P2	**Poster**
DS 21.1–21.10	Fri	9:30–12:30	REC/C213	**Optical Analysis of Thin Films**

Members' Assembly of the Thin Films Division

Thursday 17:45–18:30 REC/C213

Sessions

– Invited, Topical, Contributed Talks, and Posters –

DS 1: Organic Thin Films

Time: Monday 9:30–10:15 Location: REC/C213

DS 1.1 Mon 9:30 REC/C213

Thin film growth on weak surfaces: influence of substrate inhomogeneities — •Eric Karajic[1], Martin Oettel[1], Edwin Mozo[2], and Fabio Reis[2] — [1]University of Tübingen, Institute of Applied Physics — [2]Universidade Federal Fluminense, Instituto de Fisica

The initial island density in the growth of thin films on perfectly smooth surfaces is set by an interplay between flux, diffusion and the stability of small clusters [1]. However, real surfaces have inhomogeneities which may trap freely diffusion adsorbates and act as initial nucleation sites. Using kinetic Monte-Carlo (KMC) simulations, we investigate the influence of trapping strength and density of inhomgeneities on the initial growth behavior. We discuss the consequences for basic growth modes on weakly interacting surfaces [2]. For layer-by-layer growth, island densities may vary grossly between first and second layer, but for island growth the possible return to smooth growth at intermediate layer thicknesses is not affected. [1] T. Michely and J. Krug, Islands, Mounds, and Atoms, (Springer, 2003) [2] E. Empting et al., Phys. Rev. E 103, 023302 (2021)

DS 1.2 Mon 9:45 REC/C213

Organic self-assembled monolayers as barrier material in Josephson junctions — •Moritz Singer[1], Harsh Gupta[1], Rui Pereira[2], Benedikt Schoof[1], and Marc Tornow[1,2] — [1]TU Munich, Garching, Germany — [2]Fraunhofer EMFT, Munich, Germany

Superconducting qubits employ Josephson junctions (JJs) to provide the nonlinearity needed to address a unique two-state system. The JJs consist of two superconducting electrodes which are separated by a nanometer-thin layer acting as tunnel barrier and is mostly fabricated from oxides. The thickness of the oxide is highly sensitive to process variations, and it hosts many two-level systems (TLS) which give rise to dielectric losses, thereby limiting the qubit coherence times. In this study, we report on JJs comprising an organic self-assembled monolayer (SAM) as the insulating barrier material. Our JJs consist of Ta electrodes on a Nb seed layer, separated by a SAM of octadecene (C18H36) molecules that are grown on the thin native TaOx layer of the bottom electrode. We fabricated JJs with three different electrode sizes in the μm - range and measured critical currents Ic between 3.7 μA and 30.6 μA at 100 mK, in good quantitative agreement with the expected values according to the Ambegaokar-Baratoff relation. We further analyzed the data using the Simmons tunneling model, adapted to account for the two-layer TaOx/SAM barrier. We obtain barrier heights ranging from 0.43-0.57 eV for the SAM-JJs, which is significantly higher than for JJs fabricated with a Ta-oxide barrier only (barrier height 0.25 eV). This shows that the properties of JJs can be modified and tuned by introducing a SAM as barrier material.

DS 1.3 Mon 10:00 REC/C213

Prediction of room-temperature two-dimensional pi-electron half-metallic ferrimagnet — •Jan Phillips[1], João C. G. Henriques[1,2], Antonio T. Costa[1,3], and Joaquín Fernández-Rossier[1,4] — [1]International Iberian Nanotechnology Laboratory (INL), Av. Mestre José Veiga, 4715-330 Braga, Portugal — [2]Universidade de Santiago de Compostela, 15782 Santiago de Compostela, Spain — [3]Universidade do Minho, R. da Universidade, 4710-057 Braga, Portugal — [4]On permanent leave from Departamento de Física Aplicada, Universidad de Alicante, 03690 San Vicente del Raspeig, Spain

We propose a strategy to obtain conducting organic materials with fully spin-polarized Fermi surface, lying at a singular flat band, with antiferromagnetically coupled magnetic moments that reside in pi-orbitals of nanographenes. We consider a honeycomb crystal whose unit cell combines two molecules with S=1/2: an Aza-3-Triangulene, a molecule with orbital degeneracy, and a a 2-Triangulene. The analyzed system is half-metallic with a ferrimagnetic order, presenting a zero net total magnetic moment per unit cell. We combine density functional theory calculations with a Hubbard model Hamiltonian to compute the magnetic interactions, the bands, and the collective spin excitations. We obtain very large intermolecular exchange couplings, in the range of 50 meV, which ensures room temperature stability. This crystal being a half-metal with fully compensated magnetic moments combines two characteristics that would make it ideal for spintronics applications.

DS 2: Focus Session: Tunable Correlations in van der Waals Quantum Materials I (joint session TT/DS/HL)

The library of strongly correlated layered materials has intensively grown, giving now access to the full breadth of symmetry broken emergent phases, ranging from excitonic, to magnetic, superconducting, or Mott insulating ground states. At the same time, also the ways of tuning these correlated phases in 2D are steadily developing, e.g, via twisting or stacking, engineered defects, or applied external fields. Taken together, this nowadays allows for sheer endless possibilities to tailor layered correlated quantum materials on demand opening unprecedented avenues towards both deep insights into emergent phenomena and novel functionalization routes based on many-body properties.

This focus session will highlight recent advancements and breakthroughs achieved in this field, which we expect to be of great interest to the broadest audience and to stimulate discussions crossing field boundaries.

Coordinators: Lennart Klebl (Uni Würzburg, Jonas Profe (Uni Frankfurt), Malte Rösner (Uni Bielefeld), Ursula Wurstbauer (Uni Münster)

Time: Monday 15:00–18:15 Location: HSZ/0003

See TT 12 for details of this session.

DS 3: Thin Film Properties I: Methods

Time: Monday 15:00–16:00 Location: REC/C213

DS 3.1 Mon 15:00 REC/C213

Update on the IBA activities in Bonn — •Henry Schumacher, Dennis Sauerland, and Sebastian Neubert — Helmholtz-Institut für Strahlen und Kernphysik, Universität Bonn

The *Bonn Isochronous Cyclotron* can accelerate protons, deuterons and light ions with nominal energies of 7 to 14 MeV/nucleon. At one of the five beam lines, a new experimental site for material analysis is in development.

This new experiment will house a small number of surface barrier detector for RBS (backwards direction) and beam characterization (off-axis, foward direction) as well as a silicon drift detector for PIXE measurements and utilize a low energy alpha particle beam.

In this talk, a general overview over the setup and progress, preliminary detector tests, count rate estimations and preparatory measurements will be presented.

DS 3.2 Mon 15:15 REC/C213

The TXPES Beamline at SESAME: A New Facility for Advanced Soft X-ray Photoelectron Spectroscopy — •Zeynep Reyhan Ozturk — TARLA, Ankara, Turkey — SESAME, Balqa, Jordan

The TXPES (Turkish X-ray Photoelectron Spectroscopy) beamline at SESAME is a newly installed soft X-ray facility dedicated to high-resolution XPS, UPS, and ARPES for advanced surface and interface analysis. With a broad tunable photon-energy range, TXPES enables detailed investigation of electronic structure, chemical composition, band dispersion, and oxidation states in a wide variety of materials.

The end station features a multi-chamber UHV system including a preparation chamber, an analysis chamber, and a high-pressure cell for in situ and near-ambient pressure studies. The analysis chamber houses a hemispherical electron energy analyzer capable of XPS/UPS/ARPES, along with an ion gun, LEED, and LEIS, enabling comprehensive structural and chemical characterization at different depth sensitivities. TXPES combines tunable soft X-rays, high-resolution electron spectroscopy, and controlled environments to study surface oxidation, adsorption, catalysis, thin-film interfaces, and electronic band alignment with exceptional sensitivity. The integration of a high-pressure cell expands these investigations to realistic gas conditions, bridging the gap between model systems and real-world applications. The beamline represents a major collaborative effort between Turkish institutions and SESAME and is progressing toward full operation and user access in the near future.

DS 3.3 Mon 15:30 REC/C213

Bringing Synchrotron-Level HAXPES to the Lab: DeepCore-X for Buried Interface Characterization — •Martin Schmid[1], Elin Cartwright[2], Eleni Anargirou[1], Marcus Lundwall[2], and Susanna Eriksson[2] — [1]Scienta Omicron GmbH, Limburger Str. 75, 65232 Taunusstein — [2]Scienta Omicron AB, Danmarksgatan 22, 75323 Uppsala

Buried interfaces in multilayer semiconductor devices, such as MOSFETs, solar cells, and memory architectures, critically impact performance and reliability. Hard X-ray Photoelectron Spectroscopy (HAXPES), with greater information depth than conventional XPS, enables nondestructive analysis of buried layers. We introduce DeepCore-X, a next-generation lab instrument combining soft and hard XPS in one system, delivering synchrotron-like performance. Powered by a Ga Kα MetalJet source (9.25 keV), it offers 1000 W continuous operation and a hundred-fold intensity advantage over other lab HAXPES sources. The system supports high-throughput measurements across complex stacks. Automated sample handling, multi-point acquisition, and operando bias capabilities make it ideal for evaluating band bending, trap states, and chemical shifts. We will present recent results and application examples, including non-destructive depth profiling, to demonstrate how DeepCore-X bridges the gap between surface analysis and full device stack characterization without requiring synchrotron access.

DS 3.4 Mon 15:45 REC/C213

Simulation-Guided GIXPS: How to Maximize Signal and Depth Sensitivity in Photoelectron Emission Experiments — •O. Rehm[1], E. Kusari[1], D. Capalbo[1], A. Gloskovskii[2], C. Schlueter[2], L. Baumgarten[3], and M. Müller[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz — [2]DESY, 22607 Hamburg — [3]FZ Jülich GmbH, PGI-6, 52425 Jülich

(Hard) X-ray Photoelectron Spectroscopy ((HA)XPS) is a powerful technique for probing the chemical and electronic structure of thin films, interfaces, and multilayers, but access to synchrotron radiation is typically highly limited. To address this constraint, we present a simulation-guided approach that optimizes (HA)XPS experiments through grazing-incidence (GI) geometries. At GI angles (0.3°-2°) refraction and total reflection of X-rays generate pronounced angle-dependent interference effects that shift the weighted contribution maximum of photoelectrons to well-defined depths within the sample. Our approach - GIXPS - predicts these conditions in advance, enabling targeted enhancement of surface, interface, or bulk sensitivity. It boosts photoemission intensity by up to two orders of magnitude at characteristic GI angles, enabling faster data acquisition and better depth resolution while preserving the element-specificity of (HA)XPS. This methodology provides a practical route to more efficient, depth-selective experiments and is a powerful tool for designing and carrying out optimized interface- and bulk-sensitive (HA)XPS measurements - thus enabling the more efficient use of limited synchrotron beamtime. O. Rehm *et al.*

DS 4: Thin Film Properties II

Time: Monday 16:30–18:15 Location: REC/C213

DS 4.1 Mon 16:30 REC/C213

Epitaxial Growth and Structural Characterization of Non-centrosymmetric B20-PtAl Thin Films — •Ayusa Aparupa Biswal[1], Darius Pohl[2], Bernd Rellinghaus[2], Edouard Lesne[1], and Claudia Felser[1] — [1]Max-Planck-Institute für Chemische Physik fester Stoffe, Dresden, Germany — [2]Dresden Center for Nanoanalysis (DCN), cfaed, TU Dresden, Dresden, Germany

Topological chiral semimetals with the non-centrosymmetric cubic B20 structure (space group P213) are distinguished by chirality in their crystal, magnetic, and electronic structures [1]. B20 compounds do not possess inversion or mirror symmetry but preserve rotational symmetries. Non-magnetic B20 compounds, such as CoSi, RhSi, PdGa, and PtAl, host multifold fermions originating from topological band crossings. These lead to large Chern numbers and produce Fermi arcs, alike those found in Weyl semimetals [2,3]. We report on the heteroepitaxial growth of crystalline PtAl thin-films with a non-centrosymmetric cubic B20 structure. We employ magnetron sputtering and explore the phase space of sample composition, growth temperature, post-annealing process, as well as resorting to suitable substrates and crystalline buffer layers. The samples are structurally characterized by a combination of X-ray diffraction and atomic-scale high-resolution transmission electron microscopy, which reveals a thickness-dependent microstructure of the B20 films, attributable to a combination of strain relaxation and the formation of extended defects, which are under detailed investigation. [1] B. Bradlyn et al., Science 353 (2016).[2] D. S. Sanchez, et al., Nature 567 (2019).[3] Z. Rao et al., Nature 567 (2019).

DS 4.2 Mon 16:45 REC/C213

high-quality Bi_2Te_3 TI thin films on [0001]-oriented sapphire substrate grown by MBE — •Ismet Gelen, Ahmet Yagmur, Luke Benson, and Satoshi Sasaki — School of Physics and Astronomy, University of Leeds, Leeds LS2 9JT, UK

Over the past decades, topological insulators (TIs) have attracted great attention for their exotic property of being insulating in the bulk while conductive on the surfaces through topological surface states [1], offering promising prospects for future spintronic technologies [2]. Molecular beam epitaxy (MBE) growth method is very important to produce high-quality epitaxial thin film TIs samples. However, producing a high-quality thin film requires careful consideration of substrate preference, growth temperature, and growth rate. This study focuses on the systematic growth of high-quality Bi_2Te_3 TI thin films on a sapphire [0001] substrate with minimal lattice mismatch. We found that growth temperature has a big influence on the surface morphology, which can lead to small or large triangular terraces. When temperature is too low it can create pillars when it is too high it creates defects/holes in films. We will report our optimization of the Bi_2Te_3 growth in terms of X-ray reflectivity/diffraction, atomic force microscopy, Raman spectroscopy, and magnetotransport properties by measuring standard Hall-bar type devices at low temperatures. Finally, we obtain films with large grain size without defects/pillars, and with high mobility and low carrier density.

[1] Li, Y., et al. (2022). ACS Nano, 16(6), 9953-9959. [2] Hasan, M. Z., et al. (2010). Reviews of Modern Physics, 82(4), 3045-3067.

DS 4.3 Mon 17:00 REC/C213

exploring ehalgogenide ABX3 perovskites: challenges and insights from physical vapor deposition — •Sebastian Zimmermann[1], Roland Scheer[2], and Torsten Hölscher[1] — [1]B5 Photovoltaics, Just Transition Center, Martin Luther Universität Halle-Wittenberg — [2]Photovoltaics Groups, Martin-Luther-Universität Halle-Wittenberg

The discovery of new solar cell materials is crucial for the next generation of multijunction systems in photovoltaics. This work focuses on synthesizing thin-film materials that are theoretically well suited for photovoltaic applications. To form these materials, we use physical vapor deposition (PVD). At the beginning, we aim to synthesize chalcogenide perovskites. Chalcogenide perovskites are crystals with a perovskite structure (typically ABX3), where X stands for selenium or sulfur, A for group II metal like Ca or Ba and B for a transition metal like Ti or Zr. Compared to other perovskites, their advantages include lower toxicity and the predicted long-term stability of the layers. This talk presents results of microstructural analysis of PVD synthesized chalcogenide perovskite films and discuss challenges encountered during synthesis. Our results provide new insights in the field of photovoltaic materials and are intended to open up new perspectives for multijunction thin-film solar cells.

15 min. break

DS 4.4 Mon 17:30 REC/C213

Molecule Adsorption at Me-polar and N-polar Sc(x)Ga(1- x)N Surfaces Investigated by Photo Electron Spectroscopy — •Fabian Ullmann[1,2] and Stefan Krischok[1,2] — [1]TU Ilmenau, Ehrenbergstraße 29, 98693 Ilmenau — [2]Zentrum für Mikro- und Nanotechnologien, Gustav-Kirchoff-Straße 7, 98693 Ilmenau

ScGaN can occur in various crystal structures. The most important ones are wurtzite and rock salt formation. Depending on the scandium concentration, a phase transition between these orientations can be found. ScGaN surfaces with different scandium concentrations and orientations were grown by molecular beam epitaxy (MBE) to investigate the near-surface electronic structure. Two different substrates were used to achieve either Me-polar (SiC) and N-polar (sapphire) wz-ScGaN surfaces. The interaction of gas molecules (oxygen and water) in vacuum were analyzed by X-ray (XPS) and ultraviolet photoelectron spectroscopy (UPS).

DS 4.5 Mon 17:45 REC/C213

Molecular Beam Epitaxy of ferrimagnetic Mn_4N — •Adriano Notarangelo, Michael Hanke, Lutz Geelhaar, Oliver Brandt, and Philipp M. John — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117 Berlin, Germany.

Mn_4N is a ferrimagnetic transition-metal nitride that crystallizes in the antiperovskite structure. With its strong perpendicular magnetic anisotropy and high Curie temperature of ≈ 743 K, Mn_4N emerges as a promising material for rare-earth-free spintronics and other magnetic device applications. Since the magnetic properties of Mn_4N are sensitive to stoichiometry, strain, and lattice defects, achieving high-quality epitaxial growth is essential.

In this work, we grow 60 nm–thick Mn_4N layers by plasma-assisted molecular beam epitaxy on sub-1% lattice-mismatched $SrTiO_3$(001) substrates. After carefully calibrating the Mn/N flux ratio to achieve a 4:1 stoichiometric balance, we obtain phase-pure Mn_4N(001) films with no detectable secondary Mn_xN_y phases. X-ray diffraction reveals that optimal crystalline quality is achieved for growth temperatures between 300 and 400°C, while substantial Mn desorption hinders growth above 600°C. The out-of-plane lattice constant decreases from 3.854 to 3.828 Å as the growth temperature increases from 300 to 500°C, indicating an increased in-plane tensile strain imposed by the epitaxial constraint to $SrTiO_3$ with its larger lattice constant.

The optimization of Mn_4N film growth on $SrTiO_3$ is a solid basis for its growth on industry-relevant substrates such as Si, SiC, and GaN.

DS 4.6 Mon 18:00 REC/C213

Investigations of cubic boron nitride nucleation using in situ RHEED during pulsed laser deposition — •Falko Jahn, Laura Dienelt und Steffen Weissmantel — Laserinstitut Hochschule Mittweida, Technikumplatz 17, 09648 Mittweida

Due to its outstanding properties such as second-highest hardness, the cubic allotrope of boron nitride (c-BN) has attracted significant interest from both academia and industry for decades. So far, challenges in the thin film deposition of this material have prevented a successful industrial application, for example as a wear-resistant coating for cutting tools. Although pulsed laser deposition (PLD) has enabled progress in this particular field, several aspects of the film formation process remain insufficiently understood. In particular, the process of nucleation from the hexagonal to the cubic phase still contains unanswered questions. In this work, the microstructure of the growing film is characterized in situ using reflection high-energy electron diffraction (RHEED). This enabled further insight into the nucleation process. The results provide support for the nucleation model of subplantation. These findings contribute to a deeper understanding of c-BN nucleation during PLD or similar PVD techniques.

DS 5: Focus Session: Tunable Correlations in van der Waals Quantum Materials II (joint session TT/DS/HL)

Time: Tuesday 9:30–10:45 Location: HSZ/0105

See TT 27 for details of this session.

DS 6: Thin Oxides and Oxide Layers

Time: Tuesday 9:30–11:45 Location: REC/C213

Invited Talk DS 6.1 Tue 9:30 REC/C213

Soft X-ray Microscopy of Ferroic Thin Films — •Tim A. Butcher[1], Simone Finizio[2], Michael Schneider[1], Jörg Raabe[2], Stefan Eisebitt[1], and Bastian Pfau[1] — [1]Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, 12489 Berlin, Germany — [2]Paul Scherrer Institut, 5232 Villigen PSI, Switzerland

Any technological advance involving ferroic thin films requires a clear picture of their domain structures at the nanoscale. These can be studied by soft X-ray microscopy at synchrotron lights sources, which combines high spatial resolution with sensitivity to ferroic order. This presentation will provide an overview of several ferroic thin films and the application of coherent diffractive imaging methods such as Fourier Transform Holography and soft X-ray ptychography to their study [1]. One example is the room-temperature multiferroic BiFeO3 for which ptychography can probe the magnetoelectric coupling by resolving both the antiferromagnetic spin cycloid and the ferroelectric domains in a single measurement [2,3]. Furthermore, an example of imaging dynamics will be provided with the ptychographic investigation of magnetic domain walls [4].

[1] T. A. Butcher et al., Rev. Sci. Instrum. 96, 123704 (2025) [2] T. A. Butcher et al., Adv. Mater. 36 (2024) [3] T. A. Butcher et al., Phys. Rev. Appl. 23, L011002 (2025) [4] T. A. Butcher et al., Phys. Rev. B 111, L220409 (2025)

DS 6.2 Tue 10:00 REC/C213

Atomic Scale Insights into the Polymorphism of Ruddlesden-Popper Nickelates and Titanates — Shihao Wei[1], Stefania Baronio[2], Bruce Davidson[2], Ke Zou[2], and •Nicolas Bonmassar[1] — [1]Materials Physics, Institute for Materials Science, University of Stuttgart, Heisenberstr. 3, 70569, Germany — [2]Quantum Matter Institute, University of British Columbia, Vancouver, Canada

Ruddlesden-Popper (RP) oxides provide an ideal platform for investigating coupled structural and electronic phenomena, as subtle variations in layering and cation coordination can significantly alter their functional properties. Using oxide molecular beam epitaxy, we can grow distinct nickelate and titanate RP phases with atomic-layer precision, demonstrating the controlled stabilization of distinct polymorphs by tuning the rock-salt and perovskite layers. Advanced scanning transmission electron microscopy provides insights into the resulting structures at an atomic scale, enabling the direct identification of the respective polymorph and the characterization of extended defects, such as stacking faults. By correlating local structure with electronic properties, we can establish clear structure-property relationships across all samples. Electron energy-loss and energy-dispersive X-ray spectroscopy reveal the differences in transition-metal oxidation states, defect density and oxygen orbital occupation between the different RP phases and polymorphs. Our results highlight how precise control of the individual layers leads to the control over the polymorphs in RP nickelates and titanates.

DS 6.3 Tue 10:15 REC/C213

Memristive behaviour in Nickelate Perovskite thin films — •Foelke Janssen[1,2] and Beatriz Noheda[1,2] — [1]Zernike Institute for Advanced Materials, University of Groningen, The Netherlands — [2]Groningen Cognitive Systems and Materials Center (CogniGron), University of Groningen, The Netherlands

Memristive devices can adopt multiple resistance states depending on the history of the electric signal applied, emulating the basic behavior of synapses and neurons. They hold great promise as low energy consumption devices for in-memory and brain-inspired computing. Materials that undergo a metal-to-insulator phase transition (MIT) are interesting as volatile memristors and can also be used as neuristors by being the active component in self-oscillating circuits. Rare-earth (RE) nickelates ($RENiO_3$) display a MIT at temperatures that can be tuned by changing the RE cations, the strain state, the film thickness or the oxygen vacancy content. Compared to other transition-metal oxides, nickelates are especially interesting as memristive devices due to the robustness of the perovskite structure under intense local heating. In this work, we demonstrate that nickelates can also be used to mimic short term memory in synapses via multilevel resistance states that can be achieved in $SmNiO_3$ thin film structures upon voltage pulsing, harnessing the metal-insulator phase transition, without involving ionic transport. Furthermore, we also demonstrate $SmNiO_3$ as a neuron and discuss the mechanisms behind both devices.

15 min. break

DS 6.4 Tue 10:45 REC/C213

Structure and optical properties of Ga2O3 thin films deposited by reactive and non-reactive sputtering — •Marcell Gajdics, Ildikó Cora, Dániel Zámbó, Zsolt Endre Horváth, Miklós Serényi, and Béla Pécz — Institute for Technical Physics and Materials Science, HUN-REN Centre for Energy Research, H-1121 Budapest, Hungary

Ga2O3, as an ultrawide bandgap semiconductor has numerous potential applications in the field of optoelectronics and high-power electronics. Gallium oxide thin films can be grown by a variety of methods, among which radio frequency sputtering is a commonly used technique. In most cases, a ceramic Ga2O3 target is used for the sputter deposition of Ga2O3. In our work, we present an alternative method, i.e. reactive sputtering of a liquid Ga target. We have shown that by using this technique, layers close to the ideal stoichiometry can be deposited with higher deposition rates than by using a Ga2O3 target. The optical properties (e.g. refractive index) were studied as a function of the oxygen concentration in the films. Post-deposition annealing experiments were also performed on the amorphous as-deposited layers to study the annealing-induced structural and optical changes. It was found that as a first step of crystallization γ-Ga2O3 phase was formed and the thermodynamically stable β-Ga2O3 appeared only at higher temperatures. The photoluminescence emission and the optical bandgap were also measured at different annealing temperatures and the results were correlated with the structural properties.

DS 6.5 Tue 11:00 REC/C213

Depth Profiling of Oxygen Migration in Ta/HfO_2 Stacks During Ionic Liquid Gating — •Martin Wortmann[1,2], Beatrice Bednarz[3], Olga Kuschel[3,4], Fabian Kammerbauer[3], Mathias Kläui[3], Andreas Hütten[1], Joachim Wollschläger[4], Gerhard Jakob[3], and Timo Kuschel[1,3] — [1]Bielefeld University, Bielefeld, Germany — [2]Bielefeld University of Applied Sciences and Arts, Bielefeld, Germany — [3]Johannes Gutenberg University Mainz, Mainz, Germany — [4]Osnabrück University, Osnabrück, Germany

Ionic-liquid gating enables electric-field-driven ion transport at thin-film interfaces to manipulate structural, electronic, optical, and magnetic properties [1]. Oxygen is driven from a donor oxide layer into an underlying acceptor metal layer, but the resulting spatial distribution and voltage dependence of oxygen migration remain poorly understood. Here, we investigate the formation of Ta_2O_5 at the interface between the HfO_2 donor and Ta acceptor layers as a function of gate voltage, time, and HfO_2 thickness using oxidation-state depth profiling by combining X-ray reflectivity measurments with multi-line angular-resolved X-ray photoelectron spectroscopy [2,3]. The results elucidate both the quantitative oxygen distribution as well as the underlying mechanism [4].

[1] Bednarz et al., Appl. Phys. Lett. 124, 232403 (2024)
[2] Wortmann et al., Small Methods 8, 2300944 (2023)
[3] Wortmann et al., Appl. Surf. Sci. 713, 164356 (2025)
[4] Bednarz et al., arxiv: 2509.05748 (2025)

Invited Talk DS 6.6 Tue 11:15 REC/C213

Charge transfer at interfaces of free-standing oxide membranes and heterostructures — Kapil Nayak[1], Lee-Kang Huang[1], Anton Kaus[1], Marcus Wohlgemuth[1], Alexandros Sarantopoulos[1], Christoph Baeumer[2], Regina Dittmann[1], and •Felix Gunkel[1,2] — [1]PGI-7, FZ Jülich — [2]MESA+, UTwente

Free-standing oxides, based on the delamination of atomically defined epitaxial thin films, provide new opportunities to combine functional complex oxides with semiconductor electronics and other typically incompatible technology environments. The nanoscale confinement of these transferable membranes enables unique structures and functionalities, applicable in hybrid electronics as well as energy applications. Here, we discuss the synthesis of transferable perovskite oxide membranes and heterostructures via the all-perovskite sacrificial-layer route. We present control strategies to achieve singly-terminated membranes, using chemical treatments as well as direct growth mode control. These yield atomically smooth membrane-based substrates, serving as ideal template for heterostructure growth on Si. We use typical charge-transfer oxide heterostructures, such as LaAlO3/SrTiO3, to probe the interfacial charge-transfer across the heterostructure interface. To disentangle growth-induced redox response and thermodynamic ion-exchange, we employ in-situ x-ray spectroscopy and correlate the interplay of confinement-phenomena, redox-chemistry & growth kinetics. Finally, we will provide an outlook on membrane-based oxide heterostructures used in electrochemical water splitting, offering new opportunities for analysis and integration.

DS 7: Thermoelectric and Phase Change Materials

Time: Tuesday 10:00–11:30 Location: REC/B214

DS 7.1 Tue 10:00 REC/B214

Voltage-Controlled Magnetism via Electrically Triggered Metal-Insulator Transitions — •Lorenzo Fratino — Laboratoire de Physique Théorique et Modélisation, CY Cergy Paris Université

Phase separation is key to understanding magnetism in correlated systems like manganites. This talk will show how the resistive switching in metal-insulator transition (MIT) materials can be used to create and control artificial phase separation with voltage. In (La,Sr)MnO*, a threshold voltage triggers an electrothermal MIT, creating a paramagnetic insulating barrier inside a ferromagnetic metallic matrix [1]. We can use this to directly tune magnetic properties, achieving effects like voltage-triggered magnetic anisotropy switching [2]. We also developed a CdS/LSMO heterostructure where light injection modulates resistance drop*comparable to a 9 T magnetic field, while surprisingly decoupling the optical and magnetic responses [3]. This work establishes a versatile pathway for voltage-controlled magnetism using MIT materials [4].

References: [1] Nat. Commun. 12, 5499 (2021) [2] Phys. Rev. B 108, 174434 (2023) [3] Phys. Rev. Appl. 19, 044077 (2023) [4] Adv. Funct. Mater. 2419840 (2025)

DS 7.2 Tue 10:15 REC/B214

Thermoelectric power factors of defective scandium nitride nanostructures from first principles — •Luigi Cigarini[1], Urszula D. Wdowik[1], and Dominik Legut[1,2] — [1]IT4Innovations, VŠB Technical University of Ostrava, Czech Republic — [2]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

In scandium nitride (ScN), structural defects and chemical impurities strongly affect thermoelectricity (TE), although transport mechanisms remain unclear [1-3]. Reported electronic transport in ScN thin films shows large variability, and strategies to enhance TE efficiency often yield conflicting results [4,5]. Here, using the Landauer approach, we analyze how different types of imperfections affect electronic transport in ScN lattice. Defects are classified according to their symmetry (isolated, multiple contiguous, involving stacking mismatches) and chemical nature (oxygen impurities, nitrogen-site vacancies). Our theoretical results identify two dominant defect classes with opposing effects on TE performance: (i) contiguous nitrogen vacancies, which enhance el. conductivity but reduce the magnitude of the Seebeck coeff. (S), and (ii) oxygen substitutions coupled with nearby stacking mismatches, which increase the magnitude of S while hindering el. conductivity. In this way, we propose a rationale that relates part of the experimental variability to its microscopic origin [6]. [1] Phys. Rev. Mater. 3, 020301 (2019), [2] J. Mater. Chem. C 4, 3905 (2016), [3] Phys. Rev. B 86, 195140 (2012), [4] J. Appl. Phys. 113, 153704 (2013), [5] Appl. Surf. Sci. Adv. 25, 100674 (2025), [6] Preprint: arXiv:2509.14762.

DS 7.3 Tue 10:30 REC/B214

Understanding Charge Transport in ZnO Quantum Dots Through Combined Thermoelectric and High-Field Measurements — •Henrik Holzhauser, Morteza Shokrani, and Martijn Kemerink — IMSEAM, Heidelberg University, Germany

ZnO Quantum Dot (QD) solids are an attractive material for a wide range of applications. ZnO QDs also make an excellent model system for QD solid in general owing to the ability to tune the effective diameter of ZnO QD via UV illumination, and the effective electronic localization length via ligands. The charge transport in QD solids is typically explained as thermally activated tunnelling or hopping between the localized states of individual QDs. As such, the electric conductivity is both electric field and temperature dependent. In comparison, the Seebeck effect in QD solids, especially in connection with the electrical conductivity, is not as precisely understood. Here, we combine measurements of the Seebeck coefficient for various ZnO QDs with electric field- and temperature-dependent conductivity measurements, all performed at lattice temperatures ranging from 100 to 300K. We used bare ZnO QDs and ZnO QDs with ligands of various lengths and measured all QD solids at multiple UV-induced effective diameters. The wide range of experiments allows us to obtain a comprehensive understanding of the dominant mechanisms and the characteristic energy and length scales in the system. We find that transport is dominated by energetic disorder resulting from a diameter-dependent charging energy, in combination with an effective localization energy that reflects both wavefunction decay and morphology.

15 min. break

DS 7.4 Tue 11:00 REC/B214

Classification of Metal - Insulator Transitions: Insights from characteristic Property Changes and related Quantum Mechanical Bonding Descriptors — •Tim Bartsch[1], Raagya Arora[4], Carl-Friedrich Schön[1], Umesh Waghmare[3], and Matthias Wuttig[1,2] — [1]I. Institute of Physics (IA), RWTH Aachen University, Germany — [2]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany — [3]Theoretical Sciences Unit, School of Advanced Materials JNCASR Jakkur, Bangalore 560064, India — [4]John A. Paulson School of Engineering and appled science, Havard University, Cambridge Massachusetts

The nature of the transition between metals and insulators is one of the most fascinating topics in condensed matter physics. The end points of this transition are well-defined, i.e. a solid which has a non-vanishing electrical conductivity σ in the limit T * 0 K is a metal, while an insulator is characterized by σ = 0 S/m (T * 0 K). In 1980, Rosenbaum and co-workers investigated the metal-insulator transition in phosphorus-doped silicon, by measuring the low-temperature resistivity of samples with different doping concentrations. Here, we are pursuing a rather different goal. We are looking at a range of different crystalline insulators and check whether they can be classified as pressure-controlled MITs based on characteristic changes in their properties. Such pressure-driven MITs occur in all insulating solids at sufficiently high pressures when the orbital overlap of neighboring atoms increases sufficiently to favor a metallic state.

DS 7.5 Tue 11:15 REC/B214

Effect of Ge doping and thickness on anomalous Nernst effect in Fe4N thin films — •Robin K. Paul[1], Jakub Vít[2], Karel Knížek[2], Petr Levinský[2], Ondřej Kaman[2], Mariia Pashchenko[2], Lenka Kubíčková[2], Kyo-Hoon Ahn[2], Markéta Jarošová[2], Joris More-Chevalier[2], Stanislav Cichoň[2], Tomáš Kmječ[3], Jaroslav Kohout[3], Marcus Hans[4], Stanislav Mráz[4], Jochen M. Schneider[4], Giovanni d'Andrea[1], Lambert Alff[1], Esmaeil Adabifiroozjaei[1], Leopoldo Molina-Luna[1], Oliver Gutfleisch[1], and Imants Dirba[1] — [1]TU Darmstadt, Darmstadt, Germany — [2]Institute of Physics of the CAS, Praha, Czech Republic — [3]Charles University, Praha , Czech Republic — [4]RWTH, Aachen, Germany

Anomalous Nernst Effect(ANE)-based devices have recently emerged as a promising alternative to Seebeck based ones, offering simpler geometries. However, their adoption is constrained by lower efficiencies compared to Seebeck-based counterparts. This study focuses on exploring materials with high ANE coefficients. Among the candidates, Fe_4N has attracted attention due to its cost-effectiveness, and tunability through elemental doping. DFT calculations indicate that doping Fe_4N with Ge can enhance its ANE coefficient. In this work, thin films of doped $Fe_{4-x}Ge_xN$ were fabricated onto MgO substrates. The evolution of crystal structure and microstructure are systematically characterized correlating with Nernst effect. ANE is also reported to increase with decrease in film thickness which was investigated by preparing Fe_4N films of thickness from 5nm to 50nm.

DS 8: Transport Properties

Time: Tuesday 14:00–15:30 Location: REC/B214

DS 8.1 Tue 14:00 REC/B214

Polaron Transport in $BiVO_4$ — •Nils Sekinger[1,2], Tsedenia Zwedie[1,2], and Ian Sharp[1,2] — [1]Walter Schottky Institute, Technical University Munich — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich

Bismuth vanadate ($BiVO_4$) has received considerable attention as a potential photoanode for photocatalytic applications, thanks to its moderate bandgap of ~2.5 eV and favourable band edge energetics. However, it is believed that photogenerated electrons localise at vanadium sites to form small polarons, while holes localise around BiO_8 units to form large polarons, thereby inhibiting their transport [1]. This study investigates charge transport in monoclinic $BiVO_4$ using temperature-dependent photoconductivity measurements. Under illumination, we observe two distinct thermally-activated transport regimes. With decreasing temperature, the large-barrier electron hopping transport characteristic transitions to a lower barrier regime that may arise from the freeze-out of electron transport, resulting in a dominant influence from minority holes. The transport barriers, hopping distances, and effective masses of both small and large polarons in the dark and with illumination at different intensities are investigated. Analysing the dependence of the resistivity on temperature and light intensity provides critical insights into the polaronic conduction mechanism and offers experimental validation for theoretical models describing polaron transport. These findings improve our understanding of charge transport in $BiVO_4$ and its use in photocatalytic and electrochemical applications.

[1] *Wiktor et al. ACS Energy Lett. 2018, 3(7), 1693-1697*

DS 8.2 Tue 14:15 REC/B214

Correlation of impedance and structural properties in oxides on the microscale — •Jan L. Dornseifer[1,2], Christopher P. Körbächer[1,2], Martin Becker[1,2], Janis K. Eckhardt[2], Matthias T. Elm[1,2], and Peter J. Klar[1,2] — [1]Institute of Experimental Physics I, Justus-Liebig-University Giessen, Germany — [2]Center for Materials Research (ZfM), Jusuts-Liebig-University Giessen, Germany

The charge transport properties of ionically and/or electronically conducting thin films are governed by their elemental composition and microstructure, including their morphology and grain architecture. Electrochemical impedance spectroscopy (EIS) is widely used to probe the electrical properties, yielding macroscopic parameters. However, linking these to the underlying microscopic transport processes requires theoretical models that have so far failed for samples with expansions comparable to their grain sizes.

Here, we present an experimental approach to directly relate impedance, microstructure and microscopic transport properties. Using cerium oxide and vanadium oxide networks with well-defined microscale transport paths, the impedance of individual networks was measured via microelectrodes. Complementary SEM, EDX, and micro-Raman spectroscopy provided detailed structural information. Correlating these data with the impedance offered new insights into the microstructural influences on the charge transport. This represents a promising way to reliably determine microscopic transport properties of polycrystalline thin films on the microscale.

DS 8.3 Tue 14:30 REC/B214

Magnetotransport and Electron Optics in Bilayer Graphene — •Florian Schöppl[1], Ming-Hao Liu[2], Alina Mrenca- Kolasinska[3], Klaus Richter[1], Korbinian Rohrmüller[1], Korbinian Schwarzmaier[1], and Angelika Knothe[1] — [1]Institut für Theoretische Physik, Regensburg, Germany — [2]Department of Physics, National Cheng Kung University, Tainan City, Taiwan — [3]AGH University of Krakow, Kraków, Poland

The remarkable sample quality of bilayer graphene (BLG), combined with the strong electrostatic tunability of its band structure, makes BLG an excellent platform for electron optics. While the system's purity enables ballistic transport on micrometer scales [1,2], trigonal warping near each K point induces a valley-dependent momentum selection, resulting in characteristic anisotropic transport and scattering phenomena [3,4]. To study the interplay between such warping effects and symmetry breaking from gate-defined potentials, we employed quantum-mechanical tight-binding models as well as semiclassical simulations and find pronounced directional conductance in BLG cavities. Motivated by these anisotropic properties, we further analyze unguided -ringless- Aharonov-Bohm configurations and used wave-matching algorithms to tailor electrostatically defined lenses [5] and mirror geometries.

[1] L. Seemann et al., Phys. Rev. B (2023) [2] L. Banszerus et al., Nano Lett. 2016 [3] C. Gold et al., Phys. Rev. Lett. (2021) [4] J. K. Schrepfer et al., Phys. Rev. B (2021) [5] C. G. Péterfalvi et al., New J. Phys. 14 (2012)

15 min. break

DS 8.4 Tue 15:00 REC/B214

Multiscale Simulation of Charge Transport Across Grain Boundaries in Organic Polycrystalline Thin-Film Semiconductors — •Junior-Wilfried Tadjeugue-Nangmo[1,2] and Harald Oberhofer[1,2] — [1]University of Bayreuth — [2]Bavarian Center for Battery Technology, Bayreuth, Germany

Grain boundaries (GBs) are known to critically limit charge carrier mobility in organic polycrystalline semiconductors as already used in e.g. organic field effect transistors. In our contribution, we address Technologies with a multiscale computational framework that correlates a GB's morphology with its influence on the charge transport properties. Our approach is, at its core, based on phase-field simulations of grain growth to generate realistic GB networks. Electronic structure calculations then reveal deep trap states and significant energetic disorder at the GB, leading to substantial injection barriers. Charge transfer rates across GBs are then calculated from a hopping model which are finally fed into kinetic Monte Carlo (KMC) simulations to demonstrate the device level influence of GBs. They elucidate the fundamental role of grain boundaries in limiting charge transport and provide critical guidelines for the development of future high-performance organic electronics devices.

DS 8.5 Tue 15:15 REC/B214

Modeling of Indium Tin Oxide Back Contacts in CIGSe Solar Cells — •Oliver Wolf[1], Merve Demir[2], Matthias Maiberg[2], Torsten Hölscher[1], and Roland Scheer[2] — [1]B5 Photovoltaics, Just Transition Center, Martin Luther University Halle-Wittenberg — [2]Photovoltaics Group, Martin Luther University Halle-Wittenberg

Copper Indium Gallium Diselenide (CIGSe) thin-film solar cells achieve high efficiencies >23% on opaque molybdenum (Mo) back contacts (BC). Substituting the molybdenum by a transparent conductive oxide, such as Indium Tin Oxide

(ITO), facilitates applications in tandem solar cells or bi-facial configurations, but leads to deteriorated Fill Factors and Open-Circuit Voltages. The origin of the inferior solar cell performance remains unclear, but impeded electronic transport at the rear CIGSe/ITO interface appears most likely, especially in view of thin Gallium Oxide interlayers. To elucidate possible transport mechanisms, temperature-dependent current-voltage (JVT) and capacitance-frequency (CfT) characteristics were performed and analysed by means of numerical simulations with Sentaurus from Synopsys. In the measurements, we observe the occurrence of temperature-dependent kinks in the JVT and steps in CfT, which clearly distinguish the measurements of the solar cells with ITO BC from those with Mo. Based on simulation, tunneling processes turn out to be the dominant transport mechanism at the rear interface. Our results are able to describe the observed performance deficits in CIGSe solar cells with ITO BC.

DS 9: Thin Film Properties III: Oxides

Time: Tuesday 14:00–15:15 Location: REC/C213

DS 9.1 Tue 14:00 REC/C213

Analysis of the MgF_2 || VO_2 Interface in Applications as Smart Windows by Secondary Ion Mass Spectrometry (SIMS) — •Yan Ravil Wollenweber-Bienerth, Peter J. Klar, Anja Henss, and Martin Becker — Institute of Experimental Physics I and Center for Materials Research, Heinrich-Buff-Ring 16, Justus-Liebig-Universität Giessen, D-35392 Giessen, Germany

Smart Windows are special fenestration devices whose transmittance switches as a function of the ambient temperature. Vanadium dioxide (VO_2) is by far the most studied material for such applications. Usually, high substrate temperatures are needed to obtain VO_2 thin films. This results in detrimental diffusion of alkaline ions from the substrate into the thermochromic layer. Buffer layers between the substrate and the VO_2 may prove a suitable option for reducing this effect. Additionally, these help to increase visible transmittance and, in case of rutile materials, yield a reduction of the VO_2 growth temperature. Magnesium fluoride (MgF_2) is one viable candidate thanks to its excellent optical properties and chemical resistance. Simulations, however, show a significant influence of the interfaces between the layers on various properties. By controlling interface morphology, an improvement of the layer properties can be anticipated.

Here, we utilize SIMS depth-profiling to analyze multi-layer stacks of VO_2 and MgF_2 grown by ion-beam sputter deposition (IBSD). The stacks werde deposited on quartz glass substrates with MgF_2 serving as buffer layer. We show that this type of buffer layer improves the layer properties.

DS 9.2 Tue 14:15 REC/C213

Modification of crystal structure of TiO_2 thin films for artificial photosynthesis — •Lauri Palmolahti — University of Würzburg, Würzburg, Germany — Tampere University, Tampere, Finland

Progressing climate change has created a need for carbon-neutral energy production methods, such as artificial photosynthesis. The corrosive nature of artificial photosynthesis requires the use of coatings to protect otherwise unstable photocatalytic materials. The crystallite structure and size significantly affect the protective properties and chemical stability of the thin film. In this work, the effect of defect composition in amorphous TiO_2 thin films on vacuum annealing induced crystallization was studied. The chemical stability and protective properties of these crystallized films were then examined under conditions similar to those in artificial photosynthesis. The defect composition of the amorphous phase, such as Ti^{3+}, O^{1-}, and precursor traces, was tuned by changing the deposition parameters. The results showed that amorphous TiO_2 thin films without Ti^{3+} defects crystallized into microcrystalline anatase, whereas a moderate number of these defects led to the formation of nanocrystalline rutile. An excessive number of defects resulted in a mixed amorphous–nanocrystalline rutile phase. Impedance spectroscopy and stability tests revealed that microcrystalline anatase was prone to grain boundary corrosion, whereas nanocrystalline rutile was chemically stable and retained its protective properties for extended periods of time, making it a suitable choice for protective coatings in artificial photosynthesis.

DS 9.3 Tue 14:30 REC/C213

Investigation of epitaxial ITO layers on YSZ as a transparent conductive back contact for photoelectrochemical applications — •Margaretha Huber[1], Sergej Levashov[1], Tsedenia Zewdie[1,2], Ian D. Sharp[1,2], and Johanna Eichhorn[1] — [1]TUM School of Natural Sciences — [2]Walter Schottky Institut

Photoelectrochemical (PEC) water splitting is a promising route toward sustainable, high-energy-density solar fuels for carbon-neutral energy storage. Transparent conducting oxides such as indium tin oxide (ITO) often serve as back contacts due to their high electrical conductivity, electrochemical stability in the oxygen evolution reaction, and favorable band alignment. ITO grown on cubic oxide substrates such as yttria-stabilized zirconia (YSZ) can act as an epitaxial template with low lattice mismatch, enabling fully epitaxial oxide heterostructures with well-defined interfaces and reduced defect densities. Here, we investigate epitaxial ITO (100) thin films on YSZ grown by e-beam evaporation through a systematic variation of deposition rate, substrate temperature, and post-deposition annealing atmosphere, thereby tuning crystallinity, lattice parameters, carrier transport, and surface morphology. The correlation between structural quality and stoichiometry, and their impact on electrical properties, is investigated using X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and atomic force microscopy (AFM). These ITO/YSZ templates are evaluated using $BiVO_4$ as a model photoanode to enable efficient charge extraction and provide design guidelines for epitaxial oxide heterostructures for PEC water splitting.

DS 9.4 Tue 14:45 REC/C213

Room-temperature H_2 gas sensing in ultra-thin SnO_2 films grown via atomic layer deposition — •Rudi Tschammer[1], Dominic Guttmann[1], Carlo Tiebe[2], Karsten Henkel[1], Carlos Morales[1], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Cottbus, Germany — [2]Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany

Transitioning to an energy system based entirely on renewable energy sources requires long-term energy storage utilizing energy vectors such as hydrogen (H_2). Given its high diffusivity, broad explosive range, and low ignition energy, the adoption of H_2 requires safety systems along the hydrogen value chain. Therefore, there is a need for sensitive, specific and selective conductometric H_2 sensors operating at room temperature (RT) and compatible with complementary metal-oxide semiconductor (CMOS) technology. Earlier work by our group investigated ultra-thin cerium oxide films grown by atomic layer deposition (ALD) and demonstrated H_2 sensing at RT. This performance was due to the abundant defects present in the films. Building on these results, we present a comprehensive investigation of ALD-grown tin oxide (SnO_2), a widely researched metal oxide for H_2 gas sensing. Using *in-situ* X-ray photoelectron spectroscopy (XPS), we observe a distinct dependence of defect concentration on film thickness and oxidant. *Ex-situ* H_2/air gas sensing measurements and near-ambient pressure XPS further link film properties and sensing behavior. These findings pave the way for novel RT H_2 gas sensors based on ALD technology.

DS 9.5 Tue 15:00 REC/C213

Composition and band gap of aluminum alloyed beta-gallium oxide determined by XPS — •Lukas Schewe[1], Jana Rehm[2], Ming-Chao Kao[3], Vedran Vonk[3], Zbigniew Galazka[2], Saud Bin Anooz[2], Andreas Popp[2], and Jan Ingo Flege[1] — [1]Fachgebiet Angewandte Physik und Halbleiterspektroskopie, BTU Cottbus-Senftenberg — [2]Leibnitz-Institut für Kristallzüchtung, Berlin — [3]CXNS-Center for X-ray and Nano Science, DESY, Hamburg

Beta-phase gallium oxide has a band gap of 4.85 eV, suggesting strong potential for high-power electronics applications. Its properties can be enhanced by increasing the band gap via aluminum alloying. Here, we discuss the structural, electronic, and surface properties of β-$(Al_xGa_{1-x})_2O_3$ bulk crystals and thin films grown by metal-organic vapor-phase epitaxy (MOVPE) with Al contents of up to 40 %. Their Al content was determined by X-ray photoelectron spectroscopy (XPS) and compared with values obtained from X-ray diffraction (XRD) and inductively coupled plasma optical emission spectroscopy (ICP-OES). Additionally, potential doping gradients towards the bulk have been investigated by acquiring spectra at different take-off angles and by XPS depth profiling, revealing different aluminum concentrations in the bulk and at the surface. Furthermore, we establish a correlation between Al content and electronic band gap, i. e., with changes in the optoelectronic properties, which were determined by a combination of XPS electron-loss spectra and optical absorbance measurements. Finally, Auger spectroscopy and XRD analysis confirm the excellent chemical and structural quality of β-$(Al_xGa_{1-x})_2O_3$ thin films.

DS 10: Focus Session: Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects I (joint session TT/DS/MA)

Nickel, a direct neighbor of copper in the periodic table, has been considered a promising candidate for high-temperature superconductivity since the early 1990s. After more than three decades of research, this prediction was confirmed with the discovery of superconductivity in nickelates, marking the beginning of the "nickel age" of superconductivity. Recent advances include Sm-based infinite-layer nickelates with transition temperatures approaching 40 K, as well as bilayer nickelates exhibiting superconductivity above 90 K under pressure and up to 60 K under compressive epitaxial strain. These results highlight the crucial roles of structural engineering, epitaxial strain, and precise synthesis control, and they open new frontiers for both fundamental understanding and materials design. This focus session aims to define key scientific challenges ahead, strengthen collaboration within Germany and Europe, and accelerate progress toward higher superconducting transition temperatures.

Coordinators: Marta Gibert (TU Wien), Mattias Hepting (MPI FKF Stuttgart), Ilya M. Eremin (Ruhr-University Bochum)

Time: Wednesday 9:30–12:45 Location: HSZ/0003

See TT 39 for details of this session.

DS 11: Layer Deposition

Time: Wednesday 9:30–11:45 Location: REC/B214

DS 11.1 Wed 9:30 REC/B214

Photo-Assisted Atomic Layer Deposition — •Paul Butler[1,2], Simon Wörle[1,2], Pengyu Hu[1,3], Manfred Stemplinger[1,2], and Ian D. Sharp[1,2] — [1]Walter Schottky Institut, Technische Universität München, 85748, Garching, Germany — [2]Physics Department, TUM School of Natural Science, Technische Universität München, 85748, Garching, Germany — [3]Department of Electrical Engineering, TUM School of Computation, Information and Technology, Technische Universität München, 85748, Garching bei München, Germany

Atomic layer deposition (ALD) is a powerful technique for uniformly coating complex surfaces with thin films, though achieving lateral control remains one of its main challenges. This work demonstrates the implementation of visible-wavelength excitation to assist in the ALD process, thereby providing an opportunity for selective-area deposition using beam-shaping. We demonstrate that optical laser excitation can be used to assist in several ALD processes. An optical laser was used to selectively photo-assist the deposition of TiO_2 on gold as well as monolayer MoS_2 at low temperatures. The molecular precursors, titanium isopropoxide (TTIP) and ozone were used for the low-temperature deposition of TiO_2 on gold, while tetrakis(dimethylamido)titanium (TDMAT) and water were used for the deposition of TiO_2 on MoS_2. Photoexcitation is also shown to reduce the nucleation delay when $MeCpPtMe_3$ and ozone are used to deposit platinum films on Si and SiO_2 surfaces, using. Samples are characterized with spectroscopic ellipsometry and AFM before and after depositions, with in-situ ellipsometry during ALD procedures.

DS 11.2 Wed 9:45 REC/B214

Epitaxial growth of wurtzite $Al_{1-x}Hf_xN$ thin films by reactive magnetron sputtering — •Valentin Walbrunn[1,2], Laura I. Wagner[1,2], Verena Streibel[1,2], Mingyun Yuan[3], and Ian D. Sharp[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Germany — [2]Physics Department, TUM School of Natural Sciences, Germany — [3]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Germany

Ternary nitrides such as transition metal (TM) wurtzite $Al_{1-x}TM_xN$ compounds offer great potential for future electromechanical and ferroelectric devices. While this class of materials is exemplified by $Al_{1-x}Sc_xN$, alternative TM elements such as Hf, Zr, and Ti remain largely underexplored, despite predictions of increased piezoelectric responses and the benefit of reduced reliance on rare earth elements. In this work, we explore reactive magnetron co-sputtering of wurtzite aluminum hafnium nitride ($Al_{1-x}Hf_xN$) to achieve epitaxial thin films suitable for high-frequency surface acoustic wave (SAW) applications. We tune the Hf content by scaling the power applied to the metallic Hf and Al targets in an Ar/N_2 atmosphere and determine optimized conditions with Hf cation fractions up to 40 %. X-ray diffraction confirms the formation of a wurtzite phase with strong c-axis orientation, and rocking curve measurements indicate improved crystalline quality, comparable to sputtered $Al_{1-x}Sc_xN$. These films demonstrate epitaxial wurtzite $Al_{1-x}Hf_xN$ as a promising material platform for high-frequency SAW applications.

DS 11.3 Wed 10:00 REC/B214

Epitaxial growth of hexagonal boron nitride (h-BN) by thermal laser epitaxy (TLE) — •Markus A. Blonski[1], Gideok Kim[2], João Marcelo Lopes[1], Audrey Gilbert[1], Lutz Geelhaar[1], Jochen Mannhart[2], Darrell G. Schlom[3], and Patrick Vogt[1,2] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [3]Cornell University, Ithaca, USA

Thermal laser epitaxy (TLE) is a novel thin film synthesis technique in which the substrate and sources are heated by high-power infrared lasers. Without heating elements, TLE achieves unprecedentedly high growth temperatures and pressures, exceeding those of traditional methods like standard chemical vapor deposition (CVD) or molecular beam epitaxy (MBE). TLE enables thermal in situ substrate termination, accelerating surface treatment and avoiding pre-growth contamination. Using TLE, we map an unrivaled growth pressure and temperature (P-T) parameter space for h-BN growth on $Al_2O_3(0001)$ substrates. To optimize substrate termination, the Al_2O_3 surface is nitridized to form an AlN adlayer at $T \sim 1800\,^{\circ}C$ under an NH_3 atmosphere with a pressure of $P = 10^{-3}$ mbar. This termination process is followed by h-BN growth at 1600 °C to 2000 °C with NH_3 pressures ranging from 10^{-6} mbar to 10^{-1} mbar. We demonstrate epitaxial h-BN growth under unprecedented P-T conditions, characterized by Reflection high-energy electron diffraction, Fourier transform infrared spectroscopy, Raman spectroscopy and atomic force microscopy.

DS 11.4 Wed 10:15 REC/B214

Local growth of GaAs on Si(001) and Si(001)4.5° by Laser-assisted MOVPE — •Christian Bruckmann, Jürgen Bläsing, Armin Dadgar, and André Strittmatter — Institute of Physics, Otto-von-Guericke-University Magdeburg, Germany

The demand for increasingly performant, energy-efficient semiconductor devices is driving the research on how to combine III/V- with Si-based components in the most efficient way possible. While the monolithic integration on the Si substrate offers advantages compared to hybrid integration schemes, the heteroepitaxy of III/V-compound semiconductors is challenging due to different material properties. The Laser-assisted MOVPE enables an additive fabrication of semiconductor devices allowing cost-efficient low-volume production of special device structures. Key part is a high-power laser diode used for local heating of the substrate surface leading to local growth. GaAs islands were grown on Si(100) as well as Si(100) 4.5 ° substrates using a two-step growth approach which consists of a low-temperature nucleation layer followed by a high-temperature buffer layer. Optimization of the growth parameters and characterization with AFM and XRD shows qualitative trends similar to conventional MOVPE. For an island with a diameter of 260 nm and a height of 230 nm a XRD FWHM of 0.47 ° (ω-Scan, GaAs(004)) was obtained. Increasing the layer thickness to 3 μm yields a FWHM of 0.26 ° at optimum. Roughness measurements in the island center lead to RMS values of 4.0 nm (5 x 5 μm^2).

15 min. break

DS 11.5 Wed 10:45 REC/B214

Interface formation in ALD-based SnO_2/CeO_x heterostructures — •Dominic Guttmann[1], Rudi Tschammer[1], Carlos Morales[1], Malgorzata Kot[2], Michal Mazur[2], Damian Wojcieszak[2], Paulina Kapuscik[2], Wiktoria Kolodzinska[2], Jarosław Domaradzki[2], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Cottbus 03046, Germany — [2]Faculty of Electronics, Photonics and Microsystems, WUST, 50-372 Wroclaw, Poland

The electrical resistance of SnO_2 ultrathin films (< 20 nm) made by atomic layer deposition (ALD) strongly depends on thickness, due to intrinsic film defects at interfaces arising from changes in the ALD reaction mechanism during the first cycles and from the film/substrate interaction. Modifying interface properties in SnO_2/CeO_x heterostructures can enhance H_2 sensing performance. We studied the initial growth of SnO_2 by ALD on CeO_x substrates prepared by either electron beam evaporation (EBE) or ALD. Employing the commercial precursor tetrakis(dimethylamino)tin (TDMASn) and ozone (O_3) as well as in vacuo and near-ambient-pressure X-ray photoelectron spectroscopy, we examined how substrate preparation affects the SnO_2 nucleation behavior in the first cycles. SnO_2 growth on EBE-CeO_x indeed starts with the first precursor cycle, whereas ALD-CeO_x requires an additional conditioning step. Connecting these findings to surface chemistry, distinct C1s and N1s signatures attributed to TDMASn adsorption indicate a slow C/N buildup, consistent with previous reports on ALD-grown SnO_2 on Si, SiO_2, and Al_2O_3.

DS 11.6 Wed 11:00 REC/B214

Enhancing the antiferroelectric response of $AgNbO_3$ thin films — •Sreelakshmi Prasanna, Juliette Cardoletti, Philipp Komissinskiy, Thorsten Schneider, and Lambert Alff — Institute of Materials Science, TU Darmstadt, Darmstadt, Germany

Dielectric capacitors are widely utilized in numerous advanced high power electronic systems due to their distinctive features of high-power density, ultrafast charge/discharge capability, long storage lifetime, etc. Among them, antiferroelectrics have attracted extensive attention for energy storage applications because of their double hysteresis loop and zero remnant polarization. Within this class of materials $AgNbO_3$-based lead-free perovskites are promising candidates due to their environmentally friendly nature and strong intrinsic antiferroelectric response. In this work, we have grown $AgNbO_3$ thin films using pulsed laser deposition and examined their structural properties using X-ray diffraction and SEM. The presence of metallic Ag particles on the $AgNbO_3$ surface with a size ranging from nanometres to micrometres indicates excessive Ag creating conductive pathways and severely compromise the electrical performance, suppressing the antiferroelectric behaviour. We demonstrate a post-annealing and post-deposition treatment to remove excessive Ag in grain boundaries and as well as on the surface, while preserving the $AgNbO_3$ phase.This procedure reduces the leakage current significantly and enables the access to the antiferroelectric properties of $AgNbO_3$. This simple and effective way to enhance the performance of $AgNbO_3$ thin films opens the way to their application in eco-friendly energy storage devices.

DS 11.7 Wed 11:15 REC/B214

Low-Temperature Atomic Layer Deposition of Rutile Titanium Dioxide Buffer Layers for Thermochromic Windows — •Jan Leithäuser, Waafa Al Nachwati, Philip Klement, Sangam Chatterjee, and Martin Becker — I. Physikalisches Institut, Justus-Liebig-Universität Gießen, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

Vanadium dioxide (VO_2) exhibits a reversible semiconductor-metal transition (SMT) at approx. 68°C and enables thermochromic smart windows that modulate solar heat gain. To achieve high solar modulation (T_{sol}) at industrially compatible temperatures, a smooth, chemically stable rutile TiO_2 buffer layer is required. Here, we demonstrate that atomic layer deposition (ALD) of TiO_2 at 200 °C, followed by low-temperature annealing, results in dominant rutile at 220 °C, provided the TiO_2 thickness is at leat 30 nm; thinner layers (10 nm) crystallize as anatase. Integrating such ALD-grown rutile buffers into VO_2 || TiO_2 || Glass structures allow for optimal VO_2 growth windows at 400 - 450 °C and yields a T_{sol} comparable to that of high-temperature sputtered rutile buffers. The ALD approach maintains nanometer-scale roughness. This low-temperature route to rutile TiO_2 represents an advancement for scalable, energy-efficient thermochromic coatings compatible with temperature-sensitive substrates.

DS 11.8 Wed 11:30 REC/B214

Interface induced ferromagnetism and Superconductivity in epitaxially engineered thin films — •Mostafa Marzouk[1,2], Anupam Singh[2], Igor Mazinchenko[2], Malli Tangi[2], Sergey Ostanin[2], Younghyuk Kim[2], Ilya Kostanovski[2], Arthur Ernst[2], Mathew Gilbert[2], and Stuart Parkin[2] — [1]Current Address: Institute for Topological Insulators, University of Wuerzburg, 97074 Würzburg, Germany — [2]Max-Planck institute of Microstructure Physics, 06120 Halle (Saale), Germany

Two-dimensional electron gases (2DEGs) at oxide interfaces offer several advantages that are not typically found in semiconductor-based 2DEGs. One key advantage is their high sheet carrier density, which is essential for achieving the high current densities required in power and memory applications.

In this talk, I will present the emergent phenomena at oxide interfaces we grew using state-of-the-art molecular beam epitaxy (MBE), with a primary focus on the two-dimensional electron gases formed at KTaO-based interfaces. We observe the development of ferromagnetism in the KTaO3(110)/LaTiO3 and KTaO3(111)/LaTiO3 2DEGs. Remarkably, these ferromagnetic 2DEGs retain high electron mobilities, reaching approximately 250 cm2/V.s at 2 K and 20 cm2/V.s at 300 K. The presence of ferromagnetism is confirmed through anomalous Hall effect hysteresis loops, butterfly-shaped magnetoresistance hysteresis loops (down to 1.7 K), out-of-plane magnetization hysteresis loops, and x-ray magnetic circular dichroism (XMCD) measurements at 2 K.

DS 12: 2D Materials I

Time: Wednesday 9:30–12:00 Location: REC/C213

DS 12.1 Wed 9:30 REC/C213

Purcell enhancement of photocurrent in a van der Waals self-cavity — •Xinyu Li — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

We report the observation of Purcell-enhanced terahertz (THz) photocurrent emission in exfoliated flakes of the van der Waals (vdW) semimetal WTe_2, which act as intrinsic plasmonic self-cavities. Unlike conventional cavities that require external mirrors, micron-scale vdW flakes confine electromagnetic fields via edge reflections, supporting standing-wave plasmonic modes in the THz range. Using ultrafast optoelectronic circuitry, we measured coherent near-field THz emission resulting from nonlinear directional photocurrents excited at crystal edges. Emission spectra reveal resonant enhancement at discrete frequencies, tunable by excitation fluence and device geometry. We attribute this effect to cavity-modified photonic density of states - i.e., the Purcell effect - acting on driven, nonlinear transport currents. An analytical model capturing the self-cavity resonance conditions accurately reproduces experimental trends across multiple devices. Our findings establish WTe_2 as a bias-free, geometry-tunable THz emitter and demonstrate the potential of self-cavity engineering for controlling nonlinear, nonequilibrium dynamics in quantum materials.

Further details are available at arXiv:2507.07987.

DS 12.2 Wed 9:45 REC/C213

Radial Rashba spin-orbit fields in commensurate twisted transition-metal dichalcogenide bilayers — •Thomas Naimer[1], Paulo E. Faria Junior[2], Klaus Zollner[1], and Jaroslav Fabian[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Department of Physics, University of Central Florida, Orlando, Florida 32816, USA

In commensurate twisted homobilayers, purely radial Rashba spin-orbit fields can emerge. We employ first-principles calculations to investigate the band structures and the spin-orbit fields close to the high-symmetry points K and Γ of several commensurate twisted transition-metal dichalcogenide homobilayers: WSe_2, $NbSe_2$, and WTe_2. The observed in-plane spin textures can for the most part be reproduced successfully using a model Hamiltonian, enabling us to extract relevant parameters. Exploring different lateral displacements between the layers, we confirm that the relevant symmetry protecting the radial Rashba is an in-plane 180° rotation axis. Our calculations on WTe_2 bilayers show that their lack of C_3 symmetry results in spin textures that are neither radial nor tangential. All authors acknowledge support by the FLAG ERA JTC 2021 project 2DSOTECH, the European Union Graphene Flagship project 2DSPIN-TECH (grant agreement No. 101135853) and SFB 1277 (Project-ID 314695032).

DS 12.3 Wed 10:00 REC/C213

Spatially Controlled Photoelectrochemical Thinning of 2D Transition Metal Dichalcogenides — •Simon Wörle[1], Lukas Wolz[1], Sergej Levashov[1], Franz Gröbmeyer[2], Johanna Eichhorn[1], Emiliano Cortes[2], Jeremy Robinson[3], and Ian Sharp[1] — [1]Technical University of Munich — [2]Ludwig Maximilian University of Munich — [3]U.S. Naval Research Laboratory

The integration of two-dimensional transition metal dichalcogenides (TMDs) into functional devices and catalytic systems requires detailed understanding and control of their behavior in reactive environments. Here, we systematically investigate the photoelectrochemical (PEC) stabilities of MoS_2, WS_2, $MoSe_2$, and WSe_2 mono- and multilayer flakes under dark and illuminated conditions, revealing two distinct oxidation mechanisms. In the dark, anodic potentials promote oxidation at defect-rich TMD edge sites, with subsequent dissolution of the oxidized species causing progressive lateral shrinkage, while the basal planes remain stable. Under white light illumination from a solar simulator, photoexcited holes drive electrochemical thinning of TMD multilayer flakes, which proceeds at anodic potentials lower than those required for lateral edge oxidation in the dark. This PEC-driven thinning enables controllable top-down fabrication of large-area TMD films with well-defined thicknesses. Importantly, the use of a focused laser beam rather than white light illumination enables precise spatial control over the PEC oxidation process, allowing localized patterning and thinning in predefined regions for the processing and integration of 2D materials into functional devices.

DS 12.4 Wed 10:15 REC/C213

Pairing symmetry of Ising superconductors via the upper critical field — •Lena Engström[1], Ludovica Zullo[2], Tristan Cren[3], Andrej Mesaros[1], and Pascal Simon[1] — [1]Université Paris-Saclay, CNRS, Laboratoire de Physique des Solides, 91405 Orsay, France — [2]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany — [3]Sorbonne Université, CNRS, Institut des Nanosciences de Paris, UMR7588, F-75252 Paris, France

Several conflicting predictions have been made for the symmetry of the pairing in transition metal dichalcogenide (TMD) superconductors. An indication of if singlet or triplet pairing is present can be given by the upper critical field (Hc2), the magnetic field required to fully suppress superconductivity. Monolayer 1H-NbSe2 and 1H-TaS2 have extremely large critical fields, due to a large Ising spin-orbit coupling (SOC), yet they do not scale with SOC and temperature as expected for other TMDs. In our work on few-layer 2H-stacked TMDs, we highlight that the Ising SOC has nodal lines in the Brillouin zone imposed by symmetry. By deriving the susceptibility, we have found that the scaling of the critical field can be traced back to whether the Fermi surface intersects with these lines or not. Reinterpreting existing experimental data, we find that a predominantly singlet order is consistent with the measured Hc2. We propose two experiments where a signature of spin-singlet pairing would be visible, while discussing the possibility of mixed-parity pairing.

DS 12.5 Wed 10:30 REC/C213

Single-Metal-Atom Chains in Transition-Metal Dichalcogenides: Electronic, Magnetic, and Catalytic Properties — •Prosun Santra, Mahdi Ghorbani-Asl, and Arkady V. Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

One-dimensional metallic nanostructures exhibit Peierls instabilities, Tomonaga-Luttinger liquid behavior, Majorana fermions, and half-metallicity, which is interesting in the context of spintronics. Stable single-metal-atom chains (SMACs) were experimentally manufactured by embedding transition metal (TM) atoms at mirror twin boundaries (MTBs) in MoS_2. Using DFT calculations, we study the energetics and properties of SMACs formed by 21 TM elements embedded in MTBs in 2D $MoSe_2$, $MoTe_2$, WS_2, and WSe_2. Spin-polarized calculations reveal localized magnetism and half-metallicity in multiple systems, ideal for nanoscale spintronics. We further study the catalytic properties of these systems. Our results indicate that selected SMACs can surpass Pt(111) in hydrogen evolution reaction activity, so that these defect-engineered structures not only are versatile 1D quantum-spintronic platforms, but may also be utilized as low-cost, high-performance electrocatalysts for green H_2 production.

15 min. break

DS 12.6 Wed 11:00 REC/C213

Magnetoelectric flat band induced by a $\sqrt{3} \times \sqrt{3}$ charge density wave in monolayer $CrSe_2$ — •Victor Pardo[1], Pablo Savino Real[1], Carmen Fuente Santiago[1], Jan Phillips[2], Javier Corral Sertal[1], Adolfo Otero Fumega[3], and Santiago Blanco Canosa[4] — [1]Instituto de Materiais iMATUS, Universidade de Santiago de Compostela, E-15782 Campus Sur s/n, Santiago de Compostela, Spain — [2]Iberian International Nanotechnology Laboratory, INL Braga, Portugal — [3]Department of Applied Physics, Aalto University, 02150 Espoo, Finland — [4]Donostia International Physics Center (DIPC), San Sebastián, Spain

We investigate the electronic and magnetic properties of the $\sqrt{3} \times \sqrt{3}$ charge-density-wave (CDW) phase of $CrSe_2$ using first-principles calculations within density functional theory. We find that the most stable configuration corresponds to a ferromagnetic ground state, which hosts a remarkably flat electronic band exactly at the Fermi level. We show that the flat band derives from an a_{1g}-like component of the Cr t_{2g} manifold in a trigonal environment, combined with bonding–antibonding splittings induced by the formation of Cr trimers in the CDW structure. Strong hybridization between Cr d and Se p orbitals is crucial for stabilizing this band exactly at the Fermi level. Spin–orbit coupling affects only the remaining d bands, leaving the flat band intact. We establish how to tune the existence of this flat-band by relating it to the electric polarization caused by the CDW, hence describing a mechanism to turn on/off strong correlations with an external tuning parameter such as an electric field.

DS 12.7 Wed 11:15 REC/C213

Topological Superconductivity in $NbSe_2$-based Ising-Type Superconductors — •Jozef Haniš[1], Marko Milivojević[2], Zoltan Tajkov[3], and Martin Gmitra[1] — [1]Institute of Experimental Physics SAS Watsonova 47 040 01 Košice, Slovak Republic — [2]Institute of Informatics, Slovak Academy of Sciences, Dúbravská cesta 9 845 07 Bratislava 45, Slovakia — [3]Eötvös Loránd University, Pázmány Péter sétány 1/A, Budapest, Hungary

Topological superconductivity offers the promise of Majorana-bound states for fault-tolerant computation. We develop a symmetry-guided framework for superconducting pairing in Ising-type transition metal dichalcogenides, focusing on $NbSe_2$-based systems. We identify multiple topological phases–classified by Chern numbers and $\mathbb{Z}_2$ invariants–enabled by spin-orbit-induced triplet pairing. We present topological phase diagrams for different doping regimes and discuss zigzag-ribbon band-structure calculations. This work was supported by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I05-03-V02-00071, and the Slovak Academy of Sciences project IMPULZ IM-2021-42.

DS 12.8 Wed 11:30 REC/C213

Modeling Pressure-Induced Exciton Screening in hBN/WSe2/hBN Heterostructures — •Adlen Smiri[1], Shalini Badola[2], Amit Pawbake[2], Clément Faugéras[2], and Iann C. Gerber[1] — [1]Université Fédérale de Toulouse Midi Pyrénées, INSA-CNRS-UPS, LPCNO, 135 Av. de Rangueil, 31077 Toulouse, France — [2]Laboratoire National des Champs Magnétiques Intenses, LNCMI-EMFL, CNRS UPR3228, Univ. Grenoble Alpes, Univ. Toulouse, Univ. Toulouse 3, INSA-T, Grenoble and Toulouse, France.

Hydrostatic pressure is an effective tool to tune excitonic properties in two-dimensional semiconductors. We investigate the pressure dependence of excitonic Rydberg states in a WSe2 monolayer encapsulated in hBN and observe a reduction of the 1s-2s and 1s-3s energy separations with increasing pressure. First-principles calculations indicate negligible changes in the band structure and effective masses, pointing to pressure-modified dielectric screening as the main mechanism. A microscopic dielectric model for the WSe2 monolayer with an effective vacuum gap reproduces the observed excitonic shifts, demonstrating that enhanced screening governs exciton renormalization. These results provide a quantitative framework for tuning excitonic interactions in van der Waals heterostructures.

DS 12.9 Wed 11:45 REC/C213

Above room temperature ferromagnetism in wafer-scale Fe_3GaTe_2/SiC and the origin of double-step hysteresis in MBE-grown Fe_3GaTe_2 films — •Tauqir Shinwari[1], Victor Ukleev[2], Chen Luo[2], Kacho Imtiyaz Ali Khan[1], Florin Radu[2], and Joao Marcelo Jordao Lopes[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Helmholtz Zentrum Berlin for Materialien und Energie, Albert-Einstein Straße 15, 12489 Berlin, Germany

Two-dimensional (2D) magnetic materials provide a versatile platform for next-generation spintronic devices, where scalable growth and robust ferromagnetism are the key factors. Fe_3GaTe_2 is a 2D ferromagnet with a high Curie temperature (~ 360K) and strong perpendicular magnetic anisotropy, making it a particularly promising candidate for energy-efficient spin-based technologies. Until now, most studies on Fe_3GaTe_2 have relied on millimeter-sized bulk crystals and exfoliated flakes, which are unsuitable for wafer-scale integration and reproducible device processing. In this work, we demonstrate high-quality, large-area epitaxial growth of Fe_3GaTe_2 thin films directly on SiC(0001) substrates by MBE. The films exhibit robust above-room-temperature ferromagnetism together with strong out-of-plane magnetic anisotropy, as confirmed by magnetometry and element-specific x-ray techniques. A double-step hysteresis loop is observed in MBE-grown Fe_3GaTe_2 films, pointing to the coexistence or coupling of distinct magnetic subsystems, which will be discussed in the context of Fe site selectivity, thickness dependence, and interfacial effects.

DS 13: Layer Properties

Time: Wednesday 15:00–16:15 Location: REC/B214

Invited Talk DS 13.1 Wed 15:00 REC/B214

Tailored thermal treatments for multi-layer, multi-material polymer devices — •Katherina Haase, Shaoling Bai, Mike Hambsch, Vojtech Millek, and Stefan C. B. Mannsfeld — Faculty of Electrical and Computer Engineering & Center for Advancing Electronics Dresden (cfaed), TUD Dresden University of Technology, 01069 Dresden, Germany

Thermal annealing constitutes an important processing step during the fabrication of organic semiconductor-based devices as it removes residue solvent and often leads to improved structural order. Recently, we have explored an additional aspect of thermal annealing - its impact on the dissolution of conjugated polymer (CP) thin films. We could show that thermal annealing induces physical cross-linking in a wide range of CPs,[1] which distinctly increased their stability in the original solvent. Hence, we suggested that tailored thermal treatments could enable polymer heterojunction devices though simple sequential coating.

In this presentation, we discuss the important finding that the thermal physical cross-linking (TPC) effect produces solvent-resistant thin films for a wide variety of CPs that could be combined into a multitude of novel devices, and explore the fabrication of solution-coated, polymer heterojunction-based synaptic transistors - devices that could not have been realized without the application of cross-linking.

[1] S. Bai, K. Haase, J. Perez Andrade, M. Hambsch, F. Talnack, V. Millek, A. Prasoon, J. Liu, K. Arnhold, S. Boye, X. Feng, S. C. B. Mannsfeld, Adv. Electron. Mater. 2024, 10, 1.

DS 13.2 Wed 15:30 REC/B214

Mechanical Stress Evolution in Polycrystalline Ge Thin Films under MeV Ion Irradiation — •Karla J. Paz Corrales[1], Aaron Reupert[2], Kevin Lubig[2], Frank A. Müller[2], Berit Marx-Glowna[3], Ralf Röhlsberger[3], Till Weickhardt[1], Giancarlo Soavi[1], Martin Hafermann[1], Elke Wendler[1], and Carsten Ronning[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, 07743 Jena, Germany — [3]Helmholtz-Institut Jena, Fraunhoferstr. 8, 07743 Jena, Germany

Polycrystalline Ge thin films were deposited by magnetron sputtering, annealed at 600 °C for 1 h, and irradiated with 1.8 MeV Au ions over a broad fluence range. Structural, optical, and in-situ mechanical stress analyses were performed to investigate irradiation-induced property modifications. At low fluences, the films show a reduction of the initial tensile residual stress from the preparation process. This stress compensation is linked to the formation of point defects, which also decrease the optical band gap. These defects can migrate to grain boundaries, where recombination enhances the resistance to amorphization compared with single-crystalline Ge. At higher fluences, defect accumulation increases tensile stress and leads to the formation of mixed polycrystalline-amorphous phases. With further irradiation, the films fully transform into an amorphous phase, as evidenced by changes in both structural and optical properties. In this amorphous state, additional stress relaxation occurs, attributed to plastic flow or to interface effects between the film and substrate.

DS 13.3 Wed 15:45 REC/B214

Optical tuning of Sr(Mo,Ti)O_3 thin films through solid solution — •Anjima Kallam Valli, Juliette Cardoletti, and Lambert Alff — Institute of Materials Science, TU Darmstadt, Darmstadt, Germany

Transparent conductive oxides are key materials in display technology and renewable energy applications, being used as transparent electrodes in solar cells and optoelectronic devices. Perovskite oxides such as $SrMoO_3$, $SrVO_3$, and $SrNbO_3$ exhibit exceptional metallic conductivity combined with optical transparency. Among them, bulk $SrMoO_3$ shows a conductivity of $2 * 10^7$ S m^{-1} exceeding that of platinum at room temperature; however, its optical transparency is limited to the UV visible range (300 to 500 nm). This work investigates the broadening of the transparency window of $SrMoO_3$ through partial B-site substitution of molybdenum by titanium. Titanium incorporation modifies the carrier density and thereby tunes the plasma frequency, shifting the optical reflection edge toward longer wavelengths. Epitaxial Ti-substituted $SrMoO_3$ thin films have been grown by pulsed laser deposition. Structural analysis was performed by XRD, and their electrical transport properties, including resistivity and carrier density, were characterised using van der Pauw and Hall-effect measurements. Optical transparency has been evaluated by spectroscopic analysis. Through tailoring of the transparency with varying Ti concentration, this work opens the door to various optoelectronic device applications.

DS 13.4 Wed 16:00 REC/B214

Automating calculations for advancing the simulations of solid interfaces — •Elisa Damiani, Margherita Marsili, and Maria Clelia Righi — Dipartimento di Fisica e Astronomia, University of Bologna, Italy

Solid-solid interfaces are ubiquitous and simulations help understanding their properties, and may represent powerful screening and designing tools. Often first-principles electronic structure methods must be used: for example to characterize their transport, electronic, optical and magnetic properties, and also their adhesion and friction. Nevertheless, these approaches comes along with computational complexity and costs. In this talk I will present how we address these computational challenges by developing TribChem, a software that automates the creation of interface models, the identification of the optimal computational parameters, job submission, and data retrieval and storage. I will also show how this code has been successfully applied to the systematic study of different classes of interfaces such as metal-metal, metal-semiconductor, and metal-2D-materials ones, and illustrate the current developments that carried out to increase the complexity of the systems that can be addressed (amorphous and molecular solids) employing a Bayesian Optimization approaches.

These results are part of the SLIDE project that has received funding from the European Research Council (ERC) under the European Union*s Horizon 2020 research and innovation program (Grant agreement No. 865633).

DS 14: 2D Materials II (joint session DS/HL)

Time: Wednesday 15:00–17:30 Location: REC/C213

DS 14.1 Wed 15:00 REC/C213

Engineering at the Thinnest Scale: Insights into the Stability of 2D GaN on Liquid Metal Catalysts — •Tomoko Yokaichiya, Karsten Reuter, and Hendrik H. Heenen — Fritz-Haber-Institut der MPG, Berlin

Hexagonal GaN (h-GaN), theorized to be metastable when confined to only a few nanometers, stands out as a promising wide-bandgap semiconductor for next-generation nanoelectronics. Although early studies report that h-GaN can be synthesized using e.g. liquid metal catalysts, its definitive experimental identification is challenging. This difficulty arises from a structural ambiguity due to possible defects, multilayer-stacking variations, and competing polymorphs of h-GaN's characteristic honeycomb structure, as predicted by pioneering, yet simplified electronic-structure studies. In this work, we use density functional theory alongside large-scale atomistic simulations based on machine-learned interatomic potentials to re-assess the stability of h-GaN at finite temperatures and in the presence of a liquid metal substrate. We systematically investigate the structural and electronic properties of h-GaN, examining how they evolve with layer thickness and possible structural variations. Furthermore, we analyze its thermodynamic competition with bulk wurtzite GaN and alternative thin-film polymorphs, including a previously suggested haeckelite phase. Our results reveal that h-GaN exists within a delicate stability window. Based on these insights, we propose key signatures to guide experimental detection and outline whether h-GaN may become synthesizable as a feasible 2D semiconductor.

DS 14.2 Wed 15:15 REC/C213

Superconducting and dielectric properties of monolayer α-$TaSi_2N_4$ — •Timon Mosko[1] and Martin Gmitra[1,2] — [1]Institute of Physics, Pavol Jozef Safarik University in Kosice, Park Angelinum 9, 04001 Kosice, Slovakia — [2]Institute of Experimental Physics, Slovak Academy of Sciences, Watsonova 47, 04001 Kosice, Slovakia

The monolayer α-$TaSi_2N_4$ belongs to the recently discovered MA_2Z_4 family of two-dimensional intercalated materials, exhibiting wide range of physical properties, including semiconducting, metallic, topological, and superconducting behavior. Members of this group, such as $MoSi_2N_4$, WSi_2N_4 have already been successfully synthesized, highlighting the structural and electronic tunability of the inspected group of materials. We investigated the superconducting and dielectric properties of monolayer α-$TaSi_2N_4$ using a combination of ab initio and effective model approaches. The phonon-mediated superconductivity is examined through first-principles calculations, an effective tight-binding Hamiltonian in Wannier basis and further analyzed within the Migda-Eliashberg theory of superconductivity. Our results reveal that α-$TaSi_2N_4$ is an anisotropic two-band superconductor. Additionally, we study the dielectric response via electric susceptibility using linear response theory within the RPA, combining Green's function formalism with tight-binding modeling.

This work was supported by the Slovak Academy of Sciences project IMPULZ IM-2021-42, and by the Ministry of Education, Research, Develop-

ment and Youth of the Slovak Republic, provided under Grant No. VEGA 1/0104/25.

DS 14.3 Wed 15:30 REC/C213

Probing the Quantum Spin Hall State in Atomic Monolayers via NanoARPES — •Cedric Schmitt[1,2], Lukas Gehrig[1,2], Kilian Strauss[1,2], Jonas Erhardt[1,2], Matthew Watson[3], Jörg Schäfer[1,2], Simon Moser[1,2,4], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Universität Würzburg — [2]Würzburg-Dresden Cluster of Excellence ct.qmat — [3]Diamond Light Source, UK — [4]AG Oberflächen, Ruhr-Universität Bochum

Our recently discovered quantum spin Hall insulator indenene [1], a triangular monolayer of indium on SiC(0001), exhibits a 120 meV gap and monodomain growth on the μm scale. To verify its topological nature, we use circular dichroism in ARPES as a bulk-sensitive probe of orbital angular momentum (OAM) linked to its Berry curvature [2]. Due to SiC's stepped morphology, stacking-dependent OAM cancellation complicates microARPES. We overcome this challenge using nanoARPES with sub-600 nm resolution, resolving OAM asymmetry at individual terraces of SiC. Our study establishes dichroism as a robust spectroscopic tool for topological classification within a single SiC terrace.

[1] M. Bauernfeind et al. Nat. Commun. 12, 5396 (2021)
[2] J. Erhardt et al. Phys. Rev. Lett. 132, 196401 (2024)

DS 14.4 Wed 15:45 REC/C213

Physical Properties of $Ti_3C_2Cl_2$ MXenes — •Moritz Vanselow[1], Maksim Riabov[2], Thierry Ouisse[2], Hanna Pazniak[2], and Ulf Wiedwald[1] — [1]University of Duisburg-Essen and Center for Nanointegration Duisburg-Essen — [2]Université Grenoble Alpes, CNRS, Grenoble INP, LMGP, France

Hydrophobic $Ti_3C_2Cl_2$ MXenes are synthesized by Lewis acid molten-salt etching of $Ti_3C_2Cl_2$ followed by delamination process[1] and subsequently deposited from acetonitrile suspension ($\sim$ 0.1 mg/mL) on Si(100)/SiO_2 substrates. Using in-situ mass spectrometry and Auger electron spectroscopy in ultrahigh vacuum, we show that $Ti_3C_2Cl_2$ exhibits enhanced thermal robustness up to 900°C as compared to conventional mixed-terminated $Ti_3C_2T_x$ MXenes with T_x = −F, = O, and −OH. Complementary ex situ XRD and XPS confirm the absence of intercalated water and uniform −Cl terminations, resulting in sharp and intense (00l) peaks with c = 2.223 ± 0.015 nm and reflecting its high degree of structural order. Low-temperature specific heat measurements reveal distinct phonon signatures expected for the two-dimensional $Ti_3C_2Cl_2$. We determined the Debye temperature to 548 K in a temperature interval 20–50 K consistent with DFT model calculations[2] and a Sommerfeld constant of γ = 19.2 mJ mol^{-1} K^{-2}. This work is supported by ANR-23-CE09-0031-01 and DFG ID 530103526.

[1] T. Zhang et al., Chem. Mater. 36, 1998 (2024). [2] M. Riabov, M. Vanselow, et al., npj 2D Materials & Applications 2025, accepted

DS 14.5 Wed 16:00 REC/C213

Phase field crystal model of out-of-plane deformations in thin crystalline sheets induced by thermal expansion — •Emma Radice[1], Marco Salvalaglio[1,2], and Axel Voigt[1] — [1]Institut für Wissenschaftliches Rechnen, Technische Universität Dresden, Dresden, Germany — [2]Dresden Center for Computational Materials Science (DCMS), TU Dresden, Dresden, Germany

Thin, flexible crystalline sheets exhibit unique elastic properties due to their ability to undergo out-of-plane deformations.Understanding this behavior requires a description that couples in-plane elasticity, out-of-plane bending and the presence of defects. We develop a mesoscale description for these systems by extending the Phase-Field Crystal (PFC) model. PFC model describes crystal structures at diffusive timescales through a periodic, microscopic density field and it allows one to incorporate both elasticity and topological defects into a continuum description. Our extension permits a spatially varying equilibrium lattice spacing, enabling the representation of localized lattice eigenstrain to mimick thermal effects or lattice mismatch in heterostructures. We validate the extended model against analytical predictions from the Föppl von Kármán equations for uniaxial compression and from Eshelby's inclusion problem. Using this validated framework, we then study how locally induced compressive stresses drive out-of-plane deformation (buckling) in the sheets. Our approach, implemented via a Fourier pseudo-spectral method, exploits the PFC model's natural ability to capture the complex, coupled interactions among elasticity, out-of-plane bending and defect dynamics.

15 min. break

DS 14.6 Wed 16:30 REC/C213

Magnetotransport in Z-Folded ABC-Stacked Trilayer Graphene Structures — •Maximilian Mischke, Lina Bockhorn, Sofiya Lazareva, and Rolf Haug — Institut für Festkörperphysik, Leibniz Universität Hannover

Folded graphene (multi)layers promise to contain rich and interesting physics [1-3], so we produced a sample to investigate the influence of such a fold on magnetotransport properties of graphene. The measurements were carried out in a 4He cryostate at 1.4 K while the samples' carrier concentration was controlled via a global backgate. The sample itself consists of a z-folded ABC-trilayer graphene partially encapsulated in hBN with electrical contacts that allow for measurements in the unfolded region as well as through the fold. We observed filling factors that are unexpected for ABC-trilayer graphene. The untypical transport behaviour can be explained by angle dependend interlayer coupling and screening effects in the z-fold.

[1] S. J. Hong et al, Phys Rev B 105, 205404 (2022)
[2] H. Schmidt et al, Nature Communications 5(1), 5742 (2014)
[3] Y. Liu et al, Phys Rev B 92, 235438 (2015)

DS 14.7 Wed 16:45 REC/C213

Quantum dots in proximitized BLG/TMD heterostructures — •Ching-Hung Chiu and Angelika Knothe — Institut für Theoretische Physik, Universität Regensburg, 93053 Regensburg, Germany

Bilayer graphene (BLG) has attracted attention recently due to the possibility of inducing layer-selective Spin-orbit coupling (SOC) by proximitizing with transition metal dichalcogenides (TMDs) [1,2]. Simultaneously, the gate-tunable band gap in BLG enables electrostatic confinement of charge carriers into gate-defined quantum point contacts and quantum dots [3,4]. Here, we theoretically investigate the interplay of proximity effects and confinement by studying confined quantum states in proximitized BLG/TMD quantum dots. We calculate the states' properties, such as their splittings and spin polarisation, as a function of SOC coupling parameters and the dot's size and shape. Our studies go alongside experimental realisations of confinement in BLG/TMD heterostructures [5,6] and pave the way for using and controlling the dot's spin and valley states as qubits.

[1] K. Zollner and J. Fabian, Phys. Rev. B 104, 075126 (2021)
[2] A. M. Seiler et al., 2025 2D Mater. 12 035009
[3] H. Overweg et al,, Phys. Rev. Lett. 121, 257702 (2018)
[4] S. Möller et al., Phys. Rev. Lett. 127, 256802 (2021)
[5] J. D. Gerber et al., Nano Lett. 2025, 25, 33, 12480-12486
[6] H. Dulisch et al., Nano Lett. 2025, 25, 26, 10549-10555

DS 14.8 Wed 17:00 REC/C213

Influence of Polymethyl Methacrylate molecular weight on Graphene transfer and its intrinsic properties — •Monika Choudhary[1], Rasuole Lukose[1], Moriom Akter[1], Christian Wenger[1,2], and Mindaugas Lukosius[1] — [1]Leibniz-Institut für Innovative Mikroelektronik (IHP), Frankfurt Oder, Germany — [2]Semiconductor Materials, BTU Cottbus-Senftenberg, Cottbus, Germany

Polymethyl methacrylate (PMMA)-assisted wet transfer is widely used for integrating large-scale graphene grown on Ge(100)/Si substrates via chemical vapor deposition onto insulating SiO2/Si substrates[1,2]. However, the influence of PMMA molecular weight (MW) on properties of transferred graphene is insufficiently quantified. To address this, we investigate graphene transferred using low (50K), medium (600K), and high (950K) MW PMMA to isolate how polymer chain length governs film integrity and contamination. Characterization by atomic force microscopy (AFM), and spatially resolved X-ray photoelectron spectroscopy (XPS) reveals reduced contamination and smoother topography for graphene with 600K transfers. Additionally, micro-Raman spectroscopy demonstrates strain-free graphene with reduced doping and a 2D peak full width at half maximum (FWHM) of 35.53 cm-1 consistent with as-grown values. 1. Akhtar F., et al. ACS Appl. Mater. Interfaces 15 (2023). 2. Lukose R., et al. Scientific Reports 11 (2021). Acknowledgement: This research was funded by the European Union*s Horizon Europe research and innovation programme under grant agreement No 101120938 (GATEPOST).

DS 14.9 Wed 17:15 REC/C213

High-performance graphene field-effect transistors on cyclic olefin copolymer substrates for advanced sensor applications — •Hamid Reza Rasouli[1], Begimai Adilbekova[1], Ghazaleh Eshaghi[1], Axel Printschler[1], David Kaiser[1], Marco Reinhard[2], Alexander Rolapp[2], Tom Reinhold[2], Uwe Hübner[3], Michael Meister[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]IMMS Institut für Mikroelektronik- und Mechatronik-Systeme gemeinnützige GmbH (IMMS GmbH), 99099 Erfurt, Germany — [3]Leibniz Institute of Photonic Technology, Albert-Einstein-Straße 9, 07745 Jena, Germany

While graphene field-effect transistors (GFETs) are highly attractive for liquid-phase sensing, their performance on SiO2/Si substrates is compromised by oxide-induced charge trapping, leading to pronounced hysteresis and reduced stability. We present arrays of GFETs microfabricated on cyclic olefin copolymer (COC) substrates, which passivate SiO2 providing a low-trap and chemically inert platform in combination with flatness. GFET devices on COC demonstrate remarkably improved Dirac point stability, negligible hysteresis even in low-ionic strength buffers, and reproducibility across the arrays. For their functionalization, we employ an ultrathin carbon nanomembrane (CNM) that enables robust immobilization of various capture molecules while preserving graphene's transport properties. The CNM/GFET/COC architecture provides stable liquid-phase operation highlighting its strong potential for scalable and advanced sensor applications.

DS 15: Focus Session: Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects II (joint session TT/DS/MA)

Time: Thursday 9:30–12:30 Location: HSZ/0003

See TT 69 for details of this session.

DS 16: Thin Film Application

Time: Thursday 9:30–12:30 Location: REC/C213

DS 16.1 Thu 9:30 REC/C213

An on-chip heating platform for localized thin-film repair, non-equilibrium microstructures, and phase control — •Nensi Toncich, Nerea Abando Beldarrain, Jacopo Simone Crippa, Henning Galinski, and Ralph Spolenak — Laboratory for Nanometallurgy, Department of Materials, ETH Zürich, Switzerland

Localized on-chip heat generation and rapid thermal quenching is critical for systematic probing of phase transitions of nanofabricated systems, tailoring non-equilibrium microstructures and localized thin-film repair. Here we introduce a reactive multilayer [1] based on-chip heating platform that enables temperatures above 1000 °C, millisecond-scale heating and self-quenching rates on the order of 10^5 °C s^{-1} while preventing chemical interdiffusion. Using a diffusion-resistant, thermally conductive barrier, this platform enables three distinct, reproducible outcomes across different material systems: (i) localized melting and reflow of Au to repair electrical discontinuities, (ii) controlled microstructural evolution of Au, transforming equiaxed grains into elongated, high-aspect-ratio structures that are difficult to achieve with conventional processing, and (iii) a monoclinic-to-tetragonal phase transformation in the ZrO_2, demonstrating precise, site-specific phase engineering.

By combining ultrafast, high-temperature thermal pulses with diffusion-stable barriers, this platform offers a unique strategy for precise, on-demand modification of thin films, with broad applications in electronics, functional coatings, and nanofabrication.

[1] Toncich N. et al., J. Appl. Phys. 137(17), 2025

DS 16.2 Thu 9:45 REC/C213

Enhanced resistive switching in hybrid perovskite-MoS2 memristors — •Georgios Chatzigiannakis[1,2], Anastasia Soultati[1], Spiros Gardelis[2], and Maria Vasilopoulou[1] — [1]INN, NCSR Demokritos, 15341 Athens, Greece — [2]Physics Department, National and Kapodistrian University of Athens, Panepistimiopolis Zografos, 15784 Athens, Greece

Memristors are emerging two-terminal devices with tunable resistance states and strong potential for next-generation non-volatile memory and neuromorphic computing. Their reversible switching between high- and low-resistance states (HRS/LRS), combined with non-volatile information retention, makes them attractive for energy-efficient data storage. Metal halide perovskites have recently gained interest in thin-film memristive technologies due to their low fabrication cost, solution processability, and rich ionic dynamics, while 2D TMDs such as MoS2 provide excellent interfacial properties that modulate charge transport and defect chemistry.

We demonstrate a hybrid perovskite memristor incorporating MoS2 nanosheets, exhibiting significantly enhanced electrical performance compared to pristine devices. The MoS*-integrated device achieves endurance up to 200 switching cycles, stable retention beyond 12 000 s, and a large memory window (HRS:LRS ~100). In contrast, the pristine device shows only ~25 cycles and a window below 50. These results highlight the crucial role of TMD:perovskite interfaces in stabilizing ion-migration pathways and improving resistive-switching reliability in hybrid thin-film memristors.

DS 16.3 Thu 10:00 REC/C213

Resistive Sensor for in situ electrical monitoring during atomic layer deposition — •Lucas Rave, Colin Schormann, Stefanie Haugg, Kristian Deneke, Jun Peng, Robert Blick, and Robert Zierold — Center for Hybrid Nanostructures, University of Hamburg, Germany

Atomic layer deposition (ALD) provides exceptional coating conformality with sub-nanometer resolution, driving the new semiconductor technology node processes. Conventional in situ diagnostics, such as spectroscopic ellipsometry and quartz crystal microbalances, focus on mass and optical morphology information during deposition. However, rich electrical information remains limited. To address this, we developed an electrical in situ monitoring detector capable of resolving resistance changes for individual precursor and purge pulses. This detector contains custom-patterned titanium electrodes on Si/SiO_2 substrates, whose resistance evolution directly reflects cycle-resolved ALD surface reactions. Using this approach, we probed the deposition process for oxides, including ZnO, Al-doped ZnO (AZO), and TiO_2, capturing characteristic signatures of nucleation delays, self-limiting ligand exchange, and dopant-induced conductivity changes. Our method reveals how different precursor chemistries manifest in distinct electrical transients and provides a quantitative link between surface reaction kinetics and film evolution. The resistance-based in situ sensing offers a practical, compact, and integrable diagnostic tool for understanding and optimizing ALD processes, enabling improved control over thin-film quality in micro- and nanofabrication.

DS 16.4 Thu 10:15 REC/C213

Molecular insights into the mechanical and dynamical properties of mechanically interlocked polymer thin films — •Yang Wang[1], Andrea Giuntoli[1], and Xuzhou Yan[2] — [1]Zernike Institute for Advanced Materials, University of Groningen, 9747 AG Groningen, Netherlands; — [2]State Key Laboratory of Synergistic Chem-Bio Synthesis, Frontiers Science Center for Transformative Molecules, School of Chemistry and Chemical Engineering, Shanghai Jiao Tong University, Shanghai 200240, P. R. China;

Mechanically interlocked networks (MINs) comprise molecular components connected by mechanical bonds, introducing topological constraints that alter deformation pathways. Coarse-grained molecular dynamics simulations are used to investigate substrate-supported and free-standing MIN thin films based on [c2]daisy chain architectures, with systematic variation of extension distance, cross-linking degree, interfacial cohesive strength, and strain rate. Strongly attractive substrates induce pronounced dynamic confinement, whereas weak adhesion leads to enhanced, free-surface-like mobility. Rings exhibit slower dynamics than axle chains, whose mobility is governed by proximity to binding sites. Pull-out and biaxial deformation simulations reveal a three-stage ring-sliding mechanism that suppresses excessive bond scission, maintains network connectivity at large strains, and delays macroscopic failure, thereby enhancing toughness and energy dissipation. These results provide molecular-level insight into MIN thin film mechanics and inform the design of adaptive, energy-dissipating polymer materials.

15 min. break

DS 16.5 Thu 10:45 REC/C213

A Pathway Towards All-Optical Light-Propagation Switching — •Jakob Lindenthal, Frithjof Pietsch, Markas Sudzius, Johannes Benduhn, and Karl Leo — TU Dresden, Institut für Angewandte Physik, Nöthnitzer Str. 61, 01187 Dresden

Dynamic switching of the light propagation is a key enabler for integrated nanophotonic circuits. Optical gratings are a widely used, versatile component for coupling light into and out of waveguides. However, their diffraction efficiency is generally set and limited well below unity by static design and process parameters such as etch depths or geometric profile quality. We experimentally demonstrate the use of a dielectric-mirror cavity for enhancing the diffraction efficiency of grating couplers beyond these intrinsic limits. Using a second counterpropagating input beam achieves near-perfect dynamic control of the coupling amplitude. The experiments are backed by analytical and numerical modeling of the cavity-enhanced diffraction efficiency and the interaction of light waves in optical-gratings multiport devices. These findings extend the concept of coherent perfect absorption (CPA) from thin absorbing layers to diffractive structures, providing an all-optical propagation switching mechanism for efficient signal input and control in compact photonic circuits and nano-optic systems.

DS 16.6 Thu 11:00 REC/C213

Investigation of Temperature-Dependent Loss Mechanisms in Tantalum and Niobium Thin-Film Coplanar-Waveguide Resonators — •Philip Schneider[1], Moritz Singer[1], Harsh Gupta[1], Benedikt Schoof[1], and Marc Tornow[1,2] — [1]TU Munich, Garching, Germany — [2]Fraunhofer EMFT, Munich, Germany

Superconducting qubits can enable scalable quantum computing. Niobium (Nb) is widely used as the base superconductor, but tantalum (Ta) can improve performance by hosting fewer two-level system (TLS) losses, especially in its native oxide. We sputter-deposited Ta and Nb thin films on silicon and studied three stacks: pure Nb, Nb with a thin Ta cap, and Ta on a thin Nb seed layer, realizing distinct interface scenarios. The thin films were characterized by resistivity,

critical temperature, RRR and X-ray diffraction. Coplanar waveguide resonators were fabricated from the ~ 200 nm films to determine their internal quality factor (Q_i) in the few GHz regime. Temperature- and power-dependent measurements (100-1700 mK, -80 to -160 dBm) were fitted with a combined TLS-quasiparticle loss model to analyze loss-channels. To probe the effect of native oxide at the metal-air interfaces, the resonators were re-measured post four weeks of air exposure. In the single-photon regime at 100 mK, the average Q_i changes from 1.38×10^6 (BOE) to 1.19×10^6 (native oxide) for Nb, from 1.58×10^6 to 1.11×10^6 for Ta-capped Nb, and from 1.07×10^6 to 1.20×10^6 for Ta on an Nb seed layer. Thus, while all stacks provide Q_i in the 10^6 range, Nb-based devices degrade post oxidation, whereas the Ta dominated film remains robust and even slightly improves.

DS 16.7 Thu 11:15 REC/C213

Gallium phosphide on insulator for integrated quantum photonics — •Tobias Bucher[1], Otto Arnold[1,2,3], Katsuya Tanaka[1,2,3,4], Muyi Yang[1,2,3,4], Carsten Ronning[1], and Isabelle Staude[1,2,3,4] — [1]Institute of Solid-State Physics, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Abbe Center of Photonics, Friedrich Schiller University Jena, 07745 Jena, Germany — [3]Institute of Applied Physics, Friedrich Schiller University Jena, 07745 Jena, Germany — [4]Max Planck School of Photonics, Germany

Gallium phosphide (GaP) emerges as a promising material for quantum nanophotonics due to its high refractive index with low absorption in the visible, combined with a strong second-order nonlinear response and the absence of linear birefringence. Growing high-quality, single-crystalline GaP thin films on low-index substrates, however, faces challenges due to lattice and thermal mismatch, and process complexity in common epitaxial methods. Here, we demonstrate ion slicing of GaP thin films and anodic bonding onto low-index glass substrates. We fabricate GaP thin films from (100) and (110) bulk crystals with thicknesses of 760 ± 40nm. Structural and optical characterisation is used to optimise the implantation and bonding conditions with the goal of achieving high-optical quality and low absorption suitable for nanophotonic applications.

DS 16.8 Thu 11:30 REC/C213

Enhancement of photoluminescence of Er3+ ions by Mie-resonant silicon nitride metasurfaces — •Fengkai Wei[1,2], Carsten Ronning[1], Duk-Yong Choi[2], Xinru Ji[3], and Tobias Kippenberg[3] — [1]Institut für Festkörperphysik, Friedrich Schiller University Jena, Germany — [2]Research School of Physics, Australian National University, Australia — [3]Institute of Physics, Swiss Fed- eral Institute of Technology Lausanne (EPFL), CH-1015 Lausanne, Switzerland

Mie-resonant high-index dielectric nanoparticles and metasurfaces have been suggested as a viable platform for enhancing both electric and magnetic dipole transitions of fluorescent emitters. While previous work has demonstrated the enhancement of magnetic dipolar transitions from Eu3+ ions using silicon nanocylinders, this approach was limited by silicon's strong absorption at the Eu3+ emission wavelength in visible range. Erbium features a characteristic infrared emission wavelength of 1550nm, which is widely used in telecommunication. It makes Er a good candidate of emitters in metasurface for infrared applications. This study explores the enhancement of Er3+ ions using dielectric metasurfaces composed of Mie-resonant silicon nitride metasurface. Er3+ ions were introduced into the metasurface via ion implantation. Strong room-temperature photoluminescence (PL) was only observed after annealing, which activates the ions.Maximum PL enhancement occurred at a nanocylinder radius of ~410 nm, aligning with simulations. This study demonstrated a significant ~40-fold PL enhancement on metasurface over a planar reference.

15 min. break

DS 16.9 Thu 12:00 REC/C213

Use of hybrid electrochromic devices for dynamic solar control in buildings — •Eleftheria Merkoulidi and George Syrrokostas — Solar Energy Laboratory, Department of Physics, University of Patras, Rion, Greece

Nowadays, the three main sectors that consume a lot of primary energy are: transport, industry, and buildings. Especially in the EU during 2023, buildings were responsible for 40% of total energy consumption, for approximately 50% of all-natural gas use, and a large portion of this energy (80%) is dedicated specifically to heating, cooling, and hot water supply for occupants. Therefore, improving the energy efficiency of buildings is critical. One effective way to improve energy efficiency is by controlling the significant energy losses (up to 60%) that occur through windows. These losses are caused by heat transfer mechanisms (conduction, convection, and radiation), as well as air leakage. A promising technological solution involves the use of adaptive chromogenic windows, such as electrochromic smart windows (ECWs). They can improve the energy efficiency of a building by modulating the sunlight and solar heat entering a building in real time, by changing their appearance (from transparent to opaque), under an applied electric field. In the present study, a way to improve their optical performance is investigated, by using a cobalt based redox electrolyte as a novel alternative to other redox couples used so far, with promising results.

DS 16.10 Thu 12:15 REC/C213

Influence of Crystal Orientation on the Oxygen Evolution Reaction in La_2NiMnO_6 Films — •Felix Tegtmeyer[1], Pia Henning[2], Shagun Thakur[2], Tobias Meyer[2], Ulrich Ross[3], Vasily Moshnyaga[4], and Jasnamol Palakkal[2] — [1]Department of Ultrafast Dynamics, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]Institute of Materials Physics, University of Göttingen, Germany — [3]4th Physical Institute, University of Göttingen, Germany — [4]1st Institute of Physics, University of Göttingen, Germany

Double perovskites such as La_2NiMnO_6 (LNMO) promise applications for catalysis in energy storage and conversion. However, investigations of the oxygen evolution reaction (OER) in LNMO remain limited to nanoparticles and powders while the effects of crystal orientation remain elusive. In this work, we study monocrystalline LNMO thin film catalysts grown by metalorganic aerosol deposition at ambient air. By controlling the facet which is in contact with the electrolyte, the influence of crystal orientation is identified. We found that the activity of LNMO films with (100) crystal orientation is enhanced by one order of magnitude compared to (111) oriented films. We attribute this to the availability of both Ni and Mn active sites for the (100) surface. Moreover, an overall enhancement of the activity is identified for higher thicknesses. In long-term chronoamperometry measurements, the LNMO film retains a high activity and excellent bulk stability while the degradation is limited to a surface-near region.

DS 17: Focus Session: High-Temperature Superconductivity in Hydride Materials at High Pressures (joint session TT/DS)

Superconductors with record transition temperatures up to 250 K have been discovered and confirmed in hydride materials at high pressures over the last decade, enabled by major advances in both computational and experimental approaches. Density functional theory, combined with structure search algorithms and machine learning methods, enables high-throughput predictions of novel high-pressure phases. Ab initio microscopic theories, including Eliashberg theory and superconducting density functional theory, successfully predict transition temperatures of identified phases, with several predictions now confirmed experimentally. The synthesis of novel hydrides has revealed the importance of including hydrogen quantum fluctuations in theoretical predictions. Experimentally, advances in high-pressure synthesis techniques have enabled the preparation of novel hydride phases, while electrical transport measurements, tunneling spectroscopy, and magnetic studies have established a strong body of evidence for superconductivity by probing zero resistance, the superconducting gap, and magnetic response. This focus session will emphasize these breakthroughs, highlight ongoing challenges in both experiment and computation, and provide an outlook for finding high-temperature superconductors at lower and ambient pressures.

Coordinators: Philipp Gegenwart (Universität Augsburg), Matthias Vojta (TU Dresden)

Time: Thursday 15:00–18:45 Location: HSZ/0003

See TT 80 for details of this session.

DS 18: Spins in Molecular Systems

Time: Thursday 15:00–17:30 Location: REC/C213

DS 18.1 Thu 15:00 REC/C213

The forgotten sister of the CISS effect: spin polarization induced via proximity of adsorbed chiral molecules — •Franziska Schölzel[1], Aybüke Gülkaya[2], Dominik Hornig[1], Rico Ehrler[1], Lokesh Rasabathina[1], Aleksandr Kazimir[3], Christina Lamers[3], Olav Hellwig[1], Michael Mehring[1], Shuxia Tao[2], and Georgeta Salvan[1] — [1]Chemnitz University of Technology, Chemnitz, Germany — [2]Eindhoven University of Technology, Eindhoven, the Netherlands — [3]Leipzig University, Leipzig, Germany

Within the past years a new research field around chirality induced spin selectivity (CISS) has emerged and gains increasing attention. The central part is often played by complex chiral or helical molecules; ferromagnetic, gold capped, sometimes structured substrates and electrical transport measurements [1]. An aspect most often forgotten within this framework is the effects static equivalent [2]. We observed the Spin Polarization Induced via the Proximity of Adsorbed Chiral Molecules (SPIPAC) effect in nickel thin films for various chiral molecules. This study probes the resulting magneto-optical signal of the Ni substrate using Circular Dichroism spectroscopy. Furthermore, the impact of film thickness of the substrate, molecule density on the surface and the chirality of the molecules is explored.

[1] B. Bloom et al., Chem. Rev. 124, 4, 1950-1991 (2024)
[2] O. Ben Dor et al., Nat Commun 8, 14567 (2017)

DS 18.2 Thu 15:15 REC/C213

Understanding interface-controlled CISS-MR (magnetoresistance) via electric dipole inversion using ambient STM — •T. N. Ha Nguyen[1], Lech Tomasz Baczewski[2], Aleksandr Kazimir[3], Christina Lamers[3], and Christoph Tegenkamp[1] — [1]Analysis of Solid Surfaces, Nanostructures and Quantum Materials, Technische Universität Chemnitz, Germany — [2]Reichenhainerstr., 70 — [3]Institute for Drug Discovery, Medical Faculty University of Leipzig, Leipzig, Germany

Recent studies have highlighted the significant influence of electric dipole moment orientation in chiral molecules on spin polarization. When chiral molecules with strong dipole moments adsorb onto a surface, their orientation breaks the interfacial symmetry, leading to enhanced spin-polarized currents. Using scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS), we measured spin-polarized electron transport through polyalanine molecules, which possess substantial dipole moments. Notably, inverting the dipole moment while maintaining the molecule*s chirality results in a reversal of the chiral-induced spin selectivity magnetoresistance (CISS-MR). Our findings not only highlight the crucial role of electric dipole moments in chiral molecules but also provide insights into the CISS mechanism, particularly regarding the interface effect.

DS 18.3 Thu 15:30 REC/C213

Effect of adsorbed chiral molecules on the magnetic properties of skyrmion-hosting multilayers — •Mariam Hassan[1,2], Ivan Saldatov[3], Lokesh Rasabathina[4], Franziska Schölzel[1,2], D.R.T Zahn[1,2], Olav Hallwig[1,4], and Georgeta Salvan[1,2] — [1]Research Center for Materials, MAIN, Chemnitz University of Technology, Germany — [2]Semiconductor Physics, Institute of Physics, Chemnitz University of Technology, Germany — [3]Institute for Metallic Materials, IFW, Dresden — [4]Functional Magnetic Materials, Institute of Physics, Chemnitz University of Technology, Germany

Chirality-induced spin selectivity (CISS) and Magnetism Induced by Proximity of Adsorbed Chiral molecules (MIPAC) effects are phenomena that caught significant interests over the last few decades because of the large spin polarizations generated by organic molecules and the alteration of the surface's magnetism upon the adsorption of chiral molecules respectively [1,2]. On the other hand, magnetic skyrmions have emerged as a promising path for next-generation information storage and processing technologies. Thus, tuning skyrmion properties is of increasing interest for application in future spintronic devices. In light of the CISS and MIPAC effects, the use of chiral molecules might represent an attractive approach to address the challenge of tuning skyrmion properties [3]. In this work, we aim to investigate how adsorbed chiral molecules interact with magnetic skyrmions that are stabilized in [Co/Ni]N ferromagnetic multilayers with PMA. We observe that the adsorbed chiral molecules locally change the magnetic properties of the film, affecting the density of skyrmion nucleation sites.

DS 18.4 Thu 15:45 REC/C213

Self-Assembly of Helical Molecular Monolayers Using a Coarse-Grained Chiral Patchy Model — •Hadis Ghodrati Saeini[1], Faezeh Shabani[1], Sibylle Gemming[1], Christoph Tegenkamp[1], Florian Günther[2], and Jeffrey Kelling[1,3] — [1]Technische Universität Chemnitz, Chemnitz, Germany — [2]São Paulo State University, Rio Claro, Brazil — [3]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

The Chiral-Induced Spin Selectivity (CISS) effect makes helical molecules promising for spintronic applications, yet their surface self-assembly remains poorly understood due to experimental and computational constraints. Although Density-Functional Tight-Binding (DFTB) potentials accurately describe polyalanine (PA) α-helix SAMs, their high computational cost limits large-scale and kinetic investigations.

We introduce a coarse-grained chiral patchy model parameterized to fit the PA-specific DFTB potential, capturing its essential chiral symmetry and interaction features while remaining computationally efficient. Validation is achieved by comparing low-energy configurations obtained from annealing Monte Carlo simulations using the DFTB-based potential with dynamic pathways from coarse-grained molecular dynamics. Dynamic simulations made feasible by this model successfully reproduce the final assembled morphologies and allow explorations of potential metastable states, demonstrating its reliability and versatility for studying the kinetics of helical molecular self-assembly.

DS 18.5 Thu 16:00 REC/C213

Exploring the Origins of Helical Bundle Stability and Their Role in the CISS Effect — •Faezeh Shabani[1], Sibylle Gemming[1], Georg Kuenze[2], Paul Kluge[2], and Florian Guenther[3] — [1]Technische Universität Chemnitz, Chemnitz, Germany — [2]Universität Leipzig, Leipzig, Germany — [3]Instituto de Geociências e Ciências Exatas, Universidade Estadual Paulista, Rio Claro, Brazil

Helical bundles provide a highly regular and tunable chiral environment, making them ideal model systems for investigating the principles of the CISS effect and exploring possibilities for generating electronic hyperpolarization through (super)helical geometries. Beyond their relevance to chiral-induced spin selectivity, helix bundles also play important roles in nature: they consist of two or more α-helices supercoiled around a central axis and function as essential structural motifs in many biological systems. In this talk, we explore these characteristics using DFTB+ calculations. This computational approach allows us to analyze the energetic origins of specific bundling motifs, assess the role of dispersion interactions, and ultimately understand why certain helix bundle architectures are favored in nature.

15 min. break

DS 18.6 Thu 16:30 REC/C213

Unwinding the Helicity-Driven Electronic Properties in Polyproline I and II Chains — •Saba Arshad, Faezeh Shabani, and Sibylle Gemming — TU Chemnitz, Chemnitz, Germany

Polyproline is a polypeptide that adopts two distinct helical conformations, polyproline I (PPI) and polyproline II (PPII), with identical primary sequence but markedly different helicities and structural behavior, providing a valuable platform for examining electronic properties and their potential impact on CISS (Chirality-Induced Spin Selectivity) effects. Here, we employed density-functional approaches for chains with different numbers of monomers to investigate how helical geometry influences the electronic properties of both conformers. Our results reveal significant differences in the HOMO-LUMO gap and density of states between PPI and PPII, with the gap consistently narrowing as additional monomers are incorporated. Dipole moments calculated for chains of increasing length display distinct scaling trends for PPI and PPII helices, highlighting how both chain length and topology govern emerging molecular electronic applications.

DS 18.7 Thu 16:45 REC/C213

Modelling spin particles in an infinite helical box — Alex Mureşan[1,2], Fabian Prasse[1], and •Sibylle Gemming[1] — [1]Institute of Physics, TU Chemnitz, Germany — [2]Faculty of Physics, Babes-Bolyai University, Cluj-Napoca, Romania

Calculating the electronic states of a quantum mechanical particle in a potential well with infinitely high walls is probably the most readily accessible, still analytically solvable textbook example of quantisation via spatial confinement. As such, it is an ideal starting point for including additional terms to the Hamiltonian in order to adapt the model to a specific experimental setting, e.g. by introducing multiple particles or external fields. Here we present an extension that assumes an externally given spatial modulation of the potential well with helical characteristics as boundary condition. We derive analytical solutions for the motion of classical, Newtonian particles on a helical path, for charged Schrödinger-type quantum particles in a one-dimensional helical confinement, and quantum-mechanical spin 1/2-particles in a helical spin-orbit-split environment, which is encountered in investigations of the chirality-induced spin selectivity effect. We show that the model extension steps successively refine the eigenspectra of the simplest case, and that the spin-orbit interaction term leads to an extra splitting within the helical confinement.

Invited Talk DS 18.8 Thu 17:00 REC/C213

Insights from Quantum Dynamics Simulations: From Molecules to Organic-Material Interfaces — •Frank Ortmann — Technical University of Munich, Munich, Germany

Understanding charge, exciton and spin dynamics in molecular systems is critical for advancing organic semiconductor-based technologies. We present insights from our work addressing distinct yet complementary aspects of these phenomena for organic-electronics materials. First, we explore charge-transfer dynamics in electron-phonon coupled model systems, identifying regimes such as polaron transport and transient localization, emphasizing their seamless transitions across vibrational modes and temperatures. Second, a comparative analysis of the Matrix Product State (MPS) and Multilayer Multiconfiguration Time-Dependent Hartree (MCTDH) methods demonstrates their efficacy in modeling non-adiabatic exciton dissociation, revealing specific sensitivities to electronic-vibrational entanglement in complex systems. Lastly, we introduce current work toward a general quantum mechanical treatment of spin transport in donor-acceptor systems. These works underline the theoretical advances in capturing the interplay of various degrees of freedom in molecular optoelectronics and spintronics.

DS 19: Members' Assembly

Time: Thursday 17:45–18:30 Location: REC/C213

All members of the Thin Films Division are invited to participate.

DS 20: Poster

Time: Thursday 18:30–20:30 Location: P2

DS 20.1 Thu 18:30 P2

Techno-Enviro-Economic Evaluation for Thin-film Solar Cells Integrated with Hybrid Renewable Energy System — •Tawfik Hussein — Mechanical Engineering Dep., National Research Centre (NRC), El Buhouth st.,Dokki, Cairo, Egypt

Thin-film solar cells (TFSC) have recently emerged as a transformative technology in renewable energy, offering advantages such as lightweight design, flexibility, and cost-effectiveness compared to conventional crystalline silicon photovoltaics. This study focuses on designing an optimal hybrid renewable energy system (HRES) that integrates TFSC to maximize the efficient use of renewable energy sources (RES). A proposed HRES, combining multiple RES with TFSC, was developed to supply reliable electricity to a scientific farm in Egypt, with full technical, environmental, and economic evaluation.

The research examines TFSC performance under diverse environmental conditions, highlighting their higher efficiency in low-light and high-temperature scenarios. System indicators including performance, net present cost, CO* emissions, and renewable fraction were analyzed. Results demonstrate that TFSC-based HRES delivers reliable, low-cost energy with notable environmental benefits. Compared to conventional systems, the proposed design achieves substantial reductions in both costs and carbon emissions, enhancing sustainability. These findings confirm TFSC as a promising solution for future renewable energy systems, addressing the increasing demand for affordable and eco-friendly power generation.

DS 20.2 Thu 18:30 P2

Structural and electronic characterization of sputtered MoSe2 and WSe2 thin films on ITO substrates using synchrotron-based XAFS/XRF techniques — •Sabit Horoz[1,2], Emre Timuçin Tabaru[1], Latif Ullah Khan[3], Messaoud Harfouche[3], and Ali Karatutlu[1,4] — [1]Sivas University of Science and Technology, Sivas, Türkiye — [2]Sivas Cumhuriyet University Nanophotonics Application and Research Center-CÜNAM, 58140 Sivas, Turkey — [3]SESAME, Allan, Jordan — [4]Bilkent University Ankara, Türkiye

Two-dimensional transition metal dichalcogenides (TMDs) such as molybdenum diselenide (MoSe2) and tungsten diselenide (WSe2) exhibit remarkable optoelectronic and catalytic properties. In this work, thin films of MoSe2 and WSe2 were fabricated on indium-tin oxide (ITO) substrates using a sputtering technique and analyzed at the SESAME Synchrotron facility through X-ray Absorption Fine Structure (XAFS) and X-ray Fluorescence (XRF) spectroscopy. XAFS results at the W L3- and Mo K-edges confirmed well-ordered W-Se and Mo-Se bonds, demonstrating crystalline TMD structures. Upon annealing up to 170 °C in air, partial oxidation led to the formation of WO3 and MoO3 phases, accompanied by a visible color change from silver to transparent. Complementary Raman, UV-VIS-NIR, and ellipsometric analyses supported these findings.

DS 20.3 Thu 18:30 P2

Investigation of a hygrosensitive polymer coating for colorimetric humidity sensing — •Ketrin Pavlova[1], Katerina Lazarova[1], Darinka Christova[2], Martina Docheva[1], and Tsvetanka Babeva[1] — [1]Institute of Optical Materials and Technologies "Acad. J. Malinowski" Bulgarian Academy of Sciences, Sofia, Bulgaria — [2]Institute of Polymers, Bulgarian Academy of Sciences, Sofia, Bulgaria

A thin coatings of newly synthesized branched copolymers of poly(vinyl alcohol) comprising graft poly(N,N-dimethylacrylamide) with different side chains were studied as sensitive media for environmental changes of the relative humidity (RH). Spin-coating method was applied to deposit the thin films of both copolymers on Si-substrates, followed by temperature heating. Reflectance spectra of the samples were measured and then used to determine coating's thickness and optical constants. Sensing abilities of the coatings when exposed to different humidity level in range 5-95 RH% were examined and parameters such as hysteresis H and thickness change Δd were calculated. Possible application of the coatings for colorimetric detection is demonstrated.

DS 20.4 Thu 18:30 P2

Sputtered germanium absorbers for building-integrated semi-transparent photovoltaics — •Nico Ruskaup[1], Kai Gehrke[1], Stephan Heise[2], and Martin Vehse[1] — [1]Institut für Vernetzte Energiesysteme, Deutsches Zentrum für Luft- und Raumfahrt e. V., Carl-von-Ossietzky-Straße 15, 26129 Oldenburg — [2]Institut für Solarforschung, Deutsches Zentrum für Luft- und Raumfahrt e. V., Carl-von-Ossietzky-Straße 15, 26129 Oldenburg

Architectural glass facades worldwide typically utilize solar-control coatings deposited in inline magnetron sputter coaters to prevent buildings from excess solar heating. To use the electricity-generating potential of these facades, we aim to enable the glass industry to integrate photovoltaic functionality into their glazing using existing production lines. This requires a semi-transparent, fully sputtered thin-film solar cell. As a first step, here we demonstrate sputtered ultrathin germanium absorber layers for semi-transparent solar cells. We compare their optoelectronic properties and their microstructure with established reference layers deposited by plasma-enhanced chemical vapor deposition (PECVD) and identify sputter-process conditions that yield germanium absorbers with PECVD-comparable properties suitable for device integration. We present a sputtered germanium layer built into a solar cell, which delivers a power conversion efficiency of 2.8%. These results demonstrate that sputtered germanium is a viable absorber for thin-film photovoltaics and represent an important step towards an industrially sputtered semi-transparent solar cell for window applications.

DS 20.5 Thu 18:30 P2

Enhanced Ferroelectric Behavior in NH4Cl-Doped SnO2/Perovskite Multilayer Memristors — •Katerina Maskanaki[1], Evangelos Evangelou[1], and Anastasia Soultati[2,3] — [1]Department of Physics, University of Ioannina, 45110 Ioannina, Greece — [2]Institute of Nanoscience and Nanotechnology (INN), National Center for Scientific Research Demokritos, 15341 Agia Paraskevi, Athens, Greece — [3]Department of Electrical & Computer Engineering, Hellenic Mediterranean University (HMU), Heraklion 71410, Crete, Greece

Perovskite-based materials have emerged as promising candidates for neuromorphic computing due to their diverse conduction mechanisms and tunable electronic properties. This study is focused on the development and characterization of multi-layered memristors with the structure ITO/SnO2:NH4Cl/RbCsMAFAPbI3/P3HT/Al. A reference device employing a pristine SnO2 layer was also fabricated to compare the memristive behavior to the modified devices incorporating an NH4Cl-doped SnO2 nanocomposite layer in various concentrations. All configurations exhibited stable memristive switching; however, the NH4Cl-modified devices demonstrated significantly enhanced ferroelectric behavior, achieving endurance over 200 switching cycles and robust data retention exceeding 10^3 s. The high reproducibility and scalability of these perovskite memristors highlight their strong potential for next-generation neuromorphic and memory applications.

DS 20.6 Thu 18:30 P2

How Matrix-Mediated Osmotic Forces Govern Spatio-Temporal Dynamics and Spreading in Two-Species Biofilms — •Anthony Pietz[1], Uwe Thiele[1], and Karin John[2] — [1]University Münster, Münster, Germany — [2]University Grenoble Alps, Grenoble, France

Biofilms are thin films of bacterial communities encased in a self-produced polymeric matrix that thrive on immersed or moist surfaces [1]. The matrix confers the biofilm mechanical resistance and drives an osmotic influx of nutrients rich water into the biofilm.

While the osmotic spreading of biofilms with only one species has been extensively studied, much less is known about how matrix-mediated osmotic forces influence the spatio-temporal organization and spreading dynamics in multispecies communities. Experiments on two-species mixtures of matrix producers / non-producers show that the latter becomes confined to the advancing biofilm edge [2].

We numerically investigate the dynamics of such a two-species biofilm where the matrix-producing species attractively interacts with the matrix. Our description supplements a thermodynamically consistent thin-film approach for a passive suspension by bioactive growth terms. We analyse the resulting spatio-temporal dynamics and identify conditions under which multispecies and monospecies biofilms develop.

[1] Wilking et al. Biofilms as complex fluids. MRS Bulletin 36: 385, 2013. [2] Yan et al. Extracellular-matrix-mediated osmotic pressure drives Vibrio cholerae biofilm expansion and cheater exclusion. Nature Communications 8: 327, 2017.

DS 20.7 Thu 18:30 P2

Coherent control in size selected semiconductor quantum dot thin films — •Victor Kärcher[1,2], Tobias Reiker[1], Pedro F. G. M. da Costa[3], Andrea S. S. de Camargo[4,5], and Helmut Zacharias[1] — [1]Center for Soft Nanoscience, University of Münster, 48149 Münster, Germany. — [2]Insititute of Physics, University of Münster, 48149 Münster, Germany. — [3]São Carlos Institute of Physics, University of São Paulo, São Carlos, SP 13566-590, Brazil. — [4]Federal Institute for Materials Research and Testing (BAM), 12489 Berlin, Germany. — [5]Friedrich-Schiller University Jena (FSU), 07743 Jena, Germany.

We introduce a novel technique for coherent control that employs resonant internally generated fields in CdTe quantum dot (QD) thin films at the L-point. The bulk band gap of CdTe at the L-point amounts to 3.6 eV, with the transition marked by strong Coulomb coupling. Third harmonic generation (λ = 343 nm, hν = 3.61 eV) for a fundamental wavelength of $\lambda = 1,030$ nm is used to control quantum interference of three-photon resonant paths between the valence and conduction bands. Different thicknesses of the CdTe QDs are used to manipulate the phase relationship between the external fundamental and the internally generated third harmonic, resulting in either suppression or strong enhancement of the resonant third harmonic, while the nonresonant components remain nearly constant. This development could pave the way for new quantum interference-based applications in ultrafast switching of nanophotonic devices.

DS 20.8 Thu 18:30 P2

Ion slicing of gallium phosphide — •Otto Arnold[1,2,3], Tobias Bucher[1], Katsuya Tanaka[1,2,3,4], Muyi Yang[1,2,3,4], Carsten Ronning[1], and Isabelle Staude[1,2,3,4] — [1]Institute of Solid-State Physics, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Abbe Center of Photonics, Friedrich Schiller University Jena, 07745 Jena, Germany — [3]Institute of Applied Physics, Friedrich Schiller University Jena, 07745 Jena, Germany — [4]Max Planck School of Photonics, Germany

Gallium phosphide (GaP) has unique non-linear and quantum optical properties, such as second harmonic generation and spontaneous parametric down-conversion. For integrated optics, preparing the single crystalline GaP on a low reflective index material would be useful, as the reflective index scales with the mode confinement of the enhanced near-field. So far, GaP thin films are grown epitaxially or with MOCVD, which are both expensive and complicated. An alternative approach is ion slicing, where a helium-irradiated GaP is bound to a borosilicate glass. We fabricated high quality GaP thin-film in (100) and (110) crystal orientation on glass, with a thickness of 760 (40) nm. Energy-dispersive X-ray spectroscopy (EDX) and Rutherford backscattering spectrometry (RBS) characterization of the fabricated thin-films allow us to further optimize the irradiation profile and bonding parameters towards best optical performance for further nanofabrication of resonant meta-surfaces operating in the visible and near-infrared.

DS 20.9 Thu 18:30 P2

Piezoelectric coatings on Fiber Bragg Gratings for electric field measurement — •Florian Schmidbauer and Jens Ebbecke — Technology Campus Teisnach Sensor Technology, Deggendorf Institute of Technology, 94244 Teisnach

Monitoring high-voltage systems is gaining increasing importance. Conventional sensors often rely on electrical components that exhibit cross-sensitivities and require electrical wiring, which can pose a source of interference in certain applications. In addition, the physical dimensions of sensor heads can limit their usability.

An alternative approach employs Fiber Bragg Gratings (FBGs) coated with piezoelectric materials. Through the piezoelectric effect, mechanical deformation of the piezoelectric layer induces strain in the FBG, resulting in a measurable shift of its resonance wavelength. This type of sensor offers several advantages, including electrical passivity, a compact form factor, and the capability for remote and rapid signal interrogation via optical fibers.

This work presents the current progress in the development of such a sensor. Barium Titanate (BaTiO3) was selected as the piezoelectric material due to its high piezoelectric coefficient and more environmentally friendly profile compared to PZT. The coating was successfully applied using two different methods: sol-gel dip coating and pulsed laser deposition. Potential application areas and opportunities for further design optimization are also discussed.

DS 20.10 Thu 18:30 P2

Thermoelectric-based position-sensitive detector — Jun Peng, Lucas Rave, Pai Zhao, Rakshith Venugopal, Kristian Deneke, Stefanie Haugg, Robert H. Blick, and •Robert Zierold — Center for Hybrid Nanostructures, University of Hamburg, Germany

Precise positioning is a never-ending goal in both fundamental science and technology. Conventional position-sensitive detectors (PSDs), which rely on lateral photoelectric effects in semiconductor junctions, are inherently restricted in operating temperature and are often unsuitable for detection beyond the optical regime. Here, we present a new detector architecture, the thermoelectric-based position-sensitive detector (T-PSD), that extracts spatial information solely from heat conduction and thermoelectric conversion. Specifically, the device incorporates an ALD-deposited Al-doped ZnO (AZO) thermoelectric thin film on an isotropic substrate, where Seebeck voltages measured across multiple electrodes encode the position of an incident heat spot. It can detect single heat spots arising from various energy sources, including electromagnetic radiation, electrons, and macroscopic mechanical heat. The thin-film design enables submicrometer spatial resolution in 1D configurations, while a two-ratio voltage decoding scheme provides robust and intensity-independent localization in 2D devices. Furthermore, the T-PSD exhibits broad temperature compatibility and is particularly well suited for high-energy beams, which remain challenging to localize with existing PSD technologies.

DS 20.11 Thu 18:30 P2

Research Infrastructure Access in NAnoscience & nanotechnology (RIANA) — •Ryan Yang — Helmholtz-Zentrum Dresden-Rosendorf, Dresden, Germany

RIANA is a Horizon Europe-funded consortium of seven Analytical Research Infrastructures in Europe (ARIE) comprising of 69 research facilities that offer open, curiosity-driven research in nanoscience and nanotechnology. By integrating advanced capabilities within Europe in simulation, material synthesis, nanofabrication, characterization, and analysis, RIANA provides a single-point entry for users to perform targeted and impact-orientated investigations.

Users can simply submit a single application to access any of the nanoscience infrastructures within RIANA. A comprehensive service, anchored by 21 Junior Scientists and supported by a panel of senior facility experts will guide users through technique selection, experimental operation, data analysis and publication. Parallel Innovation Services tailor access for industry (especially SMEs) helping mature technologies, raise TRLs, and scale production processes. The Smart Science Cluster (SSC) network of on-site Junior Scientists ensures hands-on support at every research stage, from experiment design to result interpretation. Specifically, users requiring beam-time among other methods of research can take advantage of RIANA and the FIB aspects of their projects will be delegated to the RADIATE network such as the HZDR*s Ion Beam Center.

My poster will introduce this EU project and how potential users can tap into this resource.

DS 20.12 Thu 18:30 P2

Tailoring of MoO3 Thin Films by Irradiation with Energetic Heavy Ions — •Islam Al-Hamad[1], Ayman El-Said[1], Mohammad Al-Kuhaili[1], Shavkat Akhmadaliev[2], and Stefan Facsko[2] — [1]Physics Department and Interdisciplinary Research Center for Advanced Materials, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

In recent years, energetic heavy ions have been used to modify the physical properties of various materials [1]. In this study, we investigate the influence of irradiation of molybdenum trioxide (MoO3) thin films with MeV ions of various parameters [2]. The films were deposited on fused silica using thermal evaporation technique. After irradiation, the films were characterized using optical spectroscopy and XRD techniques, showing the effectiveness of ion-irradiation in tuning the films optical and structural properties by varying ion beam parameters. This is highly important for the design of advanced metal oxide materials for sensing, switching, and energy applications.

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Helmholtz Association. A.S. El-Said acknowledges the support by KFUPM, Saudi Arabia (Project: ISP24236).

[1] A.S. El-Said, S. Rao, S. Akhmadaliev, S. Facsko, Phys. Rev. Appl. 13, 044073 (2020). [2] R. Sivakumar, et al., J. Phys.: Condens. Matter 19, 186204 (2007).

DS 20.13 Thu 18:30 P2

Quantifying surface/H-plasma interactions via in-situ observation of metal - insulator transition (MIT) in rare earth perovskites ($MNiO_3$) — •Balázs Antalicz[1], Sophia Sahoo[2], Parikshit Phadke[1], Roland Bliem[1], and Gertjan Koster[2] — [1]ARCNL, Materials & Surface Science for EUVL, Science Park 106, 1098 XG Amsterdam, The Netherlands — [2]University of Twente, Inorganic Material Science Group Hallenweg 23, 7522 NH Enschede, The Netherlands

In 'green' plasma reactors and semiconductor manufacturing, reactive H species clean surfaces, but also induce degradation, e.g. via blistering or embrittlement. To retain device performance, low-cost & complexity exposure monitoring is required – which faces fundamental challenges.

To solve this, materials with strong response to hydrogenation are of interest. For example, Pt-dissociated H_2 was shown to induce MIT in $MNiO_3$ perovskites, which was accompanied by an up to 10^7-fold electrical resistance increase. Because H-plasma contains multiple pre-activated species, we anticipate simpler sensor designs are possible, without the Pt catalyst.

Using an accelerated plasma exposure tool, we then demonstrate MIT in epitaxially grown, Pt-free $NdNiO_3$. X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS) shows partial Ni^{3+} reduction, and loss/alteration of crystallinity. Further results explore re-settability by annealing in O_2, and correlate O 1s XPS spectra with crystal-field theory, structure changes, and the onset of the insulator state.

DS 20.14 Thu 18:30 P2

Distributed Bragg Reflector-Enhanced Grating Coupler on SiON-Doped Silicon Platform for 905 nm Using Particle Swarm Optimization — •Metehan Ari[1], Iremnur Duru[1], Ali Karatutlu[1,2], and Timuçin Emre Tabaru[1] — [1]Sivas University of Science and Technology — [2]] Institute of Materials Science Nanotechnology and National Nanotechnology Research Center (UNAM) Bilkent University

A vertical grating coupler operating at 905 nm was designed on a silicon oxynitride-doped silicon (SiON-Si) platform for on-chip LiDAR. For the first time, the SiON-Si layer served as the core of a grating structure. The material exhibited a refractive index of 2.27, CMOS compatibility, and negligible two-photon absorption, with its electronic structure confirmed via soft X-ray absorption spectroscopy at the HESEB beamline (SESAME).

To enhance performance, a Distributed Bragg Reflector (DBR) consisting of three alternating SiON-Si/SiO* layers was integrated beneath the grating to suppress substrate leakage. Design optimization using Particle Swarm Optimization (PSO) and FDTD analysis demonstrated that the DBR increased coupling efficiency from ~35% to 53%. Consequently, the optimized device achieved 53% (-2.76 dB) efficiency for TM-polarized vertical coupling at 905 nm. Fabricating both the grating and waveguide within the same SiON-Si layer eliminated heterogeneous interfaces, maintained single-mode behavior, and validated the platform's potential for integrated photonic circuits.

DS 20.15 Thu 18:30 P2

XRD Data Analysis and Curve Fitting Using Differential Evolution in Python — •Simon Lorch, Tobias Pollenske, and Joachim Wollschläger — Institute of Physics, University of Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

Precise evaluation of X-ray diffraction (XRD) data is essential for understanding thin-film and interface structures at the atomic scale. In this contribution, we present a Python-based framework for automated fitting and quantitative analysis of experimental diffraction data using Differential Evolution (DE) as a global optimization strategy. The method minimizes the difference between measured and simulated intensity curves by evolving parameter sets such as layer thickness, density, and interfacial roughness toward the global minimum of an error function. Unlike conventional structure-factor-based approaches, the model deliberately omits detailed atomic scattering factors and instead focuses on the optimization of macroscopic parameters to reproduce the experimental curve shape. This allows a robust and efficient fitting of complex multilayer systems even in cases where structural details or phase information are incomplete. Compared to traditional gradientbased approaches, DE shows superior robustness against local minima and enables reliable fitting of complex multilayer systems with correlated parameters. The implementation allows user-defined boundary conditions, parallel evaluation of population members, and integration of physical models for scattering amplitude and Debye-Waller damping. This open and modular approach shows how evolutionary algorithms can make XRD data analysis more reproducible and accurate.

DS 20.16 Thu 18:30 P2

Stress Evolution in Gold Thin Films Under Ion Irradiation — •Jasmin Kahl[1], Karla Paz[1], Berit Marx-Glowna[2], and Carsten Ronning[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, 07743 Jena, Germany — [2]Helmholtz-Institut Jena, Fraunhoferstr. 8, 07743 Jena, Germany

Gold thin films are important for applications requiring mechanical stability and radiation tolerance in optoelectronic devices. This work investigates the stress evolution of polycrystalline Au films irradiated with He, Si, Ag, and Au ions at various energies and fluences. In-situ stress measurements during irradiation show that the as-deposited films are pre-stressed and the mechanical stress increases under irradiation producing a tensile stress. SEM and FIB cross-section images confirm that this stress increase is associated with grain growth, which depends strongly on the ion species. Grain growth increases local density and generates tensile stress because the films are constrained by the substrate. Large grains are advantageous in applications such as electrical interconnects and microstructures, as they reduce electromigration and optical losses. X-ray diffraction reveals structural damage, lattice distortion, and possible crystallite reorientation, while AFM shows increased surface roughness due to sputtering. These results highlight the strong influence of ion species and irradiation conditions on Au thin films, guiding the optimization of gold-based components in demanding environments.

DS 20.17 Thu 18:30 P2

Structural and magnetic properties of epitaxial Fe-Sn thin films. — •Benedikt Eberts[1], Franz Weidenhiller[2], Matthias Küss[1], Lin Chen[2], Christian Back[2], and Manfred Albrecht[1] — [1]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Magnetic Weyl semimetals exhibit strong spin-orbit coupling and nontrivial band structures, enabling efficient field-free manipulation of magnetic states through spin-orbit torque [1], which makes them highly attractive for spintronic applications. Among them, the ferromagnetic Weyl semimetal Fe3Sn2 and the antiferromagnetic Dirac semimetal FeSn provide a good platform for investigating spin-orbit-driven phenomena. Both compounds crystallize in a layered Kagome lattice, where the corner-sharing triangles lead to strong frustration. In this work, we have grown high-quality epitaxial thin films of FeSn and Fe3Sn2. The films were deposited at elevated temperatures using magnetron sputtering. A seed layer system of Pt and Ru on Al2O3(0001) substrates was used to promote epitaxial growth. Thin films of varying thickness were prepared and characterized using XRD, AFM, MFM, SEM, TEM, and SQUID magnetometry. FMR measurements on Fe3Sn2 revealed low damping and the expected sixfold symmetry associated with the Kagome lattice. These thin films will next be used to study charge-spin conversion processes [2]. [1] Lyalin, I. et al., Nano Lett. 21, 6975-6982 (2021) [2] Zhang, S.-L. et al., Phys. Rev. Lett. 123, 187201 (2019)

DS 20.18 Thu 18:30 P2

Single-crystalline Ni thin films as templates for epitaxial growth of 2D materials — •Paula Vierck, Audrey Gilbert, Domenik Spallek, Jonas Lähnemann, and J. Marcelo J. Lopes — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany

Hexagonal boron nitride (h-BN) offers multiple interesting applications as a component in heterostructures with other 2D materials, for example as a passivation layer or a tunnel barrier in electronics. However, the synthesis of large-scale high quality h-BN required for such applications remains challenging, and the vast majority of the van der Waals heterostructures having h-BN as a building block are still prepared using mechanically exfoliated h-BN flakes.

To serve as a substrate for large-scale h-BN grown by molecular beam epitaxy (MBE), in this work, we investigate the synthesis of Ni films on Al_2O_3(0001) and MgO(111) using magnetron sputtering. The structure and morphology of the Ni films is characterized using X-ray diffraction (XRD), atomic force microscopy (AFM) and electron backscatter diffraction (EBSD). The structural quality of the Ni films is improved by systematically varying experimental parameters such as substrate temperature, sputtering power, film thickness and the post-growth annealing temperature, finally resulting in single crystalline Ni films with (111) orientation only.

DS 20.19 Thu 18:30 P2

Structural and optical properties of undoped β-Ga2O3 thin films deposited by ultrasonic spray pyrolysis — •Polina Shamrovska, Narmina Balayeva, and Dietrich Zahn — Technische Universität Chemnitz, Chemnitz, Germany

β-Ga2O3 thin films have gained significant research interest due to their wide bandgap, high thermal stability and breakdown voltage, making them suitable for e.g. UV photodetectors. Here, β-Ga2O3 thin films were deposited on c-plane sapphire substrates via ultrasonic spray pyrolysis, a cost-effective technique suitable for large-scale production. The deposition was performed with Ga(NO3)3 dissolved in a 1 : 1 water-ethanol mixture at a substrate temperature of 190 °C and post-deposition annealing was performed at 1000 °C. The films were characterized by Raman, AFM, XRD, optical transmittance, and conductivity measurement.

The stoichiometric β-phase Ga2O3 films revealed a preferred (-201) orientation in agreement with previous results [1]. The samples show transparency of up to 85% in the visible range and the conductivity increases with increasing film thickness. The results obtained reveal that ultrasonic spray pyrolysis allows the fabrication of highly crystalline and transparent β-Ga2O3 films suitable for further studies as solar-blind UV photodetectors.

[1] Akazawa, Housei, Vacuum, 2016, 123: 8-16.

DS 20.20 Thu 18:30 P2

Analyzing interface properties of energy materials using thin film model systems materials — •Julius K. Dinter, Anja Henss, and Matthias T. Elm — Institute of Experimental Physics I, Justus-Liebig University, Heinrich-Buff-Ring 16, D-35392, Giessen, Germany

Energy materials used in modern electrochemical devices must provide sufficiently high ionic and electronic conductivity, as both ions and electrons are stored and/or transported during device operation. However, most ionic conductors exhibit negligible electronic conductivity, and the opposite is true for typical electronic conductors. Consequently, artificial mixed-conducting composite materials are often prepared by combining ionic and electronic conducting compounds. These artificial mixed ionic-electronic conductors exhibit a large number of internal interfaces, which strongly influence charge storage and transport in the composite.

To clarify the role of such interfaces on overall electrochemical behavior, thin-film model systems with controllable and well-defined interfaces are essential. In this work, we present the fabrication of artificial mixed-conducting thin films based on lithium-ion- and oxygen-ion-conducting oxides prepared by pulsed laser deposition. Structural and compositional characterization using XRD, Raman spectroscopy, time-of-flight secondary ion mass spectrometry, and electrochemical impedance spectroscopy confirms the successful deposition and integrity of the designed model systems.

DS 20.21 Thu 18:30 P2

InAsP quantum emitters on InP with single-photon emission from O- to C-band up to 80 K — •Yiteng Zhang[1], Doaa Abdelbarey[1], Markus Etzkorn[2], Zenghui Jiang[1], Ankita Choudhary[1], Tom Fandrich[1], Arijit Chakraborty[1], Chenxi Ma[1], Pengji Li[1], Xin Cao[1], Eddy P. Rugeramigabo[1], Michael Zopf[1,3], and Fei Ding[1,3] — [1]Leibniz University Hannover, Institute of Solid State Physics, Appelstraße 2, 30167 Hannover, Germany — [2]Technische Universität Braunschweig, Laboratory for Emerging Nanometrology (LENA), Langer Kamp 6a, 38106 Braunschweig, Germany — [3]Leibniz University Hannover, Laboratory of Nano and Quantum Engineering, Schneiderberg 39, 30167 Hannover, Germany

We grow InAsP nanostructures on InP(001) by high-temperature annealing under arsenic flux followed by controlled cooling. In situ RHEED and ex situ AFM/TEM show that this sequence produces coherent, compositionally graded InAsP islands. Low-temperature micro-photoluminescence reveals spectrally isolated emission lines from individual emitters covering the telecom O- to C-bands; power dependence and second-order correlations under continuous-wave excitation show excitonic behaviour and clear antibunching with g2(0)<0.1, confirming single-photon emission. Temperature-dependent measurements indicate that single-photon emission persists up to temperatures above 80K.

DS 20.22 Thu 18:30 P2

Investigations of point defects in Nb3Sn thin films for SRF application — •Sebastian Klug[1], Maik Butterling[2], Eric Hirschmann[1], Andreas Wagner[1], and Maciej Oskar Liedke[1] — [1]Institute of Radiation Physics, HZDR, Germany — [2]Reactor Institute Delft, Delft University of Technology, The Netherlands

Bulk Niobium cavities are the state-of-the-art option to realizes high-performing linear particle accelerators. To achieve even better performance and lowering operational costs, a thin film approach with different superconducting materials is necessary. Nb3Sn coatings are promising candidates because of its high superconducting transition temperature (Tc up to 17 K). Magnetron sputtering is a very suited PVD method which provides high deposition rates and a large spectrum of deposition parameters optimization. Maximizing the transition temperature and the lower critical magnetic field Hc1 could be correlated to the structure and point defects in thin films like vacancies, their agglomerations and pores. To study this effect, positron annihilation spectroscopy (PAS) with a high sensitivity to small void-like defects is used. PAS provides non-destructive and depth-resolved information of defect type, size and density as well as their local atomic chemistry in many material types like metals, polymers, ceramics and semiconductors. In this contribution, investigations on magnetron sputtered Nb3Sn thin film samples will be presented. A special focus is set to positron annihilation spectroscopy to study the influence of different deposition parameters on defect formation and the resulting superconducting performance.

DS 20.23 Thu 18:30 P2

Surface Investigations of Ga-polar wz-GaN Grown by Plasma Assisted MBE — •Abdul Qadir Shabaz[1,2], Anees Ul Hassan[1,2], Fabian Ullmann[1,2], and Stefan Krischok[1,2] — [1]TU Ilmenau, Ehrenbergstraße 29, 98693 Ilmenau — [2]Zentrum für Mikro- und Nanotechnologien, Gustav-Kirchoff-Straße 7, 98693 Ilmenau

Since very high polarization gradients are predicted for wz-GaN/rs-ScN interfaces, well-oriented, clean Ga-polar wz-GaN surfaces are required in order to grow rs-ScN on top of this layer in a ultra high vacuum to achieve high quality interfaces. These thin layers were grown via plasma-assisted molecular beam epitaxy on 6H-SiC substrate. X-ray photoelectron spectroscopy (XPS), ultra violet photo electron spectroscopy (UPS), scanning electron microscopy (SEM) and atomic force microscopy (AFM) were performed to investigate electronic structure, composition and morphology of the surfaces.

DS 20.24 Thu 18:30 P2

Bonding and properties in NiTe-$NiTe_2$: Transition from normal metal to Dirac semimetal — •Christian Stenz[1], Kethusan Karunanathan[1], Paul Zhuromskyy[1], Kijoon Cheong[1], Tim Bartsch[1], and Matthias Wuttig[1,2] — [1]I. Institute of Physics (IA), RWTH Aachen University, Germany — [2]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany

We investigate the evolution of bonding and electronic properties across the NiTe-$NiTe_2$ system, focusing on the transition from conventional metallic behavior in NiTe to topological Dirac semimetallicity in $NiTe_2$. NiTe exhibits isotropic bonding between Ni d- and Te p-electrons, characteristic of a normal metal. In contrast, $NiTe_2$ forms a layered structure with a pseudo van-der-Waals gap and weak Te p-p interactions, hosting Dirac nodes near the Fermi level that give rise to non-trivial topological surface states and linear magnetoresistance. By tuning the Ni content in sputtered thin films, we control the interlayer coupling mediated by Ni d-electrons, enabling systematic exploration of the transition between these bonding regimes. Using density functional theory and tight-binding calculations, we analyze how additional d-electrons influence the band structure, Berry curvature, and Dirac cone formation in $NiTe_2$. Correlations between these electronic changes and material properties - such as optical and electrical conductivity, linear positive magnetoresistance, emergence of soft anharmonic bonds and bond rupture behavior - are examined.

DS 20.25 Thu 18:30 P2

Development of sacrificial layers grown on rare-earth scandate substrates for epitaxial KNN/KTN layer transfer — •Diana Avetisyan, Jeremy Maltitz, Jutta Schwarzkopf, and Jens Martin — Leibniz-Institut für Kristallzüchtung

Future technologies in sensing, communication, and computing require integrated devices with ultra-low-loss processing, precise control of photons, electrons, and spins, fast switching, broad frequency operation, and strong nonlinearities. Silicon photonics alone cannot meet these demands, making hybrid integration via layer transfer a promising approach. A promising material is sodium-doped potassium niobate, potassium tantalate, and their alloys to enable integration with photonic and acoustic devices. These materials exhibit exceptional electro-optic coefficients, nonlinear Kerr coefficients, piezoelectric coupling coefficients, and elasto-optic coefficients. The project focuses on transferring freestanding sodium-doped potassium niobate membranes onto SiO_2/Si substrates. This involves growing sodium-doped potassium niobate on a sacrificial layer/substrate stack, chemically etching the sacrificial layer, and transferring the membrane. Different substrates and sacrificial layers are explored to achieve crack- and wrinkle-free membranes. The membranes are characterized for surface topography, crystalline structure, ferroelectric, piezoelectric, and electromechanical properties for future device applications.

DS 20.26 Thu 18:30 P2

Formation and protection of two-dimensional electron gases at SrTiO3 interfaces via redox reactions — •Shi-Hui Liu, Georg Hoffmann, and Roman Engel-Herbert — Paul-Drude-Institut für Festkörperelektroni, Berlin, Germany

Strontium titanate (SrTiO3) has been the workhorse for development of new physical phenomena over decades. Recently, new momentum was generated when the formation of a two-dimensional electron gas (2DEG) via oxygen scavenging effect at the SrTiO3/AlOx interface was observed, i.e. oxidation of the deposited metal-layer upon reduction of the SrTiO3 [1]. However, depending on the Al layer thickness, these 2DEGs degrade over time due to diffusion of oxygen from the gas phase through the AlOx layer refilling the vacancies.

In this work, amorphous aluminum layers with thicknesses ranging from 0.5 to 2.5 nm were deposited on TiO2-terminated SrTiO3 (001) substrates using molecular beam epitaxy. The complementary methods of in-situ x-ray photoelectron spectroscopy, and capacitance-voltage measurements were performed to monitor the interfacial redox reaction and to identify the spatially confined conduction channel, respectively. Since the 2DEG remains stable only for a limited time within an optimum aluminum layer thickness, strategies for protecting and stabilizing the 2DEG will be pointed out.

[1] L. M. Vicente-Arche et al., Phys. Rev. Mater. 5, 064005 (2021).

DS 20.27 Thu 18:30 P2

E-Beam Evaporation of thin metal and oxide films on Al_2O_3 (0001) — •Laurenz Hüffmeier, Tobias Pollenske, and Joachim Wollschläger — Institute of Physics, University of Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

Ultrathin metal and oxide films are used in numerous fields of application, particularly in optics, electronics, and energy applications. With the increasing importance of these technologies, the requirements for these films are also rising in order to improve their properties. Precisely manufactured films with well defined structural and physical properties are required, as even minimal deviations in thickness or structure can significantly impair device performance. A suitable method for the growth of such layers is physical vapor deposition (PVD), which enables the controlled deposition of a wide variety of materials under high vacuum conditions. Here, electron beam evaporation (EBPVD) is advantageous since extremely clean films can be deposited and high evaporation rates of up to a few micrometers per second are possible.

Hence, in this work, ultrathin magnesium oxide, praseodymium oxide, cobalt, and platinum films were deposited on insulating Al_2O_3 (0001) substrates using EBPVD. The structural properties of the resulting layers were analyzed by XRR. XPS measurements were performed on all films to examine their near-surface chemical composition. For the cobalt layers deposited with different emission currents, XPS was performed both in situ and ex situ to investigate the influence of atmosphere conditions on the oxidation states.

DS 20.28 Thu 18:30 P2

Towards Low-Temperature ALD of Topological Insulator Sb_2Te_3 — •Luise Merkwitz[1,2], Paul Pöhler[1,2], Steffen Ziller[1], Knut Ulbrich[1], Marek Ulbrich[1], Sebastian Lehmann[1], and Kornelius Nielsch[1,2] — [1]Institute for Metallic Materials, Leibniz Institute for Solid State and Materials Research, IFW Dresden, D-01069 Dresden, Germany — [2]Technical University Dresden, D-01069 Dresden, Germany

Low-Temperature ALD expands the range of applications for ALD enabling not only the deposition of thin films on temperature-sensitive substrates but also the possibility of a more ressoure-efficient setup and reaching advantages in material conformity and less sample defects.

We have designed, constructed and developed a state-of-the-art Low-Temperature ALD reactor for high-quality thin films. Our previous results demonstrate the technical functionality and reproducibility of known Low-Temperature ALD processes. In addition, our latest results reveal a never before published Sb_2Te_3 synthesis which we consider to be a highly promising Room-Temperature ALD process.

DS 20.29 Thu 18:30 P2

Using layered metamaterials in spin - ventil structures as a basis for artificial neural network — •Vladimir Boian[1], Cătălin Cimbir[1], and Vladimir M Fomin[2] — [1]Technical University of Moldova, Institute of Electronic Engineering and Nanotechnologies, Chisinau, Moldovau — [2]IET, Leibniz IFW Dresden, Dresden, Germany

Elaboration of a superconducting artificial neural network (ANN) the most promising solution in the design and development of non-von Neumann architectures. There are two main components of ANN: the nonlinear switch neuron constituting a spin valve, and the linear connection element the synapse. This study presents the results of computer modeling of superconducting spin valves on the base of Josephson Junction with weak link prepared from artificial magnetic metamaterials, and of superconducting synapses, based on hybrid layered structures superconductor/ferromagnet. The proximity effect in a superlattice formed by superconducting Nb nanolayers and ferromagnetic Co layers with different thicknesses and coercive fields is analyzed both theoretically and experimentally. In this sense, they can be applied as tunable kinetic inductors for the design of ANN synapses. Metamaterials based on Nb and Co nanolayers are a very promising class of artificial magnets for superconducting spintronics and quantum computing. The use of artificial neural networks with a radically reduced consumption of electricity are increasingly appreciated worldwide.

DS 20.30 Thu 18:30 P2

From Localised to Delocalised Charge Carriers: An Optical Investigation on Metal-Insulator Transitions — •Thomas Schmidt[1], Navjot Bamrah[2], Liron B. Michael[2], Ricardo P. M. S. Lobo[3], and Matthias Wuttig[1,2] — [1]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany — [2]I. Institute of Physics (IA), RWTH Aachen University, Germany — [3]LPEM, ESPCI Paris, CNRS, PSL University, 75231 Paris, France

Understanding metal-insulator transitions (MITs) has been a central topic in solid-state physics and materials science for decades. Various theoretical frameworks describe these transitions in terms of critical charge carrier densities (Mott MIT) or electron localisation induced by disorder (Anderson MIT). Typically, electrical conductivity measurements or their temperature-dependent derivative (TCR) are used to distinguish metallic from insulating behavior.

In this work, we propose an alternative approach based on optical spectroscopy. Reflectance spectra were recorded over a broad spectral range using a Fourier-transform infrared (FTIR) spectrometer. The optical functions were subsequently obtained through modeling of the measured data. Our analysis focuses on the evolution of the Drude response in the optical conductivity, which directly reflects the dynamics of free charge carriers. The Drude feature, defined by the ratio of the plasma edge to the scattering rate, provides valuable insight into the material-specific degree of electron (de)localisation and thus offers an alternative perspective on MITs and their relation to chemical bonding.

DS 20.31 Thu 18:30 P2

Investigating the Anisotropy of Optical Phonons in Ultrafast Optical Pump-Probe Experiments — •Felix Nöhl[1], Felix Hoff[1], Jonathan Frank[1], and Matthias Wuttig[1,2] — [1]I. Institute of Physics (IA), RWTH Aachen University, Germany — [2]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany

Phonons are quantized lattice vibrations closely linked to bond strength and atomic arrangement. A well-established tool to study incoherent optical phonons in frequency domain is Raman scattering. Ultrafast lattice dynamics and coherent phonons, capable of modulating macroscopic physical properties, are of interest to emerging research fields. In ultrafast optical pump-probe experiments, coherent optical phonons can be excited and directly measured in the time domain via transient changes in reflectivity. Due to their pronounced phononic response, bismuth and tin selenide were used to further explore the excitation and detection of coherent phonons. A pump polarization scheme for our optical pump-probe setup was implemented and polarization resolved pump-probe and Raman measurements compared. Clear symmetries were observed, highlighting the influence of the lattice structure. This improves our understanding of coherent phonon anisotropy in optical pump-probe measurements and enables modulation of the detected signal by changing the pump polarization.

DS 20.32 Thu 18:30 P2

Optimization of Reactive Ion Etching processes with Optical Emission Spectroscopy — •Daniel Breuer, Bich Nguyen, Teresa Wessels, and Markus Kaiser — Helmholtz Nano Facility, Forschungszentrum Jülich, Jülich, Germany

In modern technology, devices on the scale of micro- to nanometers play an important role. In the fabrication of those devices, the dry etching process is essential to structure them. Hereby the reactive ion etching technology has been established due to its very selective and anisotropic etching. To achieve reproducible results, process control is crucial. For this purpose, optical emission spectroscopy (OES) is employed to observe the spectra of the plasma during the process. Here, OES is used to ensure thorough cleaning of the RIE chamber after etching by defining the spectra of a clean chamber. Parameters, e.g. etching gas and time, are investigated with respect to their effect on chamber cleanliness. Finally, suggestions for a rigorous cleaning procedure are given. In addition, the endpoint detection is examined on a Si wafer with 200 nm SiN. Using OES, we aim to stop the plasma immediately when the SiN is etched through to prevent damage to the Si. We implement an endpoint detection by observing the characteristic line of the CN molecule, which is a typical product of the chemical etch reaction. The effects of various system parameters on the plasma, e.g. coupled power, chamber pressure and gas flow, are studied, as well as endpoint detection settings. In conclusion, a precise analysis of the plasma via OES allows us to specifically control the etching process.

DS 20.33 Thu 18:30 P2

Optimizing Erbium Luminescence in Silicon Nitride for Integrated Photonics via Oxygen Codoping and Thermal Annealing — •Felix Mania[1], Sören Lerner[1], Jiale Sun[2], Zheru Qiu[2], Xinru Ji[2], Tobias Kippenberg[2], and Carsten Ronning[1] — [1]Friedrich-Schiller Universität, Helmholtzweg 3, 07743 Jena, Germany — [2]École Polytechnique Fédérale de Lausanne, Switzerland

Erbium-doped fiber amplifiers revolutionized long-haul optical communications, thereby establishing erbium ions as promising candidates for amplification in integrated circuits. However, their practical application in integrated photonics is currently limited by low luminescence efficiency. In this study, we utilize ion implantation into ultralow-loss silicon nitride (Si_3N_4) and investigate the influence of oxygen codoping and thermal annealing on the formation of Er-O complexes, thereby modifying the local crystal field of the erbium ions within the host matrix. Specifically, we examine the effects of varying oxygen doping concentration and annealing temperature via photoluminescence and lifetime measurements. These findings provide a critical optimization strategy for CMOS-compatible erbium-based emitters essential for future photonic integration.

DS 20.34 Thu 18:30 P2

Domain Transfer from Simulation to Experimental Neutron and X-ray Reflectivity Data Using Probabilistic Generative Models — •Jeyhun Rustamov[1], Ritz Aguilar[1], Vedhas Pandit[1], Nico Hoffmann[2], and Jeffrey Kelling[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Helm & Walter IT-Solutions, Dresden, Germany

Machine learning (ML) models trained on simulations often fail to generalize to experimental data in neutron and X-ray reflectivity analysis. Furthermore, determining thin film parameters from reflectivity curves is an inherently ambiguous inverse problem. To address this, we employ conditional normalizing flows (cNFs) with a β-Variational Autoencoder (β-VAE) embedding network to learn the full distribution of physical parameters instead of single estimates.

To further improve performance on experimental data, we systematically explore three strategies for bridging the simulation-experiment domain gap: fine-tuning with labeled experimental data, utilizing generative models to create realistic synthetic data, and a novel physics-informed method. The proposed method incorporates a differentiable forward function based on the kinematic approximation to guide the generation of sample parameters via physics-informed loss during bidirectional training of cNFs.

Our approach distinctly leverages unlabeled experimental reflection data to address cNF performance challenges on real-world reflectivity measurements. Additionally, this methodology can be broadly applied to other inverse problems with similar domain-transfer challenges.

DS 20.35 Thu 18:30 P2

A Kramers-Kronig Consistent, Parameter Free, Probabilistic Dielectric Function Model — •Noah Stiehm[1,2], Stefan Krischok[1], Rüdiger Schmidt-Grund[1], and Jana de Wiljes[2] — [1]Technische Physik I, TU Ilmenau, Germany — [2]Mathematics of Data Science, TU Ilmenau, Germany

Utilizing a Bayesian probabilistic modeling approach to approximate the full posterior probability density $p(\theta \mid y)$ of a model's parameters θ given data y can provide greater insight into the model's performance and parameter uncertainties than point estimates provided by classic, deterministic optimization algorithms.

Here we present a parameter free dielectric function model, that might be used in a Bayesian modeling context as a substitute for the well known B-spline models. Our approach is based on Gaussian processes (GP), which are a flexible class of random functions, that enable numerical sampling in an efficient manner. We utilize a GP to model the time-domain response function $\chi(t - t')$ as a latent function, from which the dielectric function $\varepsilon(\omega)$ is constructed via a discrete Fourier transform. The resulting dielectric function is therefor Kramers-Kronig consistent by construction. We implement approximate and exact (depending on available compute resources) sampling strategies to include our model in different Bayesian modeling frameworks which utilize either Markov Chain Monte Carlo (MCMC) or particle filter methods. We demonstrate our model's performance in scenarios with significant uncertainties: a sample with a concentration gradient of a AgAl alloy, and pump-probe transient ellipsometry data.

DS 20.36 Thu 18:30 P2

Tunability of optoelectronic properties of the alpha-phase MoO3 thin films — •Zhihua Yong, Lars Steinkopf, Marin Rusu, and Thomas Unold — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

Alpha-phase MoO3 is widely used as a large bandgap hole transport layer (HTL) in solar cells due to its high work function, good hole conductivity and stability. For an appropriate energy level alignment with the active layer, the optoelectronic parameters of the MoO3 layers must be fine tuned. In this work, we fabricate uniform as well as combinatorially synthesised MoO3 films via Pulsed Laser Deposition on fused silica substrates in the temperature range of 350*480oC. The film thicknesses were targeted at approximately 15 nm, as usually applied for HTLs, and confirmed by X-Ray Reflectivity measurements. All films were found to be polycrystalline and contained only the α-phase with an orthorhombic crystal structure (Pbnm space group), as observed by X-Ray Diffraction and Raman Spectroscopy. Electronic properties of the MoO3 films were investigated by combining Kelvin probe (KP) measurements and photoelectron yield spectroscopy (PYS) under inert N2 atmosphere at ambient pressure. We show by means of KP-PYS studies that the ionisation energy and work function of the films can be fine tuned between 5.72 to 6.10 eV and 5.72 to 6.00 eV, respectively, by varying the deposition temperature. That results in a fine variation of the valence band maximum with respect to Fermi level. The degenerate state of the films is observed for deposition temperatures equal or higher than 425°C.

DS 20.37 Thu 18:30 P2

Heterodyne detection of the second harmonic signal in THz pump - optical probe experiments — •Sergei Ovcharenko, Alexey Melnikov, and Georg Woltersdorf — Institut für Physik, Martin-Luther-Universität Halle, 06120 Halle (Saale), Germany

Broadband Terahertz (THz) radiation is a widely used for resonant excitation of magnon modes or spin waves in magnetic materials. Furthermore, studying the THz emission from ferromagnetic (FM) materials allows us to investigate elementary processes in ultrafast spintronic. However, experimental investigation of such effects requires broadband THz detection: the commonly used sampling in electro-optical crystals is limited by phonon absorption, Zeeman-torque sampling requires accurate determination of the magneto-optical constants of a specific FM sample. An alternative approach is the detection of the THz field-induced second harmonic (TFISH) signal, based on third-order nonlinearity $\chi(3)$ in ambient air gases. Heterodyne detection, interference between the TFISH and SH light from a reference source, allows retrieval of the full THz pulse profile. The SH heterodyning technique is also applicable to extract weak SH signals, related to THz-induced magnetization dynamics in thin films. Our work reveals a phase modulation effect in the heterodyne TFISH signal: the air gap between TFISH and reference SH sources alters the detected THz pulse shape and spectrum through propagation effect in presence of the THz field. Using the developed instrument, we performed test experiments on heterodyne SH detection of THz-induced magnetization dynamics.

DS 20.38 Thu 18:30 P2

In_2Te_3 as a Covalent Spacer in GeSbTe-based Phase Change Superlattices — •Lucas Bothe[1], Maximilian Buchta[1], and Matthias Wuttig[1,2] — [1]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), FZJ, Jülich, Germany — [2]I. Institute of Physics (IA), RWTH Aachen University, Germany

Superlattices (SL) containing GeSbTe are promising material systems to overcome typical shortcomings of Phase Change Materials (PCM) by reducing the reset current by an order of magnitude. The reason for the increased energy-efficiency of SLs remains unclear. Typically, two metavalent materials, e.g. $GeSb_2Te_4$ and Sb_2Te_3, are used in superlattices to achieve superior switching performance. It is debated that Sb_2Te_3 plays a major role in achieving this performance increase. In this work however, Sb_2Te_3 is exchanged with In_2Te_3, replacing a metavalent with a covalent sesqui-chalcogenide to investigate its influence on the switching performance. In a first step, this work presents the growth of $GeSb_2Te_4/In_2Te_3$-SLs via MBE. XRD, RHEED, SEM and EDX were employed to characterize the samples. Pronounced Laue Fringes and clearly visible SL satellite peaks in the XRD-scans demonstrate the excellent sample quality and allow for exact characterization of the achieved SL-stacking. RHEED data allows the characterization of the coupling between $GeSb_2Te_4$ and In_2Te_3, which appears to be weak but not strictly of van-der-Waals character. As a next step the samples will be optically switched with a laser set up to compare the switching characteristics to those of $GeSb_2Te_4/Sb_2Te_3$-SLs.

DS 20.39 Thu 18:30 P2

Electrical switching dynamics of Ge-Sb-Te alloys for phase-change memories — •Alexander Kiehn[1] and Matthias Wuttig[1,2] — [1]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany — [2]I. Institute of Physics (IA), RWTH Aachen University, Germany

Off-stoichiometric Ge-Sb-Te alloys are promising candidates for next-generation phase-change memory (PCM) due to their nonvolatile nature, temperature stability, and fast switching speeds. These properties make them ideal for in-memory computing or applications in data storage, where fast, energy-efficient and reliable memory is crucial. However, in order to integrate PCM into standard semiconductor devices, it is necessary to reduce the switching voltage and current. This is greatly influenced by the composition of the sputtered Ge-Sb-Te layer, as well as the contact electrode material. Using CMOS-compatible fabrication processes, chips were manufactured based on a confined cell PCM design with new TaN contacts. Based on the electrical switching results, trends in thermal stability and the resulting voltage requirements are shown for different alloys. Further analysis also shows the SET and RESET speed as well as endurance of the devices.

DS 20.40 Thu 18:30 P2

Optimizing Crystallization Kinetics and Reducing Stochasticity of the Phase-Change Materials Sb2Se3 and Ge2SeTe through Controlled Crystalline Interface Growth — •Ramon Pfeiffer, Ramon Schmidmeier, Laura Gundermann, and Matthias Wuttig — I. Institute of Physics (IA), RWTH Aachen University, Germany

Chalcogenide phase-change material (PCM) alloys such as Antimony Triselenide (Sb2Se3) and Germanium Selenide Telluride (Ge2SeTe) can be switched repeatedly with low optical losses, making them interesting contestants for integrated photonic circuits. However, by switching from the predominately investigated as-deposited phase these materials are characterized by a relatively slow crystallization speed and high stochasticity. To address these shortcomings, we investigate methods such as the recrystallization from differently melt-quenched phases and a crystalline ring. The later approach, allows for controlled growth from a crystalline interface. An increase of crystallisation speed and decrease of stochasticity is verified by a pump probe setup and through Electron Backscatter Diffraction (EBSD) measurements respectively.

DS 20.41 Thu 18:30 P2

Hard X-Ray Momentum Microscope Measurements of $SrCoO_x$ Thin Films at Beamline P22 — •Volkmar Koller, Sourav Chowdhury, Sergii Chernov, Andrei Gloskovskii, and Christoph Schlueter — Photon Science | DESY Hamburg

Emerging memory devices are a possibility to reduce electricity expenditure in the future compared to established complementary metal-oxide-semiconductors

CMOS. For instance the Mottronic is based on a topotactic phase transition TPT associated with a metal-insulator transition MIT, instead of a manipulation of charges like in semiconductors. This might allow a further miniaturization of devices.

Here we show the Hard X-Ray Momentum Microscope HarMoMic at the beamline P22 of the PETRA III synchrotron at DESY as tool to monitor the electronic and crystalline structure of materials showing a TPT. Based on Hard X-ray Photoelectron Spectroscopy HAXPES the HarMoMic probes angle resolved the bulk electronic structure of single crystalline samples. Thus, the electronic band structure and X-ray photoelectron diffraction patterns XPD can be measured. From the XPD patterns the crystalline structure of a material can be determined by comparing it to simulations (Kikuchi Diffraction patterns).

As model system we show measurements of $SrCoO_x$(001) thin films grown via PLD on Nb-doped $SrTiO_3$(001). Upon the application of an electric bias it is electrochemically oxidized from $SrCoO_{2.5}$ (BrownMillerite, insulator, antiferromagnetic) to $SrCoO_{3-\delta}$ (Perovskite-like, metallic, ferromagnetic) undergoing a TPT.

DS 20.42 Thu 18:30 P2

Intercalation of thin Fe-films at the Graphene/SiC Interface — •Niels Rösch[1,2], Fabian Göhler[1,2], Rico Ehrler[1,2], Susanne Wolff[1,2], Olav Hellwig[1,2], and Thomas Seyller[1,2] — [1]Technische Universität Chemnitz, Institut für Physik, 09126 Chemnitz — [2]Forschungszentrum für Materialien, Architekturen und Integration von Nanomembranen, 09126 Chemnitz

The intercalation of graphene on silicon carbide (SiC) with different materials is an extensively studied field of research. The intercalation of metals into the graphene/SiC interface offers a route to tune the structural, electronic and magnetic properties of the system [1,2].

In the present study, we demonstrate the successful intercalation of iron (Fe) between graphene and SiC. 4H-SiC(0001) substrates were used to prepare the buffer layer (BL) precursor by polymer assisted sublimation growth (PASG) [3]. Intercalation was carried out under ultra-high vacuum (UHV) conditions by depositing 2 nm Fe atop the BL precursor at 300 ˚C, followed by an annealing at 750 ˚C for 30 min.

The successful intercalation of iron at the BL/SiC interface was confirmed by photoelectron spectroscopy and electron diffraction. Magnetic characterization via superconducting quantum interference device magnetometer (SQUID) revealed that the intercalated Fe layer exhibits ferromagnetic behavior.

[1] A. A. Rybkina et al., Phys. Rev. B 104 (2021) 155423.
[2] N. Briggs et al., Nanoscale 11 (2019) 15440. 4.
[3] M. Kruskopf et al., 2D Mater. 3 (2016) 041002.

DS 20.43 Thu 18:30 P2

High-Fermi velocity massless carriers in a triangular monolayer of Sb — Bing Liu[1,2], •Kilian Strauss[1,2], Philipp Eck[2,3], Jonas Erhardt[1,2], Tim Wagner[1,2], Philipp Kessler[1,2], Cedric Schmitt[1,2], Lukas Gehrig[1,2], Stefan Enzner[2,3], Martin Kamp[1,2], Jörg Schäfer[1,2], Giorgio Sangiovanni[2,3], Simon Moser[1,2], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Universität Würzburg, D-97074 Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, D-97074 Würzburg, Germany — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, D-97074 Würzburg, Germany

Two-dimensional (2D) quantum materials with high Fermi velocities are key candidates for ballistic transport and high-speed electronics. However, few 2D systems have the potential to demonstrate Fermi velocities exceeding that of graphene, remaining at the level of prediction. Here, we report the successful synthesis of a triangular monolayer of antimony (Sb) on the wide-gap semiconductor SiC. Using combined angle resolved photoemission spectroscopy (ARPES) and scanning tunneling microscopy (STM) in combination with density functional theory (DFT), we reveal orbital filtering that isolates broad-bandwidth, massless p_x and p_y states, yielding a compensated Fermi surface with an ultrahigh Fermi velocity surpassing that of pristine graphene. Linear dichroism in ARPES measurements confirm the orbital polarization of these high-velocity bands. This makes the triangular antimonene a compelling platform for next-generation quantum and high-speed electronic technologies.

DS 20.44 Thu 18:30 P2

Interfacial electronic structure of molecular adsorbates on WS2 and doped MoSe2 — •Carolin Sabrina Schüle, Michael Lämmerhofer, Joschua Bueble, Louisa Adlung, and Heiko Peisert — Institut für Physikalische und Theoretische Chemie Universität Tübingen, Germany

MoSe2 and WS2 are layered transition metal dichalcogenides (TMDCs) and promising alternative to conventional semiconductor materials. We studied interface properties of different molecules on MoSe2 and WS2. In the case of MoSe2 also p- and n-doped substrates were studied. Comparably weakly interacting phthalocyanines (CoPc, MnPc, CoPcF16) were compared to strong electron acceptors (HATCN, C60). It is known that opotoelectronic properties of TMDCs such as MoS2 can be tuned by transition metal phthalocyanines (TMPCs), depending strongly on the central metal atom of the phthalocyanine,[1], the mechanism, however, is not completely understood. Generally, for TMDCs two different interaction channels are possible: Interaction via the central metal atom and the macrocycle. It is shown that the different ionisation potential of the molecules affect the size of interface dipoles, as well as a band bending in the bulk substrates. However, the role of interface states is not negligible. Also, the doping level of MoSe2 have an influence on the strength of the interaction, although no integer charge transfer might be expected. [1] DOI: 10.1021/jacs.1c07795

DS 20.45 Thu 18:30 P2

Wannier-orbital Transient Polaron Localisation for electron and spin transport in organic semiconductors — •Nisarg Trivedi, Maximilian F.X. Dorfner, Michel Panhans, and Frank Ortmann — TUM School of Natural Sciences and Atomistic Modeling Center, Munich Data Science Institute, Technische Universität München

Transport in organic semiconductors is governed by a complex interplay between comparable energy scales of electronic coupling, thermal disorder, and electron-vibration interactions, making it difficult to describe within a unified framework. Building on the hybrid Transient Polaron Localization (TPL) model proposed by Hutsch *et al.* (npj Comput. Mater. 8, 228, 2022), we introduce an efficient extension using Wannier orbitals as a localized and orthonormal basis, enabling accurate treatment of charge transport in extended pi -conjugated systems which also allows us to generalise the framework for spin transport.

DS 20.46 Thu 18:30 P2

A Dual Time-Scale KMC-MD Approach for Simulating Self-Assembly Kinetics of Polyalanine α-Helix Monolayers — •Bo-Yue Zeng[1], Hadis Ghodrati Saeini[1], Sibylle Gemming[1], and Jeffrey Kelling[1,2] — [1]Technische Universität Chemnitz, Chemnitz, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Polyalanine α-helices show strong potential for spintronic applications because of their spin-filtering ability through the Chiral-Induced Spin Selectivity (CISS) effect. To build enhanced spin-filters and understand CISS, it is important to gain better control of molecular monolayer self-assembly. This requires large scale kinetic simulations which cover the long time scales of layer formation and annealing. The kinetics of polyalanine molecules anchored to metal substrates is governed by two separate time regimes: slow diffusion on the surface and fast relaxation of the organic ensemble.

To address these challenges, we present a dual time-scale simulation approach for 2D self-assembly that combines kinetic Monte Carlo (KMC) for slow diffusion with molecular dynamics (MD) for rapid relaxation. We demonstrate a parallel implementation based on the Alpaka abstraction layer to achieve performance portability across CPUs and GPUs. This proof of concept paves the way for large-scale simulations of mono-layer self-assembly in support of future spintronic applications.

DS 20.47 Thu 18:30 P2

Modeling intermolecular interactions and ordered packing in self-assembled monolayers of polyalanine α-helices — Hadis Ghodrati Saeini[1], Thi Ngoc Ha Nguyen[1], Christoph Tegenkamp[1], Sibylle Gemming[1], Jeffrey Kelling[2], and •Florian Günther[3] — [1]Technische Universität Chemnitz, Chemnitz, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]São Paulo State University, Rio Claro, Brazil

Polypeptide molecules are attracting attention as promising candidates for electronic spin-filters due to the phenomenon of chiral-induced spin selectivity (CISS). This motivates substantial research to characterize the structural and electrical properties of self-assembled monolayers (SAMs) of peptide helices, for example, polyalanine (PA) α-helices. In this work, we aim to characterize the intermolecular interactions governing PA-SAM film formation. We developed an empirical potential that models the interaction between two isolated helices, derived using the density functional-based tight-binding (DFTB) method. This potential allowed us to simulate the most energetically favorable arrangements in SAM films via a Monte Carlo approach employing simulated annealing and the Metropolis algorithm. Statistical analysis of the relative positioning of adjacent molecules enabled us to classify the degree of frustration in the films. For enantiopure systems, a frustration-free arrangement was found, yielding a perfect hexagonal lattice. For mixtures of chiralities, the results showed parallel-aligned domains of differently handed helices. Both findings are in excellent agreement with experimental works.

DS 20.48 Thu 18:30 P2

Spin-Dependent Transport of CISS in Polyalanine on GMR-like Au/Co/Au Interfaces — •Andreas Cordier[1], Thi Ngoc Ha Nguyen[1], Huu Thoai Ngo[1], Julian Koch[1], Lech Thomas Baczewski[2], and Christoph Tegenkamp[1] — [1]Technische Universität Chemnitz — [2]Polish Academy of Sciences, Warszawa

Chiral molecules enable the investigation of spin-selective transport in a GMR-like Au/Co/Au geometry. We studied 16-mer L-polyalanine adsorbed on such multilayers by LT-UHV-STM and STS. Topography reveals interdigitated molecular arrangements with an intermolecular spacing of ~3 nm and reduced long-range order compared to ambient conditions. STS yields a HOMO-LUMO gap of ~1.8 eV and an asymmetry of the electronic states, consistent with shifts induced by the intrinsic molecular dipole under the junction electric field. The I-V characteristics show a clear dependence on the Co magnetization orienta-

tion, evidencing CISS-driven, spin-dependent transport through the PA layer and allowing an extraction of the molecular CISS-MR.

In magnetic-field-dependent feedback measurements, the tip stabilizes at distinct equilibrium positions depending on the prior Co magnetization direction, producing a robust Δz signal that vanishes on Au/Co/Au reference samples. Using a quantitative model accounting for all resistive elements of the GMR-like stack we relate the measured Δz to the spin-dependent transmission through the molecules. In combination with forthcoming electronic-structure input, this establishes the experimental foundation for a consistent determination of the CISS-induced magnetoresistance in chiral molecules.

DS 20.49 Thu 18:30 P2

Evolution of voids in molybdenum disilicide during electromigration experiments — •Julia Baldauf, Dennis Mitrenga, Tim Fink, and Philipp Kellner — CiS Forschungsinstitut für Mikrosensorik GmbH, Erfurt, Germany

Molybdenum disilicide (MoSi2) is used in macroscopic and microscopic heating devices.

The widespread use of MoSi2 is caused by its melting point of 2030˚C and its combability with CMOS processes. Because of the high melting point MoSi2 has been considered immune to electromigration phenomena. In reality electromigration is one of the main causes of chip failure for microheaters employing MoSi2 at temperatures of 600˚C up to 900˚C.

Artificially generated voids were made by using a gallium based focused ion beam, are approximately circular in shape and located near the center of a line under test made of MoSi2. We employed a laser scanning microscopy technique to observe changes of the shape of artificially generated voids. Slight changes in the shape of the voids and the formation of hillocks on the rim of the voids have been observed. Because of the low volume of the migrated material the chemical analysis remains challenging.

Machine learning is used to determine the effective ion charges used in Finite-Element-Methode-simulations of a digital twin. The digital twin will be used in conjunction with the experimental data to evaluate the effective ion charge determined by employing the machine learning algorithm.

DS 20.50 Thu 18:30 P2

Towards Study of Charge Transport Mechanisms Across Grain Boundaries in Organic Monolayer Films via Near-Field Photocurrent Spectroscopy — •Jian Xiao, Francesca Falorsi, Lukas Renn, and Thomas Weitz — Georg-August-University Göttingen, Göttingen, Germany

Organic semiconductors, particularly emerging organic thin films (OTFs) comprising one to several molecular layers, enable diverse nanoscale (opto-)electronic devices. Device performance critically depends on the crystalline order within OTFs, where grain boundaries (GBs) between dissimilarly oriented domains are widely recognized as limiting factors for charge transport. While previous studies have identified two GB types, barriers and valleys, distinguished by whether their lowest unoccupied molecular orbitals (LUMOs) lie above or below those of bulk grains, the detailed transport mechanisms across these interfaces remain poorly understood.

We will report our current efforts to develop scanning near-field optical microscopy (SNOM) to investigate excited photocurrents across GBs in organic monolayer films under illumination with photon energies comparable to the energy differences between GBs and bulk grains. Our approach aims to elucidate charge transport pathways across GBs and their contribution to macroscopic current formation. We further examine how GB type and the magnitude of interfacial energy differences influence transport mechanisms. These insights may inform charge transport studies across barriers in other optoelectronic material systems.

DS 20.51 Thu 18:30 P2

Superconducting diode effect in in epitaxial thin films of elemental superconductors — •Shanshan Guo[1], Nikolai Peshcherenko[1], Changjiang Yi[1], Ning Mao[1], Heda Zhang[1], Heiko Reith[2], Walter Schnelle[1], Edouard Lesne[1], Kornelius Nielsch[2], Yang Zhang[3], and Claudia Felser[1] — [1]Max-Planck-Institute für Chemische Physik fester Stoffe, Dresden, Germany — [2]Leibnitz IFW Dresden, Dresden, Germany — [3]Department of Physics and Astronomy, University of Tennessee, Knoxville, USA

The superconducting diode effect allows for nonreciprocal, dissipationless electronic transport. It has the potential to enhance transfer current efficiency compared to the traditional semiconducting equivalent and hence have a significant impact on the design of future electronic devices. While the field is fast evolving, there are still many unanswered questions about the underlying mechanisms and origin of the phenomenon. Here we investigate the superconducting diode effect in epitaxial thin films of elemental superconductors (V, Nb and Ta). We probe its supercurrent nonreciprocity as a function of magnetic field and temperature and discuss the role spin-orbital-coupling strength plays in the superconducting diode effect in a combined simple material/device structure. Our work should stimulate the refinement of theoretical models and enable a deeper understanding of the supercurrent rectification effect.

DS 20.52 Thu 18:30 P2

Cavity-modified electron mobility in monolayer black phosphorus from first principles — •Qinyan Yi[1], I-Te Lu[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free-Electron Laser Science, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Initiative for Computational Catalysis, The Flatiron Institute, Simons Foundation, New York City, NY 10010, United States of America

Cavity materials engineering offers a new route to control material properties through quantum fluctuations, without requiring external driving fields such as laser pulses. However, theoretical studies of cavity-modified transport in realistic materials are still lacking. In this work, we perform an ab initio study of monolayer black phosphorus coupled to cavity photons using quantum electrodynamical density functional theory (QEDFT), which includes an additional electron-photon exchange potential in the Kohn-Sham Hamiltonian. Our results show that cavity photons can modify the electron-phonon interaction of black phosphorus and decrease the phonon-limited scattering rate, leading to an increase in electron mobility by about 10% for a realistic coupling ratio of mode strength to bare photon frequency of 0.1, which is the upper limit of a realistic device. These results demonstrate that cavity materials engineering can modify the materials transport, highlighting its promise as a practical, non-intrusive approach for tuning material properties.

DS 21: Optical Analysis of Thin Films

Time: Friday 9:30–12:30 Location: REC/C213

DS 21.1 Fri 9:30 REC/C213

From Semiconductors to Quantum Materials: Ultrafast Optical Signatures Across Chalcogenide Classes — •Timo Veslin[1], Felix Hoff[1], Jonathan Frank[1], and Matthias Wuttig[1,2] — [1]I. Institute of Physics (IA), RWTH Aachen University, Germany — [2]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany

Optical pump probe spectroscopy provides a powerful means to investigate and compare ultrafast dynamics in diverse material classes, ranging from covalently bonded semiconductors to quantum materials. In this study, we contrast the optical and structural responses of sesquichalcogenides like In2Te3 films with those of quantum materials such as Bi2Te3 or Sb2Te3. Femtosecond pump probe and complementary spectroscopic analyses reveal that In2Te3 exhibits remarkably stable optical and vibrational properties across a wide thickness range, attributed to its predominantly covalent bonding network. In contrast, quantum materials based on Bi or Sb display pronounced thickness-dependent responses and strong coupling between coherent phonons and electronic states. These materials demonstrate tunable coherent lattice motions through variations in pump fluence, polarization, and pulse sequencing, offering routes for ultrafast manipulation of quantum states. The comparison highlights a clear distinction between structurally robust semiconducting chalcogenides and highly responsive quantum materials. Together, these findings delineate how bonding character and electronic topology govern ultrafast optical behavior.

DS 21.2 Fri 9:45 REC/C213

Orientation-Dependent Near-Field Infrared Properties of a Chiral SURMOF — •Nadine von Coelln[1], Ana C. Fingolo[2], Benedikt Zerulla[3], Marjan Krstić[4], Christian Huck[1], Carsten Rockstuhl[3,4], Christof Wöll[2], and Petra Tegeder[1] — [1]Institute for Physical Chemistry, Heidelberg University, Germany — [2]Institute of Functional Interfaces — [3]Institute of Nanotechnology — [4]Institute of Theoretical Solid State Physics, Karlsruhe Institute of Technology, Germany

Chiral surface-anchored metal organic frameworks (SURMOFs) are promising candidates for enantioselective separation, molecular sensing and optoelectronic applications with circularly polarized light. Given the large possible design space, it is highly important to understand their spectral response and to be able to predictively model SURMOF structures to determine interesting candidates for experimental screening. In this work, we employ infrared scanning near-field optical microscopy (IR-SNOM) to probe anisotropic infrared properties. Crystallites with two distinct molecular orientations exhibited pronounced differences in their near-field infrared spectra. A controlled manipulation of crystal orientation confirmed that molecular orientation is the origin of these spectral differences. A multi-scale modeling approach, spanning single MOF unit cell simulations to thin-film Maxwell scattering calculations, was validated as it reproduced the spectral signatures and strong orientation sensitivity of the material [1].

[1] A. Fingolo, N. von Coelln et al., *Adv. Funct. Mater.* e24088 (2025).

DS 21.3 Fri 10:00 REC/C213

Pressure-dependent photoluminescence and Raman spectra of GeSn alloys — •Stefan Zollner[1], Sonam Yadav[1], Meghan A. Worrell[1], Preston T. Webster[2], Rigo A. Carrasco[2], and Perry C. Grant[3] — [1]New Mexico State University, Las Cruces, NM, USA — [2]AFRL Space Vehicles Directorate, Albuquerque, NM, USA — [3]Arktonics LLC, Fayetteville, AR, USA

Optical spectra of $Ge_{1-x}Sn_x$ alloys (x<10%) grown on Si by chemical vapor deposition were acquired in a gas-membrane diamond anvil cell at pressures up to 10 GPa. The Si substrate contracts hydrostatically under pressure and imposes a biaxial stress on the thin epitaxial layer. The tetragonal distortion of the layer can be calculated from the bulk modulus of the substrate and the elastic constants of the layer. Room temperature Raman spectra of bulk Ge with 532 nm excitation show a parabolic blueshift from 300 cm^{-1} at atmospheric pressure to 335 cm^{-1} at 10 GPa. The blueshift due to pressure is linear and slightly larger for Ge on Si. We also acquired photoluminescence spectra of $Ge_{1-x}Sn_x$ alloys as a function of temperature and pressure. We observe a blueshift of the infrared $Ge_{1-x}Sn_x$ emission at 10 K of 46 meV/GPa which quenches at 0.6 GPa. For MWIR III/V multiple quantum wells, the blueshift is larger at 77 meV/GPa and the emission quenches at 1.3 GPa.

15 min. break

DS 21.4 Fri 10:30 REC/C213

VIPR: A Modular Machine Learning Framework for Inverse Problems with Application to Reflectometry — •Sascha Creutzburg[1,6], Jeyhun Rustamov[2], Alexandros Koutsioumpas[4], Jens Bornschein[1,6], Marina Ganeva[4], Stefan Häusler[4], Bernd Helm[1,6], Alexander Hinderhofer[5], Mykhailo Levytskyi[4], Valentin Munteanu[5], Robert Juzak[1,6], Vedhas Pandit[2], Frank Schreiber[5], Jeffrey Kelling[2,3], and Nico Mothes[1,6] — [1]Helm & Walter IT-Solutions GmbH, Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf — [3]Chemnitz University of Technology — [4]Jülich Centre for Neutron Science, Heinz Maier-Leibnitz Zentrum — [5]University of Tübingen — [6]Saxony.AI

Ambiguous inverse problems are ubiquitous in experimental physics, where multiple parameter configurations can reproduce the same measurement and classical iterative approaches are often too slow for online analysis. We present the VIPR framework, a modular machine-learning approach for such problems in thin-film reflectometry. Its reflectometry plugin for X-ray and neutron reflectometry combines three approaches: (i) Reflectorch for fast parameter estimation, (ii) prior-amortized neural posterior estimation, and (iii) neural spline flows to capture multimodal posteriors and reveal alternative plausible structures. VIPR features streaming mode for near-real-time beamline feedback and is deployed at Heinz Maier-Leibnitz Zentrum for routine analysis. The framework integrates seamlessly into existing workflows and can be extended to other inverse problems via its plugin architecture. Code: https://codebase.helmholtz.cloud/vipr/vipr-framework

DS 21.5 Fri 10:45 REC/C213

Spectroscopic Imaging Ellipsometry at Cryogenic Temperatures: Uncovering a Structural Phase Change in 2D Polar Ga — •Jakob Henz[1], Arpit Jain[2], Joshua A. Robinson[2], Su Y. Quek[3], and Ursula Wurstbauer[3] — [1]University of Münster — [2]Center for 2DLM, PennState University — [3]Centre for Advanced 2D Materials, National University of Singapore

2D polar metals are a class of atomically thin 2D materials, realized by confinement heteroepitaxial growth (CHet). Hereby, metal atoms are intercalated between a graphene and 6H-SiC interface[1]. This results in a large area, stable 2D metal film with a bonding gradient ranging from covalent over metallic to a vdW-interaction within only two to three atomic layers[2].

Here, we use cryogenic spectroscopic imaging ellipsometry to investigate the temperature dependent light-matter interaction in bilayer 2D polar gallium down to 1 K.

Contrary to theoretical expectations[1], we find a change in the local dielectric response of the material from a homogenous behavior at room temperature to a heterogenous regime at low temperatures, characterized by two absorption peaks localized to distinct surface areas on the sample[3]. This change is interpreted to indicate a structural phase transition in the material.

1 N. Briggs et al., Nat. Mater. **19**.6, 637-643 (2020).
2 M. A. Steves et al., Nano Letters **20**.11, 8312-8318 (2020).
3 J. Henz et al., in preparation (2025).

DS 21.6 Fri 11:00 REC/C213

Adsorption-Driven Vibrational and Electronic Changes on Cu(110) — •Sarang Bhasme, Mariella Denk, and Peter Zeppenfeld — Johannes Kepler University, Linz, Austria

Surface resonant Raman spectroscopy (SRRS) provides a sensitive approach for probing phonons and electron-phonon interactions on metal surfaces through resonant coupling to the surface electronic states.[1] In this work, SRRS combined with reflectance difference spectroscopy is employed to investigate adsorption induced modifications of the vibrational response of Cu(110) under ultra-high-vacuum conditions. Time-resolved SRRS measurements during controlled CO and Oxygen exposure reveal systematic evolution in phonon-related features, indicating changes in surface electronic structures and scattering pathways as adsorption progresses. These data enable comparative assessment of molecule-specific interactions and adsorption dynamics on the same surface.

[1] M. Denk et al., Phys. Rev. Lett. 128, 216101 (2022).

15 min. break

DS 21.7 Fri 11:30 REC/C213

Refining the Tanguy dispersion model for strong direct interband interactions — •Beáta Hroncová and Stefan Zollner — New Mexico State University, Las Cruces, NM, USA

In semiconductors, absorption near the band gap energy is dominated by electron valence-to-conduction band transitions. Exciton formation effectively reduces the band gap and enhances the absorption coefficient. A sharp excitonic peak corresponding to this bound state is observed in the spectral function, especially at low temperatures and low carrier concentrations [1]. At higher temperatures, the bound state is broadened and the peak disappears, but the Sommerfeld enhancement of the absorption persists.

A dispersion model of Wannier–Mott excitons with a screened Coulomb potential was derived by Tanguy [2]. However, if the band gap is small, the interactions between the conduction and valence bands are more prominent. This leads to deviations from the parabolic band curvature, and the effective mass approximation used for the calculation of the excitonic spectra is no longer accurate.

We study the dielectric response of InAs and InSb near the band edge measured by spectroscopic ellipsometry in a wide range of temperatures 50-800 K. With the use of $k \cdot p$ theory, we find the non-parabolicity of the electronic band structure, and describe how to include it in the Tanguy model. Herewith we achieve a better agreement between the theory and the experimental data.

[1] Schweizer et. al., Phys. Rev. Lett. **51**, (1983)
[2] Tanguy, Phys. Rev. B **60**, (1999)

DS 21.8 Fri 11:45 REC/C213

A Novel Characterization Tool for Optical Coatings and Thin Films — •Fabian Felixberger[1,2], Ayesha Khan[1,3], Jonathan Noé[1], Michael Förg[1], Manuel Nutz[1], Simone Strohmair[1], Ines Amersdorffer[1,3], David Hunger[3], Theodor Hänsch[2], and Thomas Hümmer[1] — [1]Qlibri GmbH, Munich — [2]Ludwig Maximilian University of Munich — [3]Karlsruhe Institute of Technology

Thin films and nanostructured surfaces play a crucial role in modern science and technology, with their applications ranging from optical components to biosensors. Their precise characterization is therefore essential for understanding and optimizing their function.

We show that inserting such materials in an optical resonator [1] offers a platform which allows the investigation of minimal amounts of scattering and absorption. In addition, it can be utilised for the detection of defects, deviations from surface flatness and local changes of the refractive index.

By raster-scanning the sample, we obtain spatially resolved maps that allow us to distinguish between point-like defects and extended surface features.

Our results prove that we have developed a versatile and open-access tool for non-destructive and quantitative analysis of optical coatings and thin films, suitable for a wide range of materials.

[1] T. Hümmer et al., Nat Commun. 7, 12155 (2016)

DS 21.9 Fri 12:00 REC/C213

Measuring sub-nanometer oscillations of a thin gold film by a combination of ultrafast imaging ellipsometry and interferometry — •Markus Olbrich[1,2], Theo Pflug[1,3], Andy Engel[1], Andrés Lasagni[2,4], and Alexander Horn[1] — [1]Laserinstitut Hochschule Mittweida, Hochschule Mittweida, Technikumplatz 17, 09648 Mittweida, Germany — [2]Institut für Fertigungstechnik, Technische Universität Dresden, George-Bähr-Str. 3c, 01069 Dresden, Germany — [3]Carl Zeiss SMT GmbH, Carl-Zeiss-Promenade 10, 07745 Jena, Germany — [4]Fraunhofer-Institut für Werkstoff- und Strahltechnik IWS, Winterbergstr. 28, 01277 Dresden, Germany

Measuring the transient dielectric function of laser-excited surfaces by ultrafast optical metrology is crucial for understanding fundamental processes such as the absorption of laser radiation, the dynamics of the electron-phonon non-equilibrium, or material ablation. Thereby, the measured transient dielectric function always represents the sum of changes in the optical properties and topography. To distinguish between these two contributions, a combination of ultrafast ellipsometry and ultrafast interferometry enables solving this problem. To demonstrate the advantage of the combination of both methods, the transient changes in the dielectric function and the surface topography in terms of periodic oscillations due to the induced shock and rarefaction waves are exemplarily demonstrated for an excited thin gold film upon single-pulsed irradiation with ultrafast laser radiation (λ = 800 nm, τ_H = 40 fs) at a fluence of 50 % of the ablation threshold.

DS 21.10 Fri 12:15 REC/C213

Long-term studies of the defect types in tritiated graphene using Raman microscopy — •Genrich Zeller[1], Magnus Schlösser[1], and Helmut H. Telle[2] — [1]KIT-IAP, Karlsruhe, Germany — [2]UAM, Madrid, Spain

Tritium loading of graphene and graphene-like materials is of interest, e.g., in astroparticle physics, where such materials are proposed as sources and targets for neutrino experiments like KATRIN or PTOLEMY, or in hydrogen-isotope separation membranes for nuclear fusion. Although hydrogenation of graphene is well established, the radioactive nature of tritium introduces additional experimental challenges and open questions.

Only in recent years has tritiation of graphene been demonstrated using self-radiolysis of tritium. In that initial proof-of-principle study, we found that tritium exposure not only led to the adsorption of atomic tritium but also to the creation of vacancy defects. A key component of the analysis of tritiated graphene is high-resolution Raman spectroscopy, which allows us to measure defect densities and to determine the nature of the defects. In this work, we follow up on our initial studies, and we observe the evolution of defect types during three years of storage under ambient conditions. We find that graphene adsorption sites become strongly depleted, evidenced by the recovery of the characteristic 2D band and an overall decrease in defect density as tracked by the D/G band ratio. The magnitude of this depletion substantially exceeds the annual reduction expected from tritium β-decay alone, indicating additional removal pathways besides radioactive decay.

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The Dynamics and Statistical Physics Division covers theoretical and experimental activities in all areas of statistical physics, quantum dynamics and many-body systems, nonlinear dynamics and pattern formation, data analysis and machine learning as well as active matter, fluid physics, soft matter, and complex fluids. The DY Division has strong links and joint sessions with the Divisions of Biological Physics (BP), Chemical Physics and Polymers (CPP), Socio- and Econophysics (SOE), and Low Temperatures (TT).

Overview of Invited Talks and Sessions

(Lecture halls HÜL/0186, ZEU/0160, ZEU/0118, and ZEU/0114; Poster P5-ZEU/0250)

Invited Talks

DY 7.1	Mon	9:30–10:00	ZEU/0114	**Fast Rare Events in Exit Times Distributions of Jump Processes** — •Raffaella Burioni
DY 7.6	Mon	11:15–11:45	ZEU/0114	**Large deviations in resetting Brownian motions** — •Satya Majumdar
DY 8.5	Mon	10:30–11:00	ZEU/0118	**Mean-field approach to finite-size fluctuations in coupled oscillator systems** — •Oleh Omelchenko, Georg Gottwald
DY 15.1	Mon	15:00–15:30	ZEU/0114	**Monte Carlo Simulation Methods for Rare-Event Sampling** — •Wolfhard Janke
DY 17.8	Mon	17:00–17:30	ZEU/0160	**Topological transition in filamentous cyanobacteria: from motion to structure** — •Marco Mazza
DY 19.1	Tue	9:30–10:00	HÜL/S186	**Mechanics of entangled fibers** — •Olivier Pouliquen, Aubin Archambault, Ignacio Andrade, Jerome Crassous, Henri Lhuissier, Joël Marthelot
DY 21.7	Tue	11:15–11:45	ZEU/0114	**Why Life Is Hot** — •Tanja Schilling, Patrick Warren, Wilson Poon
DY 28.1	Tue	14:00–14:30	ZEU/0118	**Geometry of turbulent mixing in thermal convection** — •Jörg Schumacher
DY 29.5	Tue	15:00–15:30	ZEU/0160	**Designing topological edge states in bacterial active matter** — Yoshihito Uchida, Daiki Nishiguchi, •Kazumasa A. Takeuchi
DY 34.1	Wed	9:30–10:00	ZEU/0160	**Active turbulence and odd viscosity in a colloidal chiral active system in bulk and in patterned environments** — Joscha Mecke, Yongxiang Gao, •Marisol Ripoll
DY 37.1	Wed	11:15–11:45	ZEU/0118	**Topological defects in 2D amorphous ensembles** — •Peter Keim
DY 40.1	Wed	15:00–15:30	ZEU/0114	**Learning the statistical folding of bacterial chromosomes** — •Chase Broedersz
DY 49.1	Thu	9:30–10:00	ZEU/0160	**Active memory and non-reciprocity as pathways to pattern formation in conserved scalar fields** — •Supropriya Saha, Vaishnavi Gajendragad
DY 55.1	Thu	15:00–15:30	ZEU/0160	**Out-of-equlibrium synthetic cells: the future of active matter** — •Laura Alvarez
DY 55.3	Thu	15:45–16:15	ZEU/0160	**Chemotactic like behavior in by active Brownian particles: from single particles to to polymers** — •Hidde Vuijk
DY 55.5	Thu	16:45–17:15	ZEU/0160	**From non-reciprocal torques towards shape-flexible and res-ponsive prototypic worms** — •Holger Stark, Jeanine Shea
DY 59.7	Fri	11:15–11:45	HÜL/S186	**Anyon dynamics in driven topologically ordered quantum systems** — •Francesco Petiziol
DY 62.1	Fri	9:30–10:00	ZEU/0160	**Morphogenesis, transport, and computation in micro-scale swarms** — •Akira Kakugo

Invited Talks of the joint Symposium SKM Dissertation Prize 2026 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	HSZ/0002	**Stochastic-Calculus Approach to Non-equilibrium Statistical Physics** — •Cai Dieball
SYSD 1.2	Mon	10:00–10:30	HSZ/0002	**Nonuniform magnetic spin textures for sensing, storage and computing applications** — •Sabri Koraltan
SYSD 1.3	Mon	10:30–11:00	HSZ/0002	**Anomalous Quantum Oscillations beyond Onsager's Fermi Surface Paradigm** — •Valentin Leeb
SYSD 1.4	Mon	11:00–11:30	HSZ/0002	**Coherent Control Schemes for Semiconductor Quantum Systems** — •Eva Schöll
SYSD 1.5	Mon	11:30–12:00	HSZ/0002	**On stochastic thermodynamics under incomplete information: Thermodynamic inference from Markovian events** — •Jann van der Meer

Invited Talks of the joint Symposium The Sustainability Challenge: A Decade of Transformation (SYSC)

See SYSC for the full program of the symposium.

SYSC 1.1	Mon	15:00–15:30	HSZ/AUDI	**Open-Endedness and Community-Based Approaches to Sustainability Challenges** — •Hiroki Sayama
SYSC 1.2	Mon	15:30–16:00	HSZ/AUDI	**Education as a Social Tipping Element: Evidence from Climate and Physics Education Research** — •Thomas Schubatzky
SYSC 1.3	Mon	16:00–16:30	HSZ/AUDI	**Mechanistic and Material Perspectives on Enzymatic Hydrolysis of Semicrystalline Polyesters** — •Birte Höcker
SYSC 1.4	Mon	16:45–17:15	HSZ/AUDI	**Decarbonization Options for Industry** — •Uwe Riedel
SYSC 1.5	Mon	17:15–17:45	HSZ/AUDI	**Impacts of Cosmic Dust and Space Debris in the Terrestrial Atmosphere** — •John Plane

Invited Talks of the joint Symposium Fluids with Broken Time-Reversal Symmetry: Odd/Hall Viscosity between Active Matter and Electron Flows (SYBS)

See SYBS for the full program of the symposium.

SYBS 1.1	Tue	9:30–10:00	HSZ/AUDI	**Odd viscosity in three-dimensional fluids: flows, wakes, and eddies** — •Tali Khain
SYBS 1.2	Tue	10:00–10:30	HSZ/AUDI	**Odd viscosity in two-dimensional hydrodynamic electron transport** — •Igor Gornyi, Dmitry Polyakov
SYBS 1.3	Tue	10:30–11:00	HSZ/AUDI	**Odd slip on chiral active surfaces** — •Andrej Vilfan, Yuto Hosaka
SYBS 1.4	Tue	11:15–11:30	HSZ/AUDI	**Parity-odd transport in electron fluids** — •Johanna Erdmenger
SYBS 1.5	Tue	11:30–11:45	HSZ/AUDI	**Curved Odd Elasticity** — Lazaros Tsaloukidis, Yuan Zhou, Jack Binysh, Nikta Fakhri, Corentin Coulais, •Piotr Surówka

Invited Talks of the joint Symposium France: Soft, Active and Alive: Emergent Properties in Living Matter (SYGF)

See SYGF for the full program of the symposium.

SYGF 1.1	Wed	15:00–15:30	HSZ/AUDI	**Liquid crystal geometries in type I collagen-based tissues** — •Nadine Nassif
SYGF 1.2	Wed	15:30–16:00	HSZ/AUDI	**Self-organization of the cytoplasm by physical instabilities** — •Jan Brugues
SYGF 1.3	Wed	16:00–16:30	HSZ/AUDI	**From morphogenesis to space partitioning by microtubules and molecular motors.** — •Manuel Thery
SYGF 1.4	Wed	16:45–17:15	HSZ/AUDI	**More than the sum: how composite interfaces govern function** — •Alba Diz-Muñoz
SYGF 1.5	Wed	17:15–17:45	HSZ/AUDI	**Swimming and Swarming of Intelligent Active Particles** — Segun Goh, Priyanka Iyer, Rajendra Singh Negi, •Gerhard Gompper
SYGF 1.6	Wed	17:45–18:15	HSZ/AUDI	**Perturbing the collective motion of fish with challenging environments** — •Aurélie Dupont

Invited Talks of the joint Symposium Tipping Points in Social and Climate Systems (SYTP)

See SYTP for the full program of the symposium.

SYTP 1.1	Thu	15:00–15:30	HSZ/AUDI	**Social Tipping in Heterogeneous and Polarized Populations** — •Sara Constantino, Sonke Ehret, Elke Weber, Sonja Vogt, Charles Efferson
SYTP 1.2	Thu	15:30–16:00	HSZ/AUDI	**Tipping points and regime shifts in coupled social-climate systems** — •Chris Bauch
SYTP 1.3	Thu	16:00–16:30	HSZ/AUDI	**How to tune Earth system models toward tipping?** — •Sebastian Bathiany, Niklas Boers
SYTP 1.4	Thu	16:45–17:15	HSZ/AUDI	**Algorithmic amplification and contextual sensitivity in political information exposure** — Iris Damião, Ana Vranic, Paulo Almeida, Lília Perfeito, •Joana Gonçalves de Sá
SYTP 1.5	Thu	17:15–17:45	HSZ/AUDI	**The complex interplay between democracy and platform power** — •Philipp Lorenz-Spreen

Sessions

DY 1.1–1.2	Sun	16:00–18:15	HSZ/0004	**Tutorium: Physics of Behavior (joint session SOE/TUT/DY)**
DY 2.1–2.5	Mon	9:30–12:15	HSZ/0003	**Focus Session: New Routes to Localization and Quantum Non-Ergodicity I (joint session TT/DY)**
DY 3.1–3.11	Mon	9:30–12:30	HSZ/0101	**Quantum-Critical Phenomena (joint session TT/DY)**
DY 4.1–4.11	Mon	9:30–12:45	BAR/SCHÖ	**Active Matter I (joint session BP/CPP/DY)**
DY 5.1–5.10	Mon	9:30–12:45	GÖR/0226	**Focus Session: Physics of Behavior (joint session SOE/DY)**
DY 6.1–6.13	Mon	9:30–13:00	HÜL/S186	**Machine Learning in Dynamics and Statistical Physics I**
DY 7.1–7.10	Mon	9:30–12:45	ZEU/0114	**Focus Session: Large Deviations and Rare Events I**
DY 8.1–8.10	Mon	9:30–12:30	ZEU/0118	**Nonlinear Dynamics, Synchronization, and Chaos**
DY 9.1–9.10	Mon	9:30–12:15	ZEU/0160	**Statistical Physics far from Thermal Equilibrium I**
DY 10.1–10.5	Mon	9:30–11:00	ZEU/0260	**Wetting, Fluidics and Liquids at Interfaces and Surfaces I (joint session CPP/DY)**
DY 11.1–11.5	Mon	11:30–12:45	ZEU/0260	**Wetting, Fluidics and Liquids at Interfaces and Surfaces II (joint session CPP/DY)**
DY 12.1–12.6	Mon	15:00–18:00	CHE/0089	**Focus Session: Relaxation Timescales in Open Quantum Systems (joint session TT/DY)**
DY 13.1–13.9	Mon	15:00–17:30	CHE/0091	**Focus Session: New Routes to Localization and Quantum Non-Ergodicity II (joint session TT/DY)**
DY 14.1–14.13	Mon	15:00–18:30	HÜL/S186	**Machine Learning in Dynamics and Statistical Physics II**
DY 15.1–15.12	Mon	15:00–18:30	ZEU/0114	**Focus Session: Large Deviations and Rare Events II**
DY 16.1–16.13	Mon	15:00–18:30	ZEU/0118	**Droplets, Wetting, and Microfluidics (joint session DY/CPP)**
DY 17.1–17.12	Mon	15:00–18:30	ZEU/0160	**Active Matter II (joint session DY/BP/CPP)**
DY 18.1–18.12	Tue	9:30–12:45	BAR/SCHÖ	**Active Matter III (joint session BP/CPP/DY)**
DY 19.1–19.10	Tue	9:30–12:45	HÜL/S186	**Franco-German Session on Granular Matter I**
DY 20.1–20.5	Tue	9:30–11:00	ZEU/LICH	**Focus Session: Water – from Atmosphere to Space I (joint session CPP/DY)**
DY 21.1–21.11	Tue	9:30–12:45	ZEU/0114	**Stochastic Thermodynamics**
DY 22.1–22.10	Tue	9:30–12:15	ZEU/0118	**Pattern Formation**
DY 23.1–23.12	Tue	9:30–12:45	ZEU/0160	**Complex Fluids and Soft Matter (joint session DY/CPP)**
DY 24.1–24.6	Tue	11:15–12:45	ZEU/LICH	**Focus Session: Water – from Atmosphere to Space II (joint session CPP/DY)**
DY 25.1–25.5	Tue	14:00–15:30	HÜL/S186	**Franco-German Session on Granular Matter II**
DY 26.1–26.5	Tue	14:00–15:30	ZEU/LICH	**Focus Session: Water – from Atmosphere to Space III (joint session CPP/DY)**
DY 27.1–27.6	Tue	14:00–15:30	ZEU/0114	**Statistical Physics far from Thermal Equilibrium II**
DY 28.1–28.4	Tue	14:00–15:15	ZEU/0118	**Fluid Physics and Turbulence**
DY 29.1–29.5	Tue	14:00–15:30	ZEU/0160	**Active Matter IV (joint session DY/BP/CPP)**
DY 30.1–30.12	Wed	9:30–12:45	CHE/0091	**Nonequilibrium Quantum Systems I (joint session TT/DY)**
DY 31.1–31.4	Wed	9:30–11:00	GÖR/0226	**Networks, From Topology to Dynamics – Part I (joint session SOE/DY)**
DY 32.1–32.12	Wed	9:30–12:45	HÜL/S186	**Many-body Systems: Equilibration, Chaos, and Localization (joint session DY/TT)**
DY 33.1–33.12	Wed	9:30–12:45	ZEU/0114	**Statistical Physics of Biological Systems I (joint session DY/BP)**
DY 34.1–34.10	Wed	9:30–12:30	ZEU/0160	**Focus Session: Fluids with Broken Time-Reversal Symmetry – Odd/Hall Viscosity Between Active Matter and Electron Flows**
DY 35.1–35.4	Wed	9:30–10:45	ZEU/0260	**Focus Session: Water – from Atmosphere to Space IV (joint session CPP/DY)**

DY 36.1–36.4	Wed	11:00–12:00	ZEU/0260	**Focus Session: Water – from Atmosphere to Space V (joint session CPP/DY)**
DY 37.1–37.5	Wed	11:15–12:45	ZEU/0118	**Glasses and Glass Transition (joint session DY/CPP)**
DY 38.1–38.9	Wed	15:00–17:30	HSZ/0105	**Nonequilibrium Quantum Systems II (joint session TT/DY)**
DY 39.1–39.3	Wed	15:00–15:45	GÖR/0226	**Networks, From Topology to Dynamics – Part II (joint session SOE/DY)**
DY 40.1–40.5	Wed	15:00–16:30	ZEU/0114	**Statistical Physics of Biological Systems II (joint session DY/BP)**
DY 41.1–41.16	Wed	15:00–18:00	P5	**Poster: Nonlinear Dynamics, Granular Matter, and Machine Learning**
DY 42.1–42.15	Wed	15:00–18:00	P5	**Poster: Quantum Dynamics and Many-body Systems (joint session DY/TT)**
DY 43.1–43.24	Wed	15:00–18:00	P5	**Poster: Statistical Physics**
DY 44.1–44.22	Wed	15:00–18:00	P5	**Poster: Active Matter, Soft Matter, and Fluids**
DY 45.1–45.6	Thu	9:30–11:15	GÖR/0226	**Focus Session: Physics of AI – Part I (joint session SOE/DY)**
DY 46.1–46.12	Thu	9:30–12:45	HÜL/S186	**Many-body Quantum Dynamics I (joint session DY/TT)**
DY 47.1–47.11	Thu	9:30–12:30	ZEU/0114	**Statistical Physics: General I**
DY 48.1–48.6	Thu	9:30–11:00	ZEU/0118	**Nonlinear Dynamics and Time-Delay Systems**
DY 49.1–49.11	Thu	9:30–12:45	ZEU/0160	**Active Matter V (joint session DY/BP)**
DY 50.1–50.7	Thu	10:15–12:45	BAR/0106	**Focus Session: Controlling Microparticles and Biological Cells by Ultrasound (joint session BP/CPP/DY)**
DY 51.1–51.6	Thu	11:15–12:45	ZEU/0118	**Networks: From Topology to Dynamics – Part III (joint session DY/SOE)**
DY 52.1–52.12	Thu	15:00–18:15	BAR/SCHÖ	**Statistical Physics of Biological Systems III (joint session BP/DY)**
DY 53.1–53.6	Thu	15:00–16:30	HÜL/S186	**Many-body Quantum Dynamics II (joint session DY/TT)**
DY 54.1–54.10	Thu	15:00–17:45	ZEU/0114	**Statistical Physics: General II**
DY 55.1–55.8	Thu	15:00–18:00	ZEU/0160	**Focus Session: Emergent Transport in Active Systems (joint session DY/BP)**
DY 56	Thu	18:00–19:00	ZEU/0160	**Members' Assembly**
DY 57.1–57.11	Fri	9:30–12:45	BAR/SCHÖ	**Statistical Physics of Biological Systems IV (joint session BP/DY)**
DY 58.1–58.10	Fri	9:30–12:45	GÖR/0226	**Focus Session: Physics of AI – Part II (joint session SOE/DY)**
DY 59.1–59.11	Fri	9:30–12:45	HÜL/S186	**Quantum Chaos and Coherent Dynamics (joint session DY/TT)**
DY 60.1–60.9	Fri	9:30–12:00	ZEU/0114	**Critical Phenomena and Phase Transitions**
DY 61.1–61.7	Fri	9:30–11:15	ZEU/0118	**Brownian Motion and Anomalous Transport**
DY 62.1–62.9	Fri	9:30–12:15	ZEU/0160	**Active Matter VI (joint session DY/BP)**
DY 63.1–63.5	Fri	11:30–12:45	ZEU/0118	**Nonlinear Stochastic Systems**
DY 64.1–64.1	Fri	13:15–14:00	HSZ/0002	**Closing Talk (joint session CPP/BP/DY)**

Members' Assembly of the Dynamics and Statistical Physics Division

Thursday 18:00–19:00 ZEU/0160

Sessions

– Invited Talks, Topical Talks, Tutorials, Contributed Talks, and Posters –

DY 1: Tutorium: Physics of Behavior (joint session SOE/TUT/DY)

The emerging field of the physics of behavior seeks to quantitatively characterize complex behavior in biological agents under naturalistic conditions, using tools from dynamical systems theory and statistical physics. Even in simple organisms, behavioral richness demands new methods of measurement and analysis, as well as new theoretical frameworks. In the absence of a first-principles theory, data-driven approaches are essential, and the many interacting degrees of freedom call for descriptions capable of handling high-dimensional systems.

This tutorial introduces how concepts from dynamical systems theory and statistical physics can be applied to quantify behavior across biological scales and to develop simple yet predictive models. It is intended for physicists at all levels, beginning with graduate students, who are interested in computational approaches to modeling animal behavior. The tutorial is accompanied by an openly accessible code repository to support hands-on exploration of selected topics.

Time: Sunday 16:00–18:15 Location: HSZ/0004

See SOE 1 for details of this session.

DY 2: Focus Session: New Routes to Localization and Quantum Non-Ergodicity I (joint session TT/DY)

This session explores how quantum many-body systems can fail to thermalize through mechanisms that extend beyond conventional many-body localization. Recent work has discovered new mechanisms that lead to non-ergodic behavior, including Hilbert-space fragmentation, disorder-free localization, and confinement effects that arise from destructive interference in Fock space. At the same time, experiments with ultracold atoms, trapped ions, Rydberg platforms, and superconducting qubits directly reveal many-body scars, slow relaxation, and unusual transport. This session highlights these developments and identifies the central open questions that are now driving the field forward.

Coordinators: Roderich Moessner (MPI PKS Dresden), Frank Pollmann (TU München)

Time: Monday 9:30–12:15 Location: HSZ/0003

Topical Talk DY 2.1 Mon 9:30 HSZ/0003

Eigenstate thermalization in thermal first-order phase transitions — •Maksym Serbyn — IST Austria, Am Campus 1, 3400 Klosterneuburg

In my talk I will discuss the fate of eigenstates in quantum systems in vicinity of thermal first order phase transition. The eigenstate thermalization hypothesis (ETH) posits how isolated quantum many-body systems thermalize, assuming that individual eigenstates at the same energy density have identical expectation values of local observables in the limit of large systems. In my talk I will show that ETH requires generalization in the presence of thermal first-order phase transitions. I will argue that for energies in the vicinity of the thermal phase transition, eigenstate expectation values do not need to converge to the same thermal value. The system has a regime with coexistence of two classes of eigenstates corresponding to the two branches with distinct expectation values at the same energy density, and another regime with Schrodinger-cat-like eigenstates that are inter-branch superpositions; these two regimes are separated by an eigenstate phase transition. I will also discuss potential extensions of these results to more physical models, and outline how the special structure of eigenstates near first order phase transition can be probed via quench dynamics.

Topical Talk DY 2.2 Mon 10:00 HSZ/0003

Stabilizing Floquet orders to infinite time — •Anushya Chandran[1], Shreyas Raman[2], Robin Schäfer[3], and Alicia Kollàr[4] — [1]Boston University, Boston, USA — [2]Boston University, Boston, USA — [3]Helmholtz-Zentrum Berlin, Berlin, Germany — [4]University of Maryland, College Park, USA

Floquet engineering, in which the properties of a quantum system are modified through the application of strong periodic drives, is an indispensable tool in atomic and condensed matter systems. It enables quantum simulation, the dynamic stabilization of unstable states, and the realization of exotic topological order and time crystals. However, it is inevitably limited by intrinsic heating processes, so that the engineered states are, at best, pre-thermal. I will describe a general-purpose dissipative scheme that autonomously cools a strongly driven system to close to a desired Floquet engineered state. I will demonstrate this stabilization in a driven many-body spin chain, that either spontaneously breaks a symmetry or exhibits discrete time-crystalline order in the steady state.

Topical Talk DY 2.3 Mon 10:30 HSZ/0003

Dynamical landscape of out of equilibrium emergent lattice gauge theories in two dimensions — •Nilotpal Chakraborty — University of Cambridge

Many-body models with local constraints, such as dimer, ice or generally quantum link type models often are described as emergent gauge theories. I will describe a range of recent results, comprising classical and quantum dynamics of different kind, highlighting the rich dynamical phenomenology present in these models. In line with the session's topic, I will focus more on the two-dimensional U(1) quantum link model, and highlight its potential as a new route toward localisation and non-ergodicity in the absence of quenched disorder. In doing so, I will also present spectral signatures of such localization. Finally, I will end by discussing possibilities of realising the different constrained models and their dynamics in quantum simulators, for which there appears to be palpable current interest.

15 min. break

Topical Talk DY 2.4 Mon 11:15 HSZ/0003

Interference, topology, and new Hilbert-space routes to quantum non-ergodicity — •Yi-Ping Huang[1,2,3] and Tao-Lin Tan[1] — [1]Department of Physics, National Tsing Hua University, Hsinchu 30013, Taiwan — [2]Physics Division, National Center for Theoretical Sciences, Taipei 10617, Taiwan — [3]Institute of Physics, Academia Sinica, Taipei 115, Taiwan

A central challenge in nonequilibrium quantum physics is to understand why certain many-body systems fail to thermalize even in the absence of disorder or integrability. In this talk, I will outline a different perspective in which non-ergodicity is governed by hidden geometric structures in Hilbert space rather than by conventional real-space mechanisms. This viewpoint leads to the concept of interference-caged quantum many-body scars (ICQMBS), where exact many-body destructive interference confines eigenstates to small regions of the Fock-space graph. Remarkably, interference zeros and graph automorphisms emerge as universal organizing principles, revealing a class of topological ICQMBS whose robustness originates from local Fock-space topology rather than symmetries or constraints. This framework not only explains diverse non-ergodic phenomena from one-dimensional systems to two-dimensional gauge

models but also provides new tools for systematically identifying them. I will end with a brief look at stabilizing QMBS through the lens of Kramers-Wannier duality, illustrating the challenges and possibilities that arise when studying QMBS under duality.

Topical Talk DY 2.5 Mon 11:45 HSZ/0003

Fock-space cages and their spectral signatures — •Cheryne Jonay — University of Ljubljana

Generic quantum many-body systems thermalize. Yet several mechanisms can prevent this, notable examples include integrability, many-body localization, Hilbert-space fragmentation, and scars. We will discuss a new mechanism of ergodicity breaking that arises from destructive interference in Fock space. This leads to exact eigenstates localized on polynomially many configurations within an exponentially large, fully connected Hilbert space sector. We call these states Fock-space cages. They emerge naturally in kinetically constrained models with chiral symmetry. We will present graph-theoretic methods to explicitly construct cages with support ranging from O(1) to O(L) sites, and examine how their dynamical signatures, such as return probabilities and magnetization, resist thermalization. Finally, we will explore the spectral statistics through the lens of chiral random matrix theory. The exponentially degenerate zero-energy manifold produces distinctive signatures, yet the agreement with random matrix predictions varies across energy scales - a direct consequence of localized and thermal eigenstates coexisting within the same Hilbert space sector. We will also probe the stability of these phenomena: the gap between the zero-energy manifold and the spectral bulk may give rise to protected slow dynamics.

DY 3: Quantum-Critical Phenomena (joint session TT/DY)

Time: Monday 9:30–12:30 Location: HSZ/0101

See TT 2 for details of this session.

DY 4: Active Matter I (joint session BP/CPP/DY)

Time: Monday 9:30–12:45 Location: BAR/SCHÖ

DY 4.1 Mon 9:30 BAR/SCHÖ

Bayesian inference of magnetosensing in a magnetotactic bacterium — •Sascha Lambert[1], Emilie Gachon[2], Damien Faivre[2], and Stefan Klumpp[1] — [1]University of Göttingen, Institute for the Dynamics of Complex Systems, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany. — [2]Aix Marseille Université, CEA, CNRS, BIAM, 13115 Saint-Paul-Lez-Durance, France.

Magnetotactic bacteria are often assumed to align only passively with external magnetic fields, yet recent observations of the magnetotactic bacterium SS-5 reveal a pronounced increase in swimming speed under geomagnetic conditions. Because flagellated microorganisms typically follow helical paths, magnetic torques could, in principle, straighten their trajectories and create an apparent increase in speed, offering a purely mechanical explanation. We test this hypothesis using a physical swimming model based on Active Brownian Particles that incorporates magnetic torques, rotational propulsion, and helical motion, and we explore the relevant parameter space using Bayesian inference constrained by three-dimensional trajectory data. Posterior predictive simulations demonstrate that the mechanically induced increase in apparent speed is far too small to account for the experimental observations, even under extreme parameter choices. The results quantitatively rule out swaying as a sufficient explanation for the behaviour of SS-5 and instead support the presence of an active magnetic sensing mechanism.

DY 4.2 Mon 9:45 BAR/SCHÖ

Vorticity-induced surfing and trapping in porous media — •Pallabi Das[1], Mirko Residori[1], Axel Voigt[2,3,4], Suvendu Mandal[5], and Christina Kurzthaler[1,3,4] — [1]Max Planck Institute for the Physics of Complex Systems, Germany — [2]Institute of Scientific Computing, TU Dresden, Germany — [3]Center for Systems Biology Dresden, Germany — [4]Cluster of Excellence, Physics of Life, TU Dresden, Germany — [5]TU Darmstadt, Germany

Microorganisms often encounter strong confinement and complex hydrodynamic flows while navigating their habitats. Combining finite-element methods and stochastic simulations, we study the interplay of active transport and heterogeneous flows in dense porous channels. We find that swimming always slows down the traversal of agents across the channel, giving rise to robust power-law tails of their exit-time distributions. These exit-time distributions collapse onto a universal master curve with a scaling exponent of $\approx 3/2$ across a wide range of packing fractions and motility parameters, which can be rationalized by a scaling relation. We further identify a new motility pattern where agents alternate between *trapping* along fast streams and extended *surfing* phases, the latter determining the power-law exponent. Unexpectedly, trapping occurs in the flow backbone itself – not only at obstacle boundaries – due to vorticity-induced reorientation in the highly-heterogeneous flow environment. These findings provide a fundamentally new active transport mechanism with direct implications for biofilm clogging and the design of novel microrobots capable of operating in heterogeneous media.

DY 4.3 Mon 10:00 BAR/SCHÖ

Adhesion Patterns in Gliding Filamentous Cyanobacteria — •Elias Fischer[1], Paul Nieschwitz[2], Stefan Karpitschka[2], and Holger Stark[1] — [1]Institute of Physics and Astronomy, TU Berlin, Germany — [2]Department of Physics, Universität Konstanz, Germany

Filamentous cyanobacteria play an important role in many ecosystems and the carbon cycle of our planet. They exhibit gliding motility when in contact with solid surfaces or each other. Despite their ecological relevance and increased use in biotech applications, the exact nature of the force-generating process remains not fully understood.

Our recent measurements of filamentous cyanobacteria gliding across flat surfaces and visualized in kymographs show spatio-temporal adhesion regions along the filament, indicating an intrinsic helical shape. Based on our a novel approach for modeling the mechanical aspects of individual cyanobacteria filaments, we are able to interpret the complex kymograph patterns. Each filament is modeled as a helical chain of thin cylindrical segments in 3D with bending and twisting elasticity. The filaments interact with nearby surfaces and filaments via a hard-core repulsion and an exponentially decaying adhesion force. Importantly, the propulsion forces that push the filament forward are only applied locally at surface-contacting segments.

Our simulated kymographs reveal how both the helical shape and the adhesion strength strongly influence the filament's gliding speed and the dynamics of the surface-attachment regions. Thereby, we crucially contribute to the understanding of how real filamentous cyanobacteria generate their propulsion forces.

DY 4.4 Mon 10:15 BAR/SCHÖ

The 3D chirality of malaria parasites determines their motion patterns in 2D and originates at the apical pole — •Leon Lettermann[1], Mirko Singer[2], Smilla Steinbrück[2,3], Falko Ziebert[1], Sachie Kanatani[3], Photini Sinnis[3], Friedrich Frischknecht[2], and Ulrich Schwarz[1] — [1]Institute for Theoretical Physics & BioQuant, Heidelberg University — [2]Parasitology, Center for Infectious Diseases, Heidelberg University — [3]School of Public Health and Malaria Research Institute, Johns Hopkins University

Plasmodium sporozoites, the slender forms of the malaria parasite injected by mosquitoes into the skins of their vertebrate hosts, provide a medically highly relevant model system for active chiral particles. Using 3D tracking in synthetic hydrogels, we show that sporozoites consistently move on right-handed helical trajectories. When they encounter a two-dimensional substrate, they switch to clockwise circular motion, whereas circling on glass in medium occurs with the opposite sense of rotation, suggesting on glass they try to invade the medium above. Using a sandwich assay, we demonstrate that chirality also determines the reverse transition from two-dimensional to three-dimensional motion. Combining these measurements with a theory for gliding motility allows us to identify the likely origin of chirality, namely an asymmetric distribution of adhesins. After confirming this via two-sided traction force microscopy, we finally use STED super-resolution microscopy to reveal a corresponding tilt in the apical ring complex. In summary, our analysis thus uncovers both the biological relevance and the molecular basis of chirality in the movement of malaria parasites.

DY 4.5 Mon 10:30 BAR/SCHÖ

Squirmer dynamics in porous environments — •Mirko Residori[1], Christina Kurzthaler[1], and Sebastian Aland[2] — [1]Max Planck Institute for the Physics of Complex Systems — [2]TU Freiberg

We introduce a computational framework for simulating the dynamics of microswimmers in complex porous environments. Specifically, we adopt a diffusive domain approach to represent the surface of a micro-swimmer, modeled as a squirmer. This method ensures accurate and stable finite-element simulations, even in highly confined geometries. Validation against analytical and numerical benchmarks confirms the model*s accuracy and robustness. We then apply it to explore squirmer motion in heterogeneous porous media, revealing how

hydrodynamic interactions lead to behaviors such as dynamic trapping due to hydro-dynamically induced re-orientations. Moreover, we demonstrate that the squirmer parameter and the repulsive potential critically influence a squirmer's ability to navigate and escape confinement. The proposed framework offers a versatile and efficient tool for studying active motion in complex fluids and provides new insights into micro-swimmer transport and control in natural and engineered systems.

DY 4.6 Mon 10:45 BAR/SCHÖ

Dynamics of passive tracers in active dumbbell suspension — •Chandranshu Tiwari and Sunil P. Singh — Department of Physics, Indian Institute of Science Education and Research, Bhopal 462066, India.

The transport of passive tracers in active fluids exhibits rich dynamics arising from persistent interactions between active agents and the tracer. In our work, we employ Brownian dynamics simulations to investigate the dynamical behaviour of both isotropic(circular) and anisotropic(elliptical) tracers in active dumbbell suspension, considering only steric interactions. For circular tracers, we find that the speed shows a crossover from monotonically decreasing to increasing with tracer size as the dumbbells' speed is increased. The tracer's effective diffusion also displays a non-monotonic dependence on area fraction: the diffusivity first increases and then decreases at higher area fractions.

For anisotropic tracers, the characteristic non-monotonic trend persists. Moreover, their motion along the major and minor axes differs significantly. Anisotropic accumulation of active particles around the tracer generates direction-dependent forces and fluctuations, favouring motion along the major axis. Consequently, both the speed and diffusivity along the major axis exceed those along the minor axis.

15 min. break

Invited Talk DY 4.7 Mon 11:15 BAR/SCHÖ

Modeling and inference of magnetotactic motility in complex environments — •Stefan Klumpp — Institute for the Dynamics of Complex Systems, University of Göttingen, Göttingen, Germany

Magnetotactic bacteria orient themselves and swim along field lines of the geomagnetic field. Their magnetically directed self-propelled motion makes them an instance of dipolar active matter. Here we focus on the interaction of these bacteria with walls or obstacles. Experiments in microfluidic systems show that interactions with walls result in (possibly transient) alignment parallel to the wall, which may compete with the alignment with the magnetic field. The dynamic behavior arising from the competition of the two alignments includes U-turn trajectories in circular chambers and trapping and escape dynamics in channels with overlapping cylindrical obstacles. In a phenomenological picture, the resulting motion can be described in an Active Brownian Particle model by introducing a wall torque that competes with the magnetic torque, which results in good agreement with experimental observations. Systematic Bayesian inference of the wall torque from observations shows that only a part of the torque function (dependence on incident angle) can be learned reliably from the data.

DY 4.8 Mon 11:45 BAR/SCHÖ

Quantifying aggregation behaviour of filamentous cyanobacteria — •Elias Illing and Stefan Karpitschka — Fachbereich Physik, Universität Konstanz

Cyanobacteria are ubiquitous in nature, frequently causing ecological and economic harm by explosive growth, so called blooms.

We investigate the collective dynamics of entangled filamentous cyanobacteria in open liquid media, reminiscent of their aggregates found during later stages of blooms. We investigate the impact of illumination on the clustering and spreading of the bacteria and quantify the morphology of the bacterial aggregates by image analysis. We determine the critical density necessary for initial clustering and track the evolution of the subsequent stages, ranging from stable clusters to spreading mats. These states can be modulated by light intensity variations, potentially allowing for control of the morphological evolution of cyanobacterial aggregates.

DY 4.9 Mon 12:00 BAR/SCHÖ

Dynamically Induced Spatial Segregation in Multi-Species Bacterial Bioconvection — •Mingqi Yan[1,2], Chenxi Wang[3], Oscar Gallardo-Navarro[4], Rinat Arbel-Goren[4], Joel Stavans[4], and Erwin Frey[1,2] — [1]Department of Physics, Ludwig-Maximilians-Universität München, Theresienstraße 37, 80333 München, Germany — [2]Max Planck School Matter to Life, Hofgartenstraße 8, 80539, München, Germany — [3]School of Science, Harbin Institute of Technology, 518055, Shenzhen, China — [4]Department of Physics of Complex Systems, Weizmann Institute of Science, 7610001, Rehovot, Israel

Bacterial bioconvection is a classic example of collective behavior in active matter, where upward-swimming bacteria create density instabilities leading to large-scale fluid flows. While this phenomenon is well-studied in single-species suspensions, natural environments are typically inhabited by diverse microbial communities. Here, we investigate the collective dynamics of multi-species bacterial suspensions. Combining experiments with a continuum model, we show that different bacterial species can spontaneously segregate into stable, spatially interlocked domains. Our theoretical analysis reveals that this segregation is not driven by biochemical antagonism but rather by the interplay between species-specific motility characteristics and the self-generated hydrodynamic flows. This work provides new insights into how physical interactions alone can drive the spatial organization of complex microbial communities.

DY 4.10 Mon 12:15 BAR/SCHÖ

Light-switchable microbial rafts at air-liquid interfaces — •Gustav F. Nolte, Alexandros A. Fragkopoulos, Timo Völkl, Mechthild Rappold, and Oliver Bäumchen — University of Bayreuth, Experimental Physics V, 95447 Bayreuth, Germany

In biological active matter, clustering occurs across a wide range of time and length scales, from molecular assemblies such as actomyosin networks to macroscopic systems like fire ant rafts. Here, we report on a fast, light-switchable, and fully reversible clustering phenotype on the microscale, observed at air-liquid interfaces: the raft formation of the biciliated microalga *Chlamydomonas noctigama*.

C. noctigama is a relative of the model organism *Chlamydomonas reinhardtii*, which exhibits light-switchable adhesion and subsequent clustering at solid-liquid interfaces [1,2]. We show how the cluster morphology depends on cell density and discuss potential growth mechanisms by analyzing dynamics of individual clusters. Furthermore, we characterize the dependence of raft formation on the light spectrum and interfacial free energy. Using micropipette force spectroscopy [3], we show that single cells exploit capillary forces for light-switchable ciliary adhesion to the air-liquid interface, enabling raft formation. In their natural habitats, reversible clustering may provide an advantage by allowing cells to accumulate in locations optimal for photosynthesis while increasing resilience to environmental stress.

[1] C. T. Kreis, et al., *Nat. Phys.* **14**, 45 (2018).
[2] S. Till, et al., *Phy. Rev. Res.* **4**, L042046 (2022).
[3] M. Backholm and O. Bäumchen, *Nat. Protoc.* **14**, 594-615 (2019).

DY 4.11 Mon 12:30 BAR/SCHÖ

Circadian gravitaxis: Photosynthetic microswimmers remodel local pH to actively tune vertical migration — Arkajyoti Ghoshal[1], Soumitree Mishra[1], Jayabrata Dhar[2], Hans-Peter Grossart[3,4], and •Anupam Sengupta[1,5] — [1]Physics of Living Matter, Department of Physics and Materials Science, University of Luxembourg, Luxembourg — [2]Department of Mechanical Engineering, National Institute of Technology Durgapur, India — [3]Department of Plankton and Microbial Ecology, Leibniz Institute of Freshwater Ecology and Inland Fisheries, Stechlin, Germany — [4]Institute of Biochemistry and Biology, Potsdam University, Germany — [5]Institute for Advanced Studies, University of Luxembourg, Luxembourg

Motile phytoplankton shuttle between bright surface waters and deeper nutrient rich layers, usually controlled by internal circadian clocks. Yet many species show irregular movements, defying the expected circadian rhythm. Studying a bloom forming photosynthetic species, we found that cells adjust their vertical migration by altering local pH, mediated by a shift in their gravitactic behavior. This self-modulation of pH generates sub-populations which are physiologically similar but swim differently, remaining vertically separated even under uniform conditions. Supported by a cell-level analysis and mathematical model, we confirm that the pH-mediated circadian shift is underpinned by morphological adjustments. Our results support a circadian gravitactic model in which diurnal pH control drives diversified migration, enhancing fitness particularly in acidifying oceans.

DY 5: Focus Session: Physics of Behavior (joint session SOE/DY)

Organizers: Greg Stephens (Vrije Univ. Amsterdam), Pawel Romanczuk (HU Berlin)

Physics has made important contributions to the remarkable progress in characterizing the molecules, cells, and circuits that generate natural behavior. Yet our understanding of behavior at the scale of the whole organism and in ecological and social contexts remains significantly less advanced. Even in simpler organisms, natural behavior is complex, requiring new tools for measurement (often through novel imaging), analysis, and theoretical insight. The emerging field of the physics of behavior addresses this gap by seeking to quantitatively characterize complex behavior in naturalistic settings. This focus session will highlight recent advances at the intersection of physics, neuroscience, biology, and social sciences with contributions from both theorists and experimentalists.

Time: Monday 9:30–12:45 Location: GÖR/0226

See SOE 2 for details of this session.

DY 6: Machine Learning in Dynamics and Statistical Physics I

Time: Monday 9:30–13:00 Location: HÜL/S186

DY 6.1 Mon 9:30 HÜL/S186

Reservoir Computing with Hydrodynamically Coupled Active Colloidal Oscillators — •Veit-Lorenz Heuthe[1], Lukas Seemann[1], Samuel Tovey[2], and Clemens Bechinger[1,3] — [1]Universität Konstanz, Konstanz, Germany — [2]Universität Stuttgart, Stuttgart, Germany — [3]Centre for the Advanced Study of Collective Behavior, Konstanz, Germany

Reservoir computing is a newly emerging framework that exploits the dynamical response of complex physical systems to external perturbations. The high-dimensional, non-linear dynamics of active matter systems with hydrodynamic interactions offsers great potential for highly tunable physical reservoirs. Here, we present a physical reservoir that exploits the hydrodynamic interactions between several hundred colloidal oscillators for chaotic timeseries forecasting. We demonstrate that the inherent memory in this system facilitates detection of hidden anomalies in non-Markovian time-signals. Our results highlight the potential of active matter for locating subtle, non-disruptive signatures in e.g. financial stock markets, physiological measurements or seismic and climate data. Achieving such computing functinalities in physical systems could enable the development of intelligent hardware for edge-computing.

DY 6.2 Mon 9:45 HÜL/S186

From Phase-Space Fluctuations to Predictive Power: Entropy Production as a Metric for Swarm Reservoir Computing — •Patrick Egenlauf[1,2] and Miriam Klopotek[1,3] — [1]University of Stuttgart, Stuttgart Center for Simulation Science, SimTech Cluster of Excellence EXC 2075, Stuttgart, Germany — [2]University of Stuttgart, Interchange Forum for Reflecting on Intelligent Systems, IRIS3D, Stuttgart, Germany — [3]Heidelberger Akademie der Wissenschaften, WIN-Kolleg, Heidelberg, Germany

In reservoir computing, a time-varying input is projected onto a high-dimensional state space, allowing a simple linear readout to retrieve task-relevant features. Physical substrates such as active-matter swarms promise efficient, low-energy computation, but a quantitative selection criterion, that reliably indicates a good reservoir, is missing. We simulated an interacting swarm subjected to an external driver and evaluated two entropy measures: system entropy, quantifying phase-space density fluctuations, and environment entropy, representing heat dissipation. For each parameter set of the swarm interactions, we computed the relative differences for the system and environment entropy between undriven and driven cases and measured the driver work performed on the system. Both relative differences display robust linear correlations with forecast accuracy, while the driver work matches the performance curve almost perfectly, indicating that driver-induced entropy production dominates the reservoir's information-processing capacity. Consequently, entropy production offers a quantitative metric for tuning swarm-based reservoirs toward optimal performance.

DY 6.3 Mon 10:00 HÜL/S186

Performing inference with physical response: Reservoir computing with active matter substrates — Mario U. Gaimann[1] and •Miriam Klopotek[1,2] — [1]University of Stuttgart, Stuttgart Center for Simulation Science, SimTech Cluster of Excellence EXC 2075, Stuttgart, Germany — [2]WIN-Kolleg of the Young Academy, Heidelberg Academy of Sciences and Humanities, Heidelberg, Germany

We explore questions of real-time inference and forecasting of chaotic signals, re-interpreting them in terms of nonequilibrium physical response, by studying a model of information processing with an active matter substrate used in the reservoir computing (RC) paradigm. The system becomes robustly optimal for computing in a particular dynamical regime due to its intrinsic ability to relax efficiently, which, under driving, unlocks maximal dynamical diversity and susceptibility to chaotic input signals; the mechanisms include self-healing, multi-step dynamical response, and adaptive morphological reorganization [1,2]. Shifting the system's response away from direct-agent toward collective variables is key, as evidenced by cross-correlative functions in dynamics [2]. These ideas shed light on self-optimizing inference in bio-inspired or material computing that flexibly exploits dynamics across diverse collective scales.

[1] M. U. Gaimann and M. Klopotek, arXiv:2505.05420 (2025).
[2] M. U. Gaimann and M. Klopotek, arXiv:2509.01799 (2025).

DY 6.4 Mon 10:15 HÜL/S186

Learning single and multiple chaotic systems with minimal reservoir computers — •Francesco Martinuzzi and Holger Kantz — Max Planck Institute for the Physics of Complex Systems

Chaotic dynamics are present in a multitude of natural and engineered systems. Recently, chaos has been modeled using machine learning (ML) methods thanks to their ability to infer underlying governing equations without directly accessing them. Among ML models, echo state networks (ESNs) have been widely investigated because of their simple construction and efficient training. However, ESNs typically rely on randomly initialized reservoirs whose stochastic connectivity makes them difficult to interpret and tune. To what extent are random and complex reservoir topologies actually necessary for learning chaotic dynamics with ESNs? We show that deterministic constructions of the reservoir matrix outperform random initializations for the reconstruction of chaotic attractors. By testing ten distinct deterministic topologies against random reservoirs on over 90 different attractors, our results demonstrate consistently better performance for deterministic reservoirs. Furthermore, we show how the same deterministic reservoir topologies can be leveraged to learn multiple chaotic systems with a single reservoir computer, thereby showcasing multifunctionality.

DY 6.5 Mon 10:30 HÜL/S186

Understanding task performance of time-multiplexed optical reservoir computing via polynomial expansion — •Elias Koch[1], Julien Javaloyes[2], Svetlana V. Gurevich[1,3], and Lina Jaurigue[4] — [1]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str.9 48149 Münster, Germany — [2]Departament de Física and IAC3, Universitat de les Illes Balears, Campus UIB 07122 Mallorca, Spain — [3]Center for Data Science and Complexity (CDSC), University of Münster, Corrensstrasse 2, Münster, 48149, Germany — [4]Institute of Physics, Technische Universität Ilmenau , 98693 Ilmenau, Germany

We study the dynamics of a reservoir computer, realized as a linear optical microcavity with a time-multiplexed injection stream. In the first step, the output is processed with different nonlinearities, allowing to analyze the resulting polynomials and to what extend they can approximate different tasks. To that end, we compare two different discrete tasks, both derived from the Lorenz system through integration with a Runge-Kutta (4) scheme, but sampled to different stepsizes. There, we identify the respective underlying polynomial map and discuss the occuring terms. We compare these results with the impact of employing nonlinear nodes by introducing a Kerr nonlinearity in the optical microcavity.

DY 6.6 Mon 10:45 HÜL/S186

Physical Reservoir Computing with Ferroelectric Oxides for Time-series Classification Tasks — •Atreya Majumdar[1], Yan Meng Chong[2], Dennis Meier[1,2,3], and Karin Everschor-Sitte[1] — [1]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [2]Department of Materials Science and Engineering, Norwegian University of Science and Technology (NTNU), Trondheim, Norway —

[3]Research Center Future Energy Materials and Systems, Research Alliance Ruhr, Bochum, Germany.

Physical reservoir computing leverages the intrinsic complexity, non-linearity, and fading memory of material systems to process temporal data for solving time-series pattern recognition tasks. Magnetic and ferroelectric materials have recently emerged as promising reservoir computers, offering dynamics well suited for processing time-dependent signals [1]. Here, we demonstrate that the photocurrent dynamics of the ferroelectric semiconductor ErMnO3 can be harnessed as an effective physical reservoir for real-time time-series classification. Moreover, the relaxation time of the photocurrent can be controllably tuned, providing flexibility to capture different temporal features and thereby enhancing performance. Altogether, the results highlight the potential of ferroelectric oxides as scalable, energy-efficient platforms for real-time physical reservoir computing.

[1] K. Everschor-Sitte, et al., Topological magnetic and ferroelectric systems for reservoir computing. Nat. Rev. Phys. 6, 455 (2024).

15 min. break

DY 6.7 Mon 11:15 HÜL/S186

Checking the superiority of multi-model mean forecasts by reservoir computing — Daniel Estevez Moya[1,3], Erick A. Madrigal Solis[1,2], Ernesto Estevez Rams[3], and •Holger Kantz[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]University of Techology, Dresden, Germany — [3]Faculdad de Física, Universidad de La Habana, Cuba

In weather prediction and climate forecasts it has been observed that taking the arithmetic mean forecast of an ensemble of different models is often superior to most of the individual models. We use Reservoir Computing to generate easily a large ensemble of models and study their performance on deterministic toy models. While each individually trained reservoir comes with its own model error which is a systematic error, we verify that the arithmetic mean of these forecasts is closer to the truth than most of the individual forecasts. We present a detailed dynamical explanation for this observation.

DY 6.8 Mon 11:30 HÜL/S186

Controlling dynamical systems into unseen target states using machine learning — Daniel Köglmayr[1,2], Alexander Haluszczynski[3], and •Christoph Räth[1,2] — [1]Deutsches Zentrum für Luft- und Raumfahrt (DLR) — [2]Ludwig-Maximilians-Universität (LMU) — [3]Allianz Global Investors (AGI)

Controlling nonlinear dynamical systems is a central task in many different areas of science and engineering. Combining previous work on controlling chaotic systems to arbitrary states [1] and extrapolating the system behavior into unseen parameter regions [2] using machine learning, we present here a novel, model-free, and data-driven methodology for controlling complex dynamical systems into previously unseen target states, including those with significantly different and complex dynamics. Leveraging a parameter-aware realization of next-generation reservoir computing (NGRC), our approach accurately predicts system behavior in unobserved parameter regimes, enabling control over transitions to arbitrary target states utilizing a new prediction evaluation and selection scheme [3]. By extending the applicability of machine learning-based control mechanisms to previously inaccessible target dynamics, this methodology opens the door to transformative new applications while maintaining exceptional efficiency. Our results highlight reservoir computing as a powerful alternative to traditional methods for dynamic system control.

[1] A. Haluszczynski & C. Räth, Sci Rep 11, 12991 (2021), [2] D. Köglmayr & C. Räth, Sci Rep 14, 507 (2024), [3] D. Köglmayr, A. Haluszczynski & C. Räth, submitted (https://arxiv.org/abs/2412.10251)

DY 6.9 Mon 11:45 HÜL/S186

Noise-Balanced Sparse Grid Surrogates for Multiscale Coupling of Monte Carlo and Continuum Models — •Tobias Hülser and Sebastian Matera — Fritz-Haber-Institut der MPG, Berlin

Incorporating a high-fidelity microscopic Monte Carlo model into multiscale simulations can easily become intractable, implying the necessity of surrogate models in many practical applications. Unfortunately, if the microscopic model depends on many macro-variables this can become quite challenging due to the 'curse of dimensionality'. Furthermore, the sampling noise in the underlying Monte Carlo data can lead to uncontrolled errors corrupting the surrogate even though it would be highly accurate in the case of noise-free data. To address these points, we have developed a novel sparse grids interpolation approach which balances interpolation and noise induced errors complemented by a multilevel on-the-fly construction during the multi-scale simulation. Besides its efficiency, an appealing feature is the ease of use of the approach with a single hyperparameter controlling the whole surrogate construction - from which data needs to be created (and how accurately) to the surrogate's accuracy with guaranteed convergence. We demonstrate the approach on examples from heterogenous catalysis, incorporating microscopic kinetic Monte Carlo models into convection-diffusion type reactor scale simulations.

DY 6.10 Mon 12:00 HÜL/S186

Learning Time Trajectories of a Stochastic Dynamical System with a Slowly Varying Parameter — •Changho Kim[1], Zihan Xu[1], Andrew Nonaka[2], and Yuanran Zhu[2] — [1]University of California, Merced, California, USA — [2]Lawrence Berkeley National Laboratory, Berkeley, California, USA

The statistics-informed neural network (SINN) is a reliable machine learning approach for learning and reproducing stochastic trajectories based on the statistical properties of sample trajectory data, particularly for stationary, Gaussian-like, multidimensional stochastic processes. However, to enable practical applications–such as surrogate modeling for the development of hybrid simulation methods–SINN must be extended to learn quasi-stationary dynamics driven by a slowly varying parameter. We enhance the SINN framework by incorporating this parameter as an additional input and by introducing loss functions to capture its influence, as well as proposing a new neural network structure that takes both white noise sequences and time trajectories of the slowly varying parameter as inputs. Additionally, we propose an alternative method for estimating a conditional probability density function to address computational constraints. We validate our approach through two benchmark problems: the dissociative adsorption problem and Langevin dynamics in an oscillating double-well potential.

DY 6.11 Mon 12:15 HÜL/S186

Learning spatiotemporal patterns from mean-field data — •Edmilson Roque dos Santos[1] and Tiago Pereira[2] — [1]MPI-PKS,Germany — [2]University of São Paulo, Brazil

Networks of coupled dynamical systems are fundamental models across the sciences, from physics to neuroscience. Despite their success, the governing equations of such systems are often unknown, limiting our ability to predict and control their dynamics. A major current effort is to learn these governing equations directly from data. However, existing approaches typically require access to the time series of all node states, which is rarely available outside controlled experiments. In most realistic scenarios, only aggregate or mean-field data, such as linear combinations of node states, can be measured. In this case, learning the governing equations from mean-field data inevitably becomes a secondary goal, since one must first learn the network trajectory that generated the observed measurements. This task is inherently challenging because distinct network states can yield identical macroscopic observations. Here, we address the problem of learning the network trajectory from random mean-field measurements. We show that accurate reconstruction becomes possible when the network exhibits structured spatiotemporal patterns, such as traveling waves. By representing these patterns sparsely in the Fourier domain, we leverage compressive sensing theory to formulate a convex optimization problem that robustly reconstructs the network trajectory. We illustrate our findings using a unidirectional ring of coupled Stuart-Landau oscillators.

DY 6.12 Mon 12:30 HÜL/S186

Discovering Mechanisms and Governing Laws with Sparse Regression — •Gianmarco Ducci, Maryke Kouyate, Juan Manuel Lombardi, Artem Samtsevych, Karsten Reuter, and Christoph Scheurer — FHI Berlin

Interpretable data-driven methods have proven viable for deriving complex vector fields directly from experimental data. Their inherent differential formulation, however, make them vulnerable to noise, which can compromise the sparsity of the inferred models. In order to promote sparsity, a weak formulation can be employed. Then, finding the optimal set of basis functions is a necessary prerequisite, yet a challenging task to determine in advance.

We present the release version of the Data-Driven Model Optimizer `ddmo`, a symbolic regression tool which provides fine-grained control over the admissible space of candidate terms. Its core contribution lies in the systematic optimization of the library of functions, implemented through two complementary engines: a standard SINDy-based differential formulation and a weak-form variant. Its modular structure further enables the optimization of test functions within the weak formulation. An overview of the software capabilities is provided, alongside with a case study illustrating the reconstruction of effective kinetics from experimental reactor data.

DY 6.13 Mon 12:45 HÜL/S186

POD-Subspace Reconstruction of Convective Reversal Dynamics from Limited Sensor Data — •Tim Kroll and Oliver Kamps — CDSC ,University of Münster

We introduce a data-driven modelling framework that leverages a hybrid LSTM-neural-network architecture to capture convection reversals from limited time-series measurements.. The method operates entirely in POD space, enabling efficient and accurate reconstruction of complex dynamical systems from limited observations by modelling non-orthogonal modes as a superposition of POD modes. The corresponding dynamics are modelled by an LSTM, incorporating knowledge about the history of the timeseries. We demonstrate its effectiveness on convection processes, showing that measurements from a single sensor - of either temperature T or velocity V - are sufficient to recover the full spatiotemporal dynamics, consisting of temperature, velocity or a combination of both, within the reduced representation. Furthermore this approach has potential to be applied in different scientific fields detached from convection or fluid dynamics.

DY 7: Focus Session: Large Deviations and Rare Events I

The modeling and understanding of large deviations and rare events is of crucial importance in a wide range of real-world applications, including climate science, actuarial statistics (insurance statistics), natural disaster management, or the description of financial markets. At the same time, such effects are fundamental for the understanding of many systems in condensed-matter physics. In first-order phase transitions, for instance, the coexisting phases are connected by transition states involving droplet excitations whose probability is suppressed by dozens or hundreds of orders of magnitude as compared to the pure-phase peaks. Likewise, for many disordered systems the behavior of typical cases is incompatible with that of the average sample as the problem is described by very broad, heavy-tailed distributions, where averages are dominated by rare events. For many models, like the Kadar-Parisi-Zhang equation or random-graph properties, there has been considerable analytical progress in the last decade. Likewise, new or improved numerical techniques have been proposed that now allow for the treatment of previously inaccessible problems or regimes. This focus session is devoted to an update on the state of the art in this rapidly evolving area.

Organized by Alexander K. Hartmann (Oldenburg) and Martin Weigel (Chemnitz)

Time: Monday 9:30–12:45 Location: ZEU/0114

Invited Talk DY 7.1 Mon 9:30 ZEU/0114

Fast Rare Events in Exit Times Distributions of Jump Processes — •Raffaella Burioni — Department of Mathematics, Physics and Computer Sciences, University of Parma, Italy — INFN - Sezione di Milano Bicocca - Parma, Italy

Rare events in first-passage and exit-time statistics of jump processes can play a decisive role in triggering anomalous reactions and extreme responses in a wide range of systems. This is particularly relevant when jump lengths or waiting times follow broad, heavy-tailed distributions, for which rare events are not exponentially suppressed and can significantly affect macroscopic observables. Interestingly, in the presence of heavy-tailed distributions, large fluctuations follow the Big Jump Principle, a counterintuitive mechanism according to which rare events arise not from the accumulation of many small deviations, but from a single, dominant fluctuation.

We present a general framework for estimating the contribution of fast rare events to exit probabilities in jump processes with fat-tailed distributions. We apply this approach to discrete-time random walks, Lévy walks, and the Lévy-Lorentz gas, which are widely used to describe transport in biological systems and disordered media. We derive the scaling form of the probability distribution for fast exit events, in which the process leaves a finite interval over distances much larger than the typical scale and on timescales orders of magnitude shorter than the characteristic timescale of the dynamics. We discuss extensions to N independent walkers, where collective effects can further enhance the contribution of fast rare events to exit statistics.

DY 7.2 Mon 10:00 ZEU/0114

Rare Events, Many Searchers, and Fast Target Reaching in a Finite Domain — Elisabetta Ellettari[1], Giacomo Nasuti[1], •Alberto Bassanoni[1,2], Alessandro Vezzani[1,3], and Raffaella Burioni[1,2] — [1]University of Parma, Italy — [2]INFN, Parma associated group, Italy — [3]IMEM-CNR, Parma, Italy

Finding a target in a complex environment is a fundamental challenge in nature. An effective strategy to reduce the time needed to reach a target is to deploy many searchers, increasing the likelihood that at least one will succeed by using the statistics of rare events. When the underlying stochastic process involves broadly distributed step sizes, rare long jumps dominate the dynamics, making the use of multiple searchers particularly powerful. We investigate the statistics of extreme events for the mean first passage time in a system of N independent walkers moving with jumps distributed according to a power law, where target-reaching is governed by single, large fluctuations. We show that the mean first passage time of the fastest walker scales as $\langle \tau_N \rangle \sim 1/N$, representing a dramatic speed-up compared to classical Brownian search strategies. We derive a scaling law relating the number of walkers required to reach a target within a given time to the size X of the search region. As an application, we model biological fertilization, predicting how the optimal number of spermatozoa scales with uterus size across species. Our predictions match empirical data, and this theory applies broadly to any population of searchers operating within a region of size X, providing a universal framework for efficient search in disordered environments.

DY 7.3 Mon 10:15 ZEU/0114

Large deviations and uncertainty relations for self-interacting jump processes — •Francesco Coghi[1,2], Amarjit Budhiraja[3], and Juan P. Garrahan[1,2] — [1]School of Physics and Astronomy, University of Nottingham, Nottingham, NG7 2RD, UK — [2]Centre for the Mathematics and Theoretical Physics of Quantum Non-Equilibrium Systems, University of Nottingham, Nottingham, NG7 2RD, UK — [3]Department of Statistics and Operations Research, University of North Carolina, Chapel Hill, NC 27599, USA

Self-interacting jump processes are stochastic systems where transition rates depend on the process' own empirical occupation measure – that is, the time-averaged distribution of the states visited by the process – introducing a feedback that breaks Markovianity. In this talk, I will present a large deviation framework for such systems. Specifically, I will derive the level-2.5 rate functional describing the joint fluctuations of occupation and flux, obtained via an exponential tilting construction extended to the non-Markovian setting. From this, I will show how memory modifies fluctuation bounds, leading to kinetic and thermodynamic uncertainty relations that generalise those of standard Markov processes. I will conclude with two examples that illustrate how feedback reshapes fluctuation-dissipation trade-offs: a minimal two-state model and a collective exploration process inspired by ant dynamics.

DY 7.4 Mon 10:30 ZEU/0114

A pedestrian's approach to large deviations in semi-Markov processes with an application to entropy production — •Jonas H. Fritz, Alexander M. Maier, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Semi-Markov processes play an important role in the effective description of partially accessible systems. They occur, for instance, in coarse-graining procedures such as state lumping and when analyzing waiting times between few visible Markovian events. The finite-time measurement of any coarse-grained observable in a stochastic system depends on the specific realization of the underlying trajectory. Moreover, the fluctuations of such observables are encoded in their rate function that follows from the rate function of the empirical measure and the empirical flow in the respective process. Derivations of the rate function of empirical measure and empirical flow in semi-Markov processes with direction-time independence (DTI) exist in the mathematical literature, but have not received much attention in the stochastic thermodynamics community. We present an accessible derivation of the rate function of the tuple frequency in discrete-time Markov chains and extend this to the rate function of the empirical semi-Markov kernel in semi-Markov processes without DTI [1]. From this, we derive an upper bound on the rate function of the empirical entropy production rate, which leads to a lower bound on the variance of the mean entropy production rate measured along a finite-time trajectory. We illustrate these analytical bounds with simulated data. [1] Alexander M. Maier, Jonas H. Fritz and Udo Seifert, arXiv:2509.15077, 2025

DY 7.5 Mon 10:45 ZEU/0114

Concentration of observables in slow-fast dynamical systems with noise — •Xizhu Zhao[1,2] and Aljaž Godec[1,2] — [1]Mathematical Physics and Stochastic Dynamics, Institute of Physics, University of Freiburg, Freiburg, Germany — [2]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany

Stochastic differential equations involving separated timescales play an important role in modeling the dynamics of complex systems in physics, biology, and climate science. We explore the concentration of observables, i.e. functions or functionals of dynamical variables, in slow-fast dynamical systems with noise. Using stochastic analysis and singular perturbation theory, we determine the domains of concentration for observables in systems with a stable manifold or undergoing a bifurcation. We also derive bounds for the distribution of the first-exit time from these domains. The results show that the concentration of observables exhibits behavior distinct from that of microscopic sample paths.

15 min. break

Invited Talk DY 7.6 Mon 11:15 ZEU/0114

Large deviations in resetting Brownian motions — •Satya Majumdar — CNRS, LPTMS, Universite Paris-Saclay, Orsay 91405, France

After a brief introduction to large deviations, I will focus on one dimensional resetting Brownian motions, first on a single particle and then on a gas of multiparticles. I will show that for a single partcle, while the position distribution of a resetting Brownian motion approaches a stationary form at long times, the

relaxation to this stationary state is unusual: it is described by a large deviation function that undergoes a second order dynamical phase transition. The same rate function also shows up in the distribution of the maximum up to time t of a set of independent resetting Brownian motions with a distributed initial positions. I will discuss the difference between the 'quenched' and 'annealed' initial positions and how they affect the statistics of the maximum.

DY 7.7 Mon 11:45 ZEU/0114

Large deviations and condensation in the cost of stochastic resetting — •John C. Sunil[1], Martin R. Evans[1], Richard A. Blythe[1], and Satya N. Majumdar[2] — [1]SUPA, School of Physics and Astronomy, University of Edinburgh, Peter Guthrie Tait Road, Edinburgh EH9 3FD, United Kingdom — [2]Université Paris-Saclay, CNRS, LPTMS, 91405 Orsay, France

Searching for misplaced objects is a task that we are all familiar with. In particular, the way we search for a misplaced object, such as keys, is by repeatedly resetting to the object*s last known location. It has been shown that such resetting expedites the mean time to complete the search process. However, in practice, resets must also incur costs, whether in time, energy, or money. This motivates examining the probabilities of rare cost fluctuations that deviate significantly from typical behaviour. In this talk, I will demonstrate the effect of costly resets and the large deviations exhibited by the tails of the total cost distribution using an exactly solvable model of diffusion with stochastic resetting. Further, I will discuss the eventual breakdown of the large deviation principle for certain classes of cost, resulting in a phase transition known as condensation.

(i) J. C. Sunil, R. A. Blythe, M. R. Evans and S. N. Majumdar, The cost of stochastic resetting, J. Phys. A: Math. Theor. 56 (2023) 395001.

(ii) M. R. Evans and J. C. Sunil, Stochastic Resetting and Large Deviations, SciPost Phys. Lect. Notes, vol. 103, 2025.

DY 7.8 Mon 12:00 ZEU/0114

Perturbative framework for finding the transition rates for active particles — •Vito Seinen[1], Peter Bolhuis[1], Daan Crommelin[2], Michel Mandjes[3], and Sara Jabbari-Farouji[1] — [1]University of Amsterdam — [2]Centrum Wiskunde & Informatica — [3]University Leiden

Activated escape or transition rates between metastable states have been a growing topic of research due to their relevance in many physical processes and their roles in certain non-equilibrium phase transitions. In the context of motility-induced phase separation (MIPS), such active transition rates are known to govern the nucleation processes that initiate phase separation. To gain insight into these phenomena, we develop a projection-operator formalism for a generic model of an active particle in a multi-well potential. We compute the transition rates perturbatively in two asymptotic regimes: one in which the dynamics of the activity (the driving process) is much faster than that of the particle (the driven process), and one in which the activity dynamics is much slower. From these asymptotic expansions, we construct an approximation that interpolates across the intermediate regime, thereby capturing all parameter ranges relevant in the rare-event limit. Our results provide deeper understanding of the complex dependence of active transition rates on the magnitude of the activity, the thermal noise strength, and the dynamical timescale of the active (driving) process*its persistence time

DY 7.9 Mon 12:15 ZEU/0114

Large deviation properties of Brownian particles in switching harmonic traps — •Chinmay Pradeep Chandratre and Alexander K. Hartmann — Institut of Physics, University of Oldenburg, Oldenburg (Germany)

For N independent particles in a harmonic trap with stiffness switching between μ_1 and μ_2, a complete characterization of the non-equilibrium steady state including the computation of joint distribution of particle positions has been performed under the stochastic-resetting protocol [1]. In the large-N limits, this allows for the computation of observables such as the distribution of the position M_k of the k-th rightmost particle (Extreme value statistics), spacing distributions $D_k = M_k - M_{k+1}$ and the particle count $N_L = \left|\{\, i : |x_i| \le L \,\}\right|$ for an interval $[-L, L]$. However, the finite-N regime with significant large-deviation corrections is analytically unknown. The numerical limitations in resolving the support of the distribution, especially in the tails, are circumvented through specialized large-deviation algorithms [2] by deploying modified Markov Chain Monte Carlo methods. The distributions $P(M_k)$, $P(D_k)$ and $P(N_L)$ and corresponding rate functions were obtained numerically from simulations performed for several system sizes. Conditional distribution rendered further insight into the correlations between M_k, D_k, and N_L.

[1] Biroli, Marco and Kulkarni, Manas and Majumdar, Satya N. and Schehr, Grégory, Phys. Rev. E **109**, 032106 (2024)

[2] A.K. Hartmann, Phys. Rev. E **89**, 052103 (2014)

DY 7.10 Mon 12:30 ZEU/0114

Optimal escape processes of run-and-tumble particles — Karthik Cheruvary[2], •Rafael Diaz Hernandez Rojas[1], and Peter Sollich[1] — [1]University of Göttingen — [2]IISER Pune

Run-and-tumble (RT) motion is a fundamental mode of self-propulsion observed across diverse biological systems from bacterial chemotaxis to immune cell migration. Modelling this non-equilibrium system is challenging due to the non-Gaussian noise governing the self-propulsion direction, θ. To address this, we investigate the trajectories of a particle confined by a potential in $d = 2$ and subject to both thermal fluctuations and RT motion. We incorporate tumbling by modelling changes in θ as Poisson shot noise process with rate λ and generic distribution of angle changes, Δ. Employing a path-integral formalism in the weak noise limit, we derive exact equations of motion for all degrees of freedom, valid for arbitrary λ and distributions of Δ. This allows us to map the problem of finding the most likely escape trajectory to the minimisation of an appropriate action. Our analysis reveals that the effects of the non-Gaussian noise are more prominent in the limit of small λ, which corresponds to highly persistent RT motion. There, we show analytically that, regardless of the distribution of Δ, RT escape paths are exponentially more probable –exhibiting a lower action– than their active Brownian particle equivalent. The optimal RT trajectories are non-trivial and can exhibit discontinuities or very rapid changes in θ, implying that RT particles will exploit their tumbling ability to optimize escape from potential wells. We verify our theoretical predictions through extensive numerical simulations.

DY 8: Nonlinear Dynamics, Synchronization, and Chaos

Time: Monday 9:30–12:30 Location: ZEU/0118

DY 8.1 Mon 9:30 ZEU/0118

Coherence properties of collective modes in oscillator networks — •Arkady Pikovsky — University of Potsdam, Potsdam, Germany

Synchronization transition in populations of coupled oscillators is manifested by an appearance of a global oscillating mode. While oscillations are perfect in the thermodynamic limit, for finite ensembles the collective mode is subject to fluctuations. Here we focus on the properties of diffusion of the global phase, which determine coherence time of the collective oscillations. We discuss scaling of the diffusion constant with the system size, and describe cases where the coherence is perfect.

DY 8.2 Mon 9:45 ZEU/0118

Phase locking and multistability in the topological Kuramoto model on cell complexes — •Iva Bačić[1,2], Michael T. Schaub[3], Jürgen Kurths[4], and Dirk Witthaut[1,5] — [1]Institute of Climate and Energy Systems: Energy Systems Engineering (ICE-1), Forschungszentrum Jülich, 52428 Jülich, Germany — [2]Institute of Physics Belgrade, University of Belgrade, Serbia — [3]RWTH Aachen University, Aachen, Germany — [4]Potsdam Institute for Climate Impact Research (PIK), Potsdam, Germany — [5]Institute for Theoretical Physics, University of Cologne, 50937 Köln, Germany

Higher-order group interactions fundamentally shape the dynamics and stability of oscillator networks. The topological Kuramoto model captures these effects by extending classical synchronization models to include interactions between cells of arbitrary dimension within simplicial and cell complexes. We present the topological nonlinear Kirchhoff conditions algorithm, a nonlinear generalization of Kirchhoff's circuit laws, that systematically identifies all phase-locked states in the topological Kuramoto model and reveals how higher-order topology governs multistability. Applying this framework to rings, Platonic solids, and simplexes, we uncover structural cascades of multistability inherited across dimensions, and demonstrate that cell complexes can exhibit richer multistability patterns than simplicial complexes of equal dimension. We find evidence hinting at universal multistability classes. Our results reveal how higher-order interactions affect synchronization and open new directions for understanding collective dynamics in systems with non-pairwise interactions.

DY 8.3 Mon 10:00 ZEU/0118

From quaternion order parameter to extreme synchronization transitions — •Moritz Thümler[1], Seungjae Lee[1], Lennart J. Kuklinski[1], and Marc Timme[1,2] — [1]Chair of Network Dynamics, Center for Advancing Electronics Dresden (cfaed) and Institute of Theoretical Physics, TUD Dresden University of Technology, 01062 Dresden, Germany — [2]Lakeside Labs, Lakeside B04b , 9020 Klagenfurt, Austria

Synchrony plays a fundamental role in the operation of many systems across physics, biology, and engineering. Fifty years after the introduction of

the paradigmatic Kuramoto model*which provides a mathematically tractable framework for studying transitions to synchrony*several open questions remain, particularly concerning finite-size systems. An analytic continuation of the Kuramoto model from real to complex variables has been proposed to address this challenge [1]. Here, we introduce a generalized quaternion order parameter that captures complex-valued state vectors and demonstrate its effectiveness by uncovering a link between real-valued Kuramoto dynamics and complex locked states calculated via self-consistency and newly uncovered explosive transitions to synchrony [2].

[1]*Moritz Thümler et al., Synchrony for Weak Coupling in the Complexified Kuramoto Model, Physical Review Letters 130:187201 (2023).

[2] Lee, Seungjae, Kuklinski, Lennart J., Thümler, Moritz and Timme, Marc. "Hopf-induced desynchronization" Zeitschrift für Naturforschung A, vol. 80, no. 11, 2025,

DY 8.4 Mon 10:15 ZEU/0118

Transition to turbulence in wind turbine wakes: synchronisation and nonlinear dynamics — •Thomas Messmer, Michael Hölling, and Joachim Peinke — Carl von Ossietzky Universität Oldenburg, School of Mathematics and Science, Institute of Physics, Oldenburg, Germany

The wake of a wind turbine is a typical shear flow that transitions from near- to far-wake, ultimately reaching fully developed turbulence. In this study, we investigate experimentally in a wind tunnel the wake dynamics of a periodically excited model wind turbine*a scenario motivated by applications such as floating wind turbines and periodic control strategies. Our findings reveal distinct excitation regimes with unique wake behaviours.

In one regime, the wake synchronises with the excitation period, forming an organised flow structure that accelerates the transition to turbulence. In another regime, nonlinear quasi-periodic dynamics emerge, characterised by the formation of multiple coherent structures that interact nonlinearly and also accelerate the transition to the far wake.

At the conference, we will discuss the mechanisms underlying synchronisation and quasi-periodic dynamics, as well as their implications for the fundamental problem of the transition to turbulence.

Invited Talk DY 8.5 Mon 10:30 ZEU/0118

Mean-field approach to finite-size fluctuations in coupled oscillator systems — •Oleh Omelchenko[1] and Georg Gottwald[2] — [1]University of Potsdam, Germany — [2]University of Sydney, Australia

Networks of coupled phase oscillators are one of the most studied dynamical systems with numerous applications in physics, chemistry, biology, and engineering. A variety of methods exists to explain their properties and dynamics in the thermodynamic limit, when the network size tends to infinity. However, the behavior of such systems in the more realistic case of a finite number of oscillators still remains poorly understood. In this talk, we revisit the paradigmatic Kuramoto-Sakaguchi model describing synchronization transitions in networks of all-to-all coupled heterogeneous phase oscillators, and propose an ab initio approach for characterizing analytically the statistical properties of finite-size fluctuations in this system. Our framework is applicable to any stationary partially synchronized state and does not require any prior knowledge about its structure. Moreover, it is sufficiently general such that it can be applied to a broader class of interacting particle systems.

15 min. break

DY 8.6 Mon 11:15 ZEU/0118

Energy Transfer in a Coupled Duffing System — •Martyna Sedlmayr and Andrzej Rysak — Faculty of Mechanical Engineering, Lublin University of Technology, 36 Nadbystrzycka St., 20-618 Lublin, Poland

The Duffing system is a non-linear prototypical chaotic system, of interest in studies of damping and energy harvesting. In this work we analyse modifications to the energy transfer in the system when it is magnetically coupled to a harmonic oscillator. The form of the magnetic interaction is obtained from a fit to experimental data. Numerical analyses then determine the power either dissipated by, or supplied to, the Duffing system by its individual components. In all simulations, the Duffing potential itself is not changed. Our analysis focuses on assessing the impact of the coupled oscillator on the energy efficiency of the system. We demonstrate the effects of changing the value of the mass, the damping and the elasticity of the perturbing system. We focus on searching for configurations of the perturbation for which an increase in efficiency occurs, which can be caused by either modifying the dynamics or by providing additional energy.

DY 8.7 Mon 11:30 ZEU/0118

Transient Signatures of Flow-Topological Transitions in Nonlinear Quantum Oscillators — •Alejandro S. Gómez and Javier del Pino — Department of Theoretical Condensed Matter Physics, (IFIMAC), Universidad Autónoma de Madrid

Non-equilibrium phases in driven-dissipative systems are ubiquitous. Often, they appear as classical fixed point attractors and limit cycles, with standard phase transitions triggered by local instabilities. Yet the flow-topology framework [1] shows that transitions can also arise from nonlocal reorganizations, leaving attractors unchanged and emerging only in transients. Stationary quantum states still reflect these structures as probability hotspots, and local changes can induce Liouvillian spectral degeneracies. However, how the nonlocal, transient reorganizations manifest in the Liouvillian remains open.

In this talk, I will introduce a topological framework that extends the classification of fixed points [1] to capture the full phase-space connectivity considering also limit cycles. By linking open quantum dynamics to the classification of Morse-Smale flows [2], Crucially, we demonstrate that our graph invariant exposes transitions the Liouvillian spectrum misses altogether, related to global flow-topology transitions. I illustrate this framework by mapping the dissipative phases of a two-photon-driven Kerr resonator with added gain.

[1] G. Villa et al., Topological classification of driven-dissipative nonlinear systems, Sci. Adv. (2025).

[2] A. A. Oshemkov, Classification of Morse-Smale flows on two-dimensional manifolds, Sbornik Math. (1998).

DY 8.8 Mon 11:45 ZEU/0118

The disordered logistic map — Joseph W. Baron[1] and •Tobias Galla[2] — [1]Department of Mathematical Sciences, University of Bath, Bath, BA2 7AY, UK — [2]Instituto de Fisica Interdisciplinar y Sistemas Complejos IFISC (CSIC-UIB), 07122 Palma de Mallorca, Spain

The logistic map is a central model of low dimensional chaos. In disordered systems with many degrees of freedom on the other hand, one finds high-dimensional chaos, induced by heterogeneous interactions.

Here, we study a system of many logistic maps with quenched random interactions. Using dynamic mean-field theory, random matrix theory and simulations we show that minimal disorder removes the period-doubling cascade in the conventional logistic map. The cascade is replaced by a sudden onset of chaos. We find a separate and qualitatively different transition to chaos with more smoothly evolving trajectories. The power spectra of fluctuations exhibit different power-law behaviour near the two transitions. In a disordered Henon map we find very similar behaviour.

Our results show that even minimal disorder can severely disrupt the behaviour of well-known dynamical systems. The work also shows that discrete-time disordered systems can exhibit rather different behaviour from their continuous-time cousins [1]. Disordered maps highlight that different chaotic behaviours can be observed in one single system, and that each of these behaviours leaves a fingerprint before chaos sets in.

[1] J. W. Baron, T. J. Jewell, C. Ryder, and T. Galla, Breakdown of random-matrix universality in persistent Lotka-Volterra communities, Physical Review Letters 130, 137401 (2023).

DY 8.9 Mon 12:00 ZEU/0118

Transient nature of recurrence based local dimension estimates from finite time series — •Reik V. Donner — Magdeburg-Stendal University of Applied Sciences, Magdeburg, Germany — Potsdam Institute for Climate Impact Research, Potsdam, Germany

Local fractal dimensions are a widely used concept in dynamical system theory. However, comparing their empirical spatial patterns across published works reveals surprising inconsistency with theoretical expectations. This points to the fact that corresponding estimates obtained from finite time series are notoriously spurious. As an example, a very long trajectory of the Lorenz-63 system in its chaotic regime is subsampled in two different ways: generating ensembles of individual state vectors drawn independently at random from the complete record versus ensembles of contiguous time series segments. In the latter situation, which is commonly present in time series analysis, one obtains a broad distribution and non-random spatial pattern of local dimension estimates, while consideration of independent samples provides much more narrowly distributed and spatially unstructured estimates. While finite-time estimates may still be useful for identifying transient structures caused by the proximity to unstable periodic orbits or similar dynamically invariant objects, their practical interpretation for real-world time series should be carefully reconciled.

DY 8.10 Mon 12:15 ZEU/0118

Two-dimensional turbulent condensates without bottom drag — •Adrian van Kan[1], Alexandros Alexakis[2], and Edgar Knobloch[3] — [1]Department of Mathematics, Texas A&M University, College Station, USA — [2]Laboratoire de Physique de l'Ecole Normale Supérieure, ENS, Université PSL, CNRS, Paris, France — [3]Department of Physics, UC Berkeley, Berkeley, California, USA

The extent to which statistical equilibrium theory applies to driven dissipative dynamics remains an important open question in many systems. We use extensive direct numerical simulations of the incompressible two-dimensional (2D) Navier-Stokes equation to examine the steady state of large-scale condensates in 2D turbulence at finite Reynolds number Re in the absence of bottom drag. Large-scale condensates appear above a critical Reynolds number $Re_c \approx 4.19$. For $Re \gtrsim Re_c$, we find a power-law scaling of the energy with $Re - Re_c$, with the energy spectrum at large scales following the absolute equilibrium form pro-

posed by Kraichnan. At larger Re, the energy spectrum deviates from this form, displaying a steep power-law range at low wave numbers with exponent −5, with most of the energy dissipation occurring within the condensate at large scales. We show that this spectral exponent is consistent with the logarithmic radial vorticity profile of the viscously saturated condensate predicted by quasilinear theory. Our findings shed new light on the classical problem of large-scale turbulent condensation in forced dissipative 2D flows in finite domains, showing that the large scales are close to equilibrium dynamics in weakly turbulent flows but not for strong condensates ($Re \gg 1$).

DY 9: Statistical Physics far from Thermal Equilibrium I

Time: Monday 9:30–12:15 Location: ZEU/0160

DY 9.1 Mon 9:30 ZEU/0160

Dissipation enables robust extensive scaling of multipartite correlations — •Krzysztof Ptaszyński[1,2], Maciej Chudak[1], and Massimiliano Esposito[2] — [1]Institute of Molecular Physics, Polish Academy of Sciences, Mariana Smoluchowskiego 17, 60-179 Poznań, Poland — [2]Complex Systems and Statistical Mechanics, Department of Physics and Materials Science, University of Luxembourg, 30 Avenue des Hauts-Fourneaux, L-4362 Esch-sur-Alzette, Luxembourg

We investigate the multipartite mutual information between N discrete-state stochastic units interacting in a network that is invariant under unit permutations [1]. We show that when the system relaxes to fixed point attractors, multipartite correlations in the stationary state either do not scale extensively with N, or the extensive scaling is not robust to arbitrarily small perturbations of the system dynamics. In particular, robust extensive scaling cannot occur in thermodynamic equilibrium. In contrast, mutual information scales extensively when the system relaxes to time-dependent attractors (e.g., limit cycles), which can occur only far from equilibrium. This demonstrates the essential role of dissipation in the generation and maintenance of multipartite correlations. We illustrate our theory with the nonequilibrium Potts model. Finally, we present a generalization of our approach to permutation-invariant open quantum systems [2].

[1] Phys. Rev. Lett. 135, 057401 (2025)
[2] Phys. Rev. E 112, 054137 (2025)

DY 9.2 Mon 9:45 ZEU/0160

Nested Stochastic Resetting: Nonequilibrium Steady States and Exact Correlations — •Callum Britton[1], Henry Alston[2], and Thibault Bertrand[1] — [1]Imperial College London, London, United Kingdom — [2]Laboratoire de Physique de l'Ecole Normale Supérieure, Paris, France

Stochastic resetting has gained a lot of traction over the past few years. It has been shown to drive the formation of nonequilibrium steady states and the optimization of first-passage properties in an analytically tractable setting. Yet, most works have thus far focused on single-particle stochastic resetting. In this talk, we introduce nested stochastic resetting, an exactly solvable, many-body stochastic resetting model achieved by harnessing resets as unilateral interactions between particles. We look at a system of n particles, where the position of particle i is independently reset to the instantaneous position of particle $i-1$ according to a Poisson process. We derive analytically the steady-state statistics of these nested stochastic resetting processes including the stationary distribution for each process as well as its moments. In this system, we go one step further and calculate exactly the steady-state two-point correlations $\langle x_i x_j \rangle$ between processes by mapping the problem to one of the ordering statistics of random counting processes. We expect this framework will both help build a model-independent framework for random processes with unilateral interactions and find immediate applications, e.g., in the modelling of lossy information propagation.

DY 9.3 Mon 10:00 ZEU/0160

Mutual linearity: A generic property of steady-state Markov networks — •Robin Bebon and Thomas Speck — Institute for Theoretical Physics 4, University of Stuttgart, Heisenbergstraße 3, 70569 Stuttgart, Germany

Nonequilibrium response theory has long sought universal principles to characterize the behavior of observables under external perturbations. While powerful tools exist near thermal equilibrium, general results far from equilibrium remain sparse and often rely on specific assumptions that severely limit their applicability, e.g., a specific parametrization of transition rates. In this work, we prove a remarkably simple, yet broadly applicable result: In a Markov network, any two steady-state probabilities remain linearly related when perturbing transition rates along a single edge of the network. This mutual linearity holds for every irreducible Markov network, arbitrarily far from equilibrium, and is independent of the chosen rate parametrization. As key implications, we demonstrate that the relative response of all states in the network is identical and show that analogous linear relations follow for a broad class of observables, including generic state-dependent and counting observables. Crucially, the coefficients that enter these linear relationships are empirically accessible, which makes our results not only conceptually significant but also provide a novel practical tool for inference and model validation in biological and chemical systems.

DY 9.4 Mon 10:15 ZEU/0160

Stochastic Path Integrals for Non-Markovian Dynamics: Fractional Operators, and Entropy Production — •Felipe Abril-Bermudez — Independent Researcher (formerly University of Aberdeen, UK)

Stochastic dynamics with long-range correlations, multiplicative noise, and memory effects give rise to rich non-equilibrium behaviors, including anomalous diffusion, metastability, and nontrivial entropy production. In this work, we develop a unified stochastic path integral (SPI) framework that extends the Parisi-Sourlas supersymmetric formalism to treat multidimensional Langevin systems with multiplicative noise, thresholds, and fractional operators driven by fractional Gaussian noise. The resulting generalized Fokker-Planck equation is solved for representative processes, enabling analytical estimation of Shannon entropy and entropy production rates, which exhibit the emergence of quasi-steady states with non-monotonic dissipation. In parallel, the formalism recovers the standard underdamped Langevin and Klein-Kramers results while providing a systematic treatment of non-Markovian dynamics responsible for anomalous transport, weak ergodicity breaking, and dynamical phases such as time glasses and time crystals. Thus, it is shown how the SPI can serve as a unified approach to study anomalous stochastic phenomena in complex systems.

DY 9.5 Mon 10:30 ZEU/0160

Thermophoresis of a tracer particle via coarse graining of an explicit nonequilibrium medium — •Wade Hodson and Aljaz Godec — Mathematical Physics and Stochastic Dynamics, Institute of Physics, University of Freiburg

We investigate the transport of a tracer particle embedded in an explicitly represented medium with a position-dependent temperature. The medium consists of a chain of harmonic oscillators, in which a temperature gradient is established by connecting each particle to its own heat reservoir. We then couple a tracer to this medium via a generic potential. Under these conditions, we find that the tracer preferentially diffuses in one direction due to the temperature gradient, a phenomenon known as thermophoresis. We study the model analytically in various regimes, including the weak coupling, low temperature, overdamped, Markovian, and hydrodynamic limits, and supplement these results with numerical computations. In the Markovian limit, we are able to coarse-grain over the medium's degrees of freedom to obtain a Langevin equation for the tracer, with a potential of mean force, a damping coefficient, and a diffusion coefficient which can be evaluated in the low-temperature regime. We focus on the analysis of this low-temperature Langevin equation, with a particular interest in the parameter regimes where the tracer can potentially exhibit negative thermophoresis, in which the tracer diffuses preferentially towards higher temperatures. Finally, we generalize our results to higher dimensions, by coupling the tracer to a two- or three-dimensional medium.

DY 9.6 Mon 10:45 ZEU/0160

Volterra Series leads to exact Dynamical Density Functional Theory — •Ion Santra — KU LEUVEN

We derive an exact Volterra series expansion for a mean mesoscopic field of an interacting particle system subject to a potential perturbation, expressing the Volterra expansion kernels in terms of the field's response functions, to any order. Applying this formalism to the mean particle density of a simple interacting fluid, we identify a form reminiscent of dynamical density functional theory, with, however, fundamental differences: A generally nonlocal mobility kernel appears, and the internal force derives from a functional of the *history* of mean density. In the limit of a slowly varying external force, the expansion kernels of this functional turn into the equilibrium direct correlation functions of the corresponding order, thereby, in this limit, recovering the equilibrium density functional. We identify a freedom in deriving this expansion, which, e.g., allows different forms of mobility kernels, and we explore two choices: A nonlocal mobility kernel results in a concise ans simple form to linear order. For interacting Brownian particles, a local mobility kernel results in a form reminiscent of previous forms for the density current.

15 min. break

DY 9.7 Mon 11:15 ZEU/0160

Thermal Relaxation on Random Graphs via Metropolis and Glauber Dynamics — •Marija Vucelja — University of Virginia, Charlottesville, US — MPI-PKS, Dresden, Germany

Efficient sampling algorithms rely on dynamics that drive a physical system rapidly toward its target state. I will introduce the Mpemba effect – an anomalous thermal relaxation phenomenon in which a system initially at a higher temperature cools down more quickly than one starting at a lower temperature – and its heating analog, in which a cooler initial state can lead to faster heating than a hotter initial state. We investigate thermal relaxation in quenched disordered systems under Metropolis and Glauber dynamics, examining how varying transition rates affect relaxation behavior. We show that Metropolis dynamics on a complete graph cannot exhibit the Mpemba effect, whereas on an incomplete graph it can. Even rank-one perturbations of the transition rates are sufficient to generate anomalous relaxation. Finally, we discuss the probability of observing the Mpemba effect in the large-temperature limit.

DY 9.8 Mon 11:30 ZEU/0160

Fermionic quantum criticality far from equilibrium — •Rohan Mittal, Tom Zander, Johannes Lang, and Sebastian Diehl — Universität Zu Köln

Driving a quantum system out of equilibrium while preserving its subtle quantum mechanical correlations on large scales presents a major challenge, both fundamentally and for technological applications. At its core, this challenge is pinpointed by the question of how quantum effects can persist at asymptotic scales, analogous to quantum critical points in equilibrium. In this work, we construct such a scenario using fermions as building blocks. These fermions undergo an absorbing-to-absorbing state transition between two topologically distinct and quantum-correlated dark states. Starting from a microscopic, interacting Lindbladian, we derive an effective Lindblad-Keldysh field theory in which critical fermions couple to a bosonic bath with hydrodynamic fluctuations associated with particle number conservation. A key feature of this field theory is an emergent symmetry that protects the purity of the fermions' state even in the presence of the thermal bath. We quantitatively characterize the critical point using a leading-order expansion around the upper critical dimension, thereby establishing the first non-equilibrium universality class of fermions. The symmetry protection mechanism, which exhibits parallels to the problem of directed percolation, suggests a pathway toward a broader class of robust, universal quantum phenomena in fermionic systems.

DY 9.9 Mon 11:45 ZEU/0160

ultrafast thermodynamics of the ferroelectric soft mode in laser-excited SrTiO3 — •Yulong Qiao and R. Matthias Geilhufe — Department of Physics, Chalmers University of Technology, Gothenburg, Sweden

Intense THz laser pulses allow to selectively pump and control optical phonon modes. This has led to the realization of metastable phases of matter, phonon-induced magnetism, and ultrafast magnetic switching. Following such a non-thermal path-way in the sub-picosecond timescale, has recently sparked questions on the temporal evolution of thermodynamic quantities, such as heat and entropy production, in the context of ultrafast thermodynamics [1].

In this work, we simulate the dynamics of the ferroelectric soft mode in SrTiO3 driven by a THz laser pulse using molecular dynamics [2]. We show that both the soft-mode dynamics and the associated energy transfer from the soft mode to other ionic degrees of freedom are accurately described by our stochastic thermodynamic theory. Moreover, the molecular dynamics simulations clearly reveal that the power spectral density of the noise is frequency-dependent. This indicates that the commonly adopted Markovian approximation breaks down. In this talk, I will also discuss the non-Markovian effects induced by the ultrafast laser pulse.

[1] L. Caprini, H. Löwen, R. M. Geilhufe, Nature Communication. 15, 94 (2024).
[2] F. Eriksson, Y. Qiao, E. Fransson, R. M. Geilhufe, P. Erhart, in preparation.

DY 9.10 Mon 12:00 ZEU/0160

Ultrafast Thermodynamics - entropy, heat and criticality on picosecond timescales — •R. Matthias Geilhufe — Chalmers University of Technology, Gothenburg, Sweden

Materials are composed of a vast number of ions and electrons, arranging themselves in regular patterns. Due to immense progress in ultrafast spectroscopy, ranging from the low-frequency infrared to high-frequency X-ray regimes, collective excitations of charge, spin, lattice, and orbital degrees of freedom can now be triggered and probed on their characteristic time and length scales. Probing such excitations far from equilibrium motivates the field of ultrafast thermodynamics, which translates well-understood concepts, such as entropy and heat, to picosecond dynamics. I will introduce the concept of ultrafast thermodynamics using the example of entropy production due to laser-driven phonons [1] and magnons [2] using stochastic thermodynamics. Furthermore, I will show extensions of the formalism to non-Markovian behavior and quantum mechanics.

[1] L. Caprini, H. Löwen, R. M. Geilhufe, Nature Communications, 15, 94 (2024) [2] F. Tietjen, R. M. Geilhufe, PNAS Nexus, 4, 3 (2025)

DY 10: Wetting, Fluidics and Liquids at Interfaces and Surfaces I (joint session CPP/DY)

Time: Monday 9:30–11:00 Location: ZEU/0260

See CPP 5 for details of this session.

DY 11: Wetting, Fluidics and Liquids at Interfaces and Surfaces II (joint session CPP/DY)

Time: Monday 11:30–12:45 Location: ZEU/0260

See CPP 8 for details of this session.

DY 12: Focus Session: Relaxation Timescales in Open Quantum Systems (joint session TT/DY)

In the quantum year 2025 many applications of quantum systems are revisited for their actual physical implementability. Realizing that no quantum system is truly isolated from its environment highlights the need for a thorough understanding of the coupling between an open system and its environment. While many standard treatments lead to Lindblad equations, the underlying approximations are not always applicable and require detailed case-by-case studies. This theoretical focus session provides a platform discussing modern developments in the field in the regime of strongly interacting or driven open systems and their impact on relaxation timescales. We aim to enhance attention and trigger also experimental activity in the field of system-environment interactions and the induced relaxation timescales.

Coordinators: Gernot Schaller (Helmholtz-Zentrum Dresden-Rossendorf), Nikodem Szpak (Universität Duisburg-Essen)

Time: Monday 15:00–18:00 Location: CHE/0089

See TT 18 for details of this session.

DY 13: Focus Session: New Routes to Localization and Quantum Non-Ergodicity II (joint session TT/DY)

Time: Monday 15:00–17:30 Location: CHE/0091

DY 13.1 Mon 15:00 CHE/0091

Localized obstructed pairs with zero superfluid stiffness from doping an antiferromagnetic insulator — •Tamaghna Hazra[1], Nishchhal Verma[2], and Jörg Schmalian[1] — [1]Institüt für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Department of Physics, Columbia University

Doping a Mott antiferromagnet is widely expected to yield mobile Cooper pairs whose kinetic energy sets the superfluid stiffness. We show instead that, when doped charges propagate on the line graph of a lattice with strong antiferromagnetic exchange, they bind into *obstructed* Cooper pairs, which are compact localized bosons that possess *zero* superfluid stiffness at leading order in the strong-coupling expansion. The pair-hopping Hamiltonian generates an exactly flat bosonic band whose compact localized states dominate the low-energy Hilbert space, yielding a ground-state manifold with extensive degeneracy and a phase stiffness that vanishes anomalously as the *third* inverse power of the pairing strength in the strong-coupling limit. At quarter filling, the frustrated dynamics maps onto a quantum dimer model at the Rokhsar-Kivelson point, realizing a d-wave resonating-valence-bond spin liquid with topological ground-state degeneracy and deconfined holon excitations. Our results establish a mechanism for interaction-driven localization without disorder, in which strong magnetically-mediated pairing produces Cooper pairs whose kinetic energy collapses to zero, revealing a distinct failure mode of unconventional superconductivity in strongly-correlated materials.

DY 13.2 Mon 15:15 CHE/0091

Disorder-free localization from mass-imbalanced fractionalization — •Shi Feng, Johannes Knolle, and Michael Knap — Technical University of Munich, Garching, Germany

We report disorder-free localization of Majorana fermions over intermediate timescales in an emergent gapless non-integrable Z_2 quantum liquid. A large density of heavy visons induced by an external magnetic field provides coherent disorder that localizes the light fermions while preserving translation symmetry. Compelling evidence of the localization within intermediate time scale is provided by the time evolution of the local energy density, which shows negligible spreading after a local quench on its ground state; and a vanishing energy current response despite the gapless energy spectrum. These results demonstrate that the disorder-free localization can also occur near equilibrium at low energy, and offer an explanation to the thermal paradox in recent experiments where a linear specific heat coexists with vanishing thermal transport in frustrated Mott insulators with disorder-free gapless quantum magnets.

DY 13.3 Mon 15:30 CHE/0091

Fock space fragmentation in quenches of disordered interacting fermions — •Ishita Modak[1], Rajesh Narayanan[2], Ferdinand Evers[3], and Soumya Bera[1] — [1]Department of Physics, Indian Institute of Technology Bombay, Mumbai, India. — [2]Department of Physics, Indian Institute of Technology Madras, Chennai, India — [3]Institute of Theoretical Physics and Halle-Berlin-Regensburg Cluster of Excellence CCE, University of Regensburg, Regensburg, Germany

Hilbert space fragmentation primarily originates from specific kinematic constraints or emergent conservation laws in many-body systems with translation invariance. It leads to non-ergodic dynamics and breakdown of the eigenstate thermalization hypothesis. We demonstrate that also in disordered systems (e.g. random-field XXZ model), fragmentation appears as a natural concept offering fresh perspectives on many-body delocalization (MBdL). We split the Fock-space into potential-energy shells, which contain the accessible phase space for the relaxation of a quenched initial state. In this construction, dynamical observables reflect properties of the shell geometry, e.g., the drastic sample-to-sample fluctuations observed in the weak disorder regime, $W < W_c$, represent fluctuations of the shell-mass. Upon crossing over to strong disorder, $W > W_c$, the potential-energy shell decays into fragments; we argue that, unlike percolation, fragmentation is a strong-coupling scenario with turn-around flow: $W_c(L)$ diverges with increasing system size. We conjecture that the slowing down of the relaxation dynamics reported in traditional MBdL studies is a manifestation of Fock-space fragmentation introduced here.

DY 13.4 Mon 15:45 CHE/0091

Non-ergodic one-magnon magnetization dynamics of the Kagome lattice antiferromagnet — Henrik Schlüter, •Jannis Eckseler, and Jürgen Schnack — Bielefeld University

The present view of modern physics on non-equilibrium dynamics is that generic systems equilibrate or thermalize under rather general conditions, even closed systems under unitary time evolution. The investigation of exceptions thus not only appears attractive, in view of quantum computing where thermalization is a threat it also seems to be necessary. Here, we present aspects of the one-magnon dynamics on the Kagome lattice antiferromagnet as an example of a non-equilibrating dynamics due to flat bands. Similar to the one-dimensional delta chain localized eigenstates also called localized magnons lead to disorder-free localization and prevent the system from thermalization [1].

[1] H. Schlüter, J. Schnack and J. Eckseler, Zeitschrift für Naturforschung A (2025) doi:10.1515/zna-2025-0249

DY 13.5 Mon 16:00 CHE/0091

Cooling dynamics of a disorder-free localized Kitaev model — •Arkadeep Mitra, Francesco Piazza, and Markus Heyl — Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

The Kitaev spin-1/2 model on a 2D honeycomb lattice has a Z_2 gauge symmetry that translates to an effective picture of free Majorana fermions on a background static charge field. This yields a ground state that realizes a quantum spin liquid (QSL) with fractional excitations. At high temperatures, however, it has recently been observed to enter a disorder-free localized phase, so that any experimental cooling of a Kitaev material has to cross this localized and associated phase transition. Motivated from this, we study theoretically the cooling dynamics upon coupling the Kitaev model to phonons with a symmetry breaking interaction. We envisage that signatures obtained from this dynamics could act as probes for QSL.

15 min. break

DY 13.6 Mon 16:30 CHE/0091

Scrambling signature of scars — •Thomas Michel[1], Mathias Steinhuber[2], Juan Diego Urbina[2], and Peter Schlagheck[1] — [1]Université de Liège, Liège, Belgique — [2]Universität Regensburg, Regensburg, Germany

We study signatures of scrambling, such as out-of-time-ordered correlators, that are associated with weakly unstable periodic orbits in a mixed or chaotic classical phase space, fulfilling Heller's criterion [1] for the existence of scars. As verified within generic dynamical systems like the kicked rotor and the driven pendulum, evaluating scrambling observables for coherent states centred in phase space about such periodic orbits gives rise to characteristic scar features both in the short and long time regimes, the latter amounting to a significant amendment of the characteristic growth exponent with respect to the generic semiclassical prediction [2,3]. Extensions to many-body scars in Bose-Hubbard rings [4] are discussed.

[1] E. J. Heller, Phys. Rev. Lett. 53, 1515 (1984).
[2] J. Rammensee, J.-D. Urbina, and K. Richter, Phys. Rev. Lett. 121, 124101 (2018).
[3] T. R. Michel, J. Diego Urbina, and P. Schlagheck, J. Phys. A: Math. Theor. 58, 275303 (2025).
[4] Q. Hummel, K. Richter, and P. Schlagheck, Phys. Rev. Lett. 130, 250402 (2023).

DY 13.7 Mon 16:45 CHE/0091

Many-Body Cages - Flat bands on the state graph — •Tom Ben-Ami[1,2], Markus Heyl[1], and Roderich Moessner[2] — [1]University of Augsburg, D-86135 Augsburg, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, Dresden 01187, Germany

We identify the many-body counterpart of flat bands, which we term many-body caging, as a general mechanism for non-equilibrium phenomena such as a novel type of glassy eigenspectrum order and many-body Rabi oscillations in the time domain. We focus on constrained systems of great current interest in the context of Rydberg atoms and synthetic or emergent gauge theories. We find that their state graphs host motifs which produce flat bands in the many-body spectrum at a particular set of universal energies. Basis states in Fock space exhibit Edwards-Anderson type order in the absence of quenched disorder, with an intricate, possibly fractal, distribution over Fock space. This is reflected in a distinctive structure of a non-vanishing post-quench long-time Loschmidt echo, an experimentally accessible quantity. In general, phenomena familiar from single-particle flat bands manifest themselves in characteristic many-body incarnations, such as a reentrant 'Anderson' delocalisation, offering a rich ensemble of experimental signatures in the abovementioned quantum simulators. The variety of single-particle flat band types suggests an analogous typology–and concomitant phenomenological richness to be explored–of their many-body counterparts.

DY 13.8 Mon 17:00 CHE/0091

Dynamics in the presence of local symmetry-breaking impurities — •Yahui Li[1,2], Pablo Sala[3,4], Frank Pollmann[1,2], Sanjay Moudgalya[1,2], and Olexei Motrunich[3,4] — [1]Technical University of Munich, Germany — [2]Munich Center for Quantum Science and Technology, Germany — [3]California Institute of Technology, USA — [4]Walter Burke Institute for Theoretical Physics, USA

Continuous symmetries lead to universal slow relaxation of correlation functions in quantum many-body systems. In this talk, I will show how local symmetry-breaking impurities affect the dynamics of these correlation functions using Brownian quantum circuits. While explicitly breaking the symmetry is generally expected to lead to eventual restoration of full ergodicity, we find that approximately conserved quantities that survive under such circumstances can still induce slow relaxation. This can be understood using a super-Hamiltonian formulation, where low-lying excitations determine the late-time dynamics. We show that in one dimension, symmetry-breaking impurities modify diffusive and subdiffusive behaviors associated with U(1) and dipole conservation at late times, e.g., by increasing power-law decay exponents of the decay of autocorrelation functions. On the other hand, for an impurity that disrupts strong Hilbert space fragmentation, it leads to prethermal plateaus in autocorrelation functions. Overall, our approach systematically characterizes how symmetry-breaking impurities affect relaxation dynamics in symmetric systems.

DY 13.9 Mon 17:15 CHE/0091

Late time dynamics of quantum entanglement — •Felix Dusel[1,2], Frank Pollmann[1,2,3], Tobias Micklitz[4], and Alexander Altland[5] — [1]Department of Physics, Technical University of Munich, 85748 Garching, Germany — [2]Munich Quantum Valley, 80807 Munich, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Schellingstraße 4, 80799 Munich, Germany — [4]Centro Brasileiro de Pesquisas Físicas, Rua Xavier Sigaud 150, 22290-180 Rio de Janeiro, Rio de Janeiro, Brazil — [5]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Straße 77, 50937 Cologne, Germany

We study entanglement spreading in quantum circuits composed of local qudits with large Hilbert space dimension, and single-particle dynamics relaxing slower than the characteristic timescale for entangling of neighboring qudits.

DY 14: Machine Learning in Dynamics and Statistical Physics II

Time: Monday 15:00–18:30 Location: HÜL/S186

DY 14.1 Mon 15:00 HÜL/S186

Machine-learned classical density functional theory in higher dimensions with convolutional layers — Felix Glitsch, Jens Weimar, and •Martin Oettel — Institut für Angewandte Physik, Universität Tübingen

Through minimization of a grand free energy functional in classical density functional theory (cDFT), inhomogeneous systems in equilibrium can be efficiently computed. For that, the functional of the excess (over ideal gas) free energy is required which is known explicitly only in a few cases. Recent advancements use machine learning for constructing this functional from simulation data, mostly for systems with one-dimensional, planar inhomogeneities. We propose a machine learning model for application in two dimensions [1] akin to density functionals in weighted density forms, as, e.g., in fundamental measure theory. We implement the model with fast convolutional layers only and apply it to a system of hard disks in fully 2D inhomogeneous situations. The model is trained on a combination of smooth and steplike external potentials in the fluid phase. Pair correlation functions from test particle geometry show very satisfactory agreement with simulations although these types of external potentials have not been included in the training. The method should be fully applicable to 3D problems.

[1] F. Glitsch, J. Weimar and M. Oettel, Phys. Rev. E 111, 055305 (2025)

DY 14.2 Mon 15:15 HÜL/S186

Scalable Boltzmann Generators for equilibrium sampling of large-scale materials — •Maximilian Schebek[1], Frank Noé[1,2,3,4], and Jutta Rogal[1,5] — [1]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin — [2]Fachbereich Mathematik und Informatik, Freie Universität Berlin, 14195 Berlin — [3]Microsoft Research AI for Science, 10178 Berlin — [4]Department of Chemistry, Rice University, Houston, Texas 77005, USA — [5]Initiative for Computational Catalysis, Flatiron Institute, New York, New York 10010, USA

Generating equilibrium ensembles is essential for modeling molecules and materials, yet traditional simulators like molecular dynamics suffer from limited sampling efficiency. Boltzmann Generators introduced the concept of one-shot deep learning for equilibrium sampling, but scalability to large systems has remained a major challenge. Here, we overcome this scaling limitation with a new Boltzmann Generator architecture that can model large materials systems. Our approach combines augmented coupling flows with graph neural networks to exploit local environments, enabling energy-based training and rapid inference. Compared to previous designs, it trains faster, uses fewer resources, and achieves superior sampling efficiency. Crucially, it transfers to much larger system sizes, allowing efficient sampling of materials with simulation cells exceeding a thousand atoms. We demonstrate its capabilities on Lennard-Jones crystals, mW water ice phases, and the silicon phase diagram, producing accurate equilibrium ensembles and free energies across scales where finite-size effects vanish.

DY 14.3 Mon 15:30 HÜL/S186

Autoencoder Learning Dynamics on MCMC Ising Dataset — •Max Weinmann[1,2,3] and Miriam Klopotek[1,3] — [1]University of Stuttgart, Stuttgart Center for Simulation Science, SimTech Cluster of Excellence EXC 2075, Stuttgart, Germany — [2]University of Stuttgart, Interchange Forum for Reflecting on Intelligent Systems, IRIS3D, Stuttgart, Germany — [3]Heidelberger Akademie der Wissenschaften, WIN-Kolleg, Heidelberg, Germany.

While consistent and abstract descriptions of learning dynamics in neural networks remain rare, they have become omnipresent and are used in many branches of science. As a result, predicting dynamics under diverse choices of ML model parameters can fail catastrophically and it remains difficult to mitigate these failures. Reliable control requires a deep understanding of the relevant mechanisms and conditions for learning particular kinds of datasets. Our study focuses on autoencoder architectures that perform well if they encode the dataset into a compressed representation that reflects core physical concepts of the data it is trained on, succeeding at a self-learned inverse model to decode this representation to reconstruct the original input (of physical origin). Some physical concepts are learned in a particular order, which depend on theoretical complexity of the representation and that of the ML architecture. We measure generalization ability against hard theoretical baselines and investigate the information geometry, stability, and physical interpretability of latent space over training time.

DY 14.4 Mon 15:45 HÜL/S186

Learning order: can neural networks discover phase transitions without symmetry functions? — •Carina Karner — Institute for Theoretical Physics, TU Wien, Vienna, Austria

Phase transitions in soft matter systems from crystallization to gelation arise from collective particle rearrangements that are challenging to capture in full microscopic detail. Conventional approaches rely on order parameters or symmetry functions to characterize emerging structures, but such descriptors may overlook crucial features in the often complex organisation of biolgical materials or synthetic super-structures. Here we investigate whether machine learning can uncover these hidden features directly from raw particle configurations. Using autoencoders trained on simulated trajectories of serveral soft matter systems, we show that the latent space encodes clear signatures of structural transitions without the need for handcrafted inputs. Our results suggest that neural networks can serve as unbiased tools to detect and interpret phase behavior in complex soft matter systems, revealing patterns that elude traditional symmetry-based analysis.

DY 14.5 Mon 16:00 HÜL/S186

Microscopy on Autopilot: Self-Supervised Transformers for Feature Detection and Control — •Damián Baláž, Gianmarco Ducci, Christoph Scheurer, Karsten Reuter, and Hendrik H. Heenen — Fritz-Haber-Institut der MPG, Berlin

The evaluation of microscopy experiments often relies on manual inspection or supervised machine learning. The former is inefficient, whereas the latter requires extensive labeling and may introduce human bias. Self-supervised learning, by contrast, learns from raw image data, capturing intrinsic visual patterns without the need for manual annotation. This improves generalization and objectivity, making it ideal for complex and dynamic microscopy data. Motivated by these advantages, we use a pre-trained self-supervised machine learning model (DINO), based on vision transformer architecture. This constitutes our central tool for feature detection and temporal analysis in microscopy experiments.

We demonstrate the versatility of our approach for two microscopy experiments: i) observing graphene flake growth on liquid copper ii) tracking crack formation in a cobalt oxide catalyst. In both cases, the model enables label-free, qualitative monitoring by identifying related structures based on similarity in the learned feature space. Beyond using it for analysis, we show how the same feature space representations can be used to predict experimental dynamics to autonomously steer processes toward desired targets via planning in feature space. Our findings highlight the potential of self-supervised vision models for real-time analysis and control in microscopy-based experiments.

DY 14.6 Mon 16:15 HÜL/S186

Learning microstructure in active matter — •Writu Dasgupta, Suvendu Mandal, Aritra Mukhopadhyay, and Benno Liebchen — Technische Universität Darmstadt, Darmstadt, Germany

Understanding the full parameter dependence of microscopic structure in active matter remains a central challenge, particularly for strong activity and high density, where simulations become increasingly expensive. Here, we present a data-driven approach that learns radial and angular correlations in terms of the pair-correlation function $g(r,\theta)$ of passive and active Brownian particles. Our predictions are in close quantitative agreement with Brownian dynamics simulations, even for parameter values that the neural networks had not previously encountered during training. Our predictions are subsequently distilled into compact, closed-form expressions using symbolic regression, providing an interpretable description of the underlying structure. Our approach offers a unified and computationally efficient route to understanding non-equilibrium correlations.

DY 14.7 Mon 16:30 HÜL/S186

Physical embodiment enabled learning for autonomous navigation of active particles in complex flow fields — •Diptabrata Paul[1], Nikola Milosevic[2], Nico Scherf[2], and Frank Cichos[1] — [1]Molecular Nanophotonics Group, Peter Debye Institute for Soft Matter Physics, Leipzig University, 04103 Leipzig, Germany — [2]Max Planck Institute for Human Cognitive and Brain Sciences, 04103 Leipzig, Germany

Autonomous navigation at the microscale is a major challenge in active matter due to strong environmental noise and hydrodynamic disturbances. While living systems rely on sophisticated sensing and feedback to regulate functions from sub-cellular processes to chemotactic navigation strategies, artificial microswimmers lack such adaptive mechanisms and therefore struggle to respond effectively to stationary or dynamic perturbations. In this work, we introduce an actor-critic reinforcement learning (RL) framework and demonstrate that physical embodiment alone enables adaptive navigation without explicit environment sensing. Training of the active particle agent in strong and spatially varying flow fields leads to emergence of robust strategies that counteract hidden hydrodynamic perturbations excluded from the agent's observation space. This reveals that embodied dynamics encode sufficient information for effective decision-making, enabling RL to exploit morphology-environment coupling as an implicit sensing channel. Our approach bridges the gap between simple stimulus response schemes and higher-level adaptive behavior and establishes a foundation for online learning, and microscale robotics.

15 min. break

DY 14.8 Mon 17:00 HÜL/S186

Machine Learning for Electric-Field Driven Nuclear Dynamics in Solids and Liquids — •Elia Stocco[1], Christian Carbogno[2], and Mariana Rossi[1] — [1]MPI for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Fritz Haber Institute of the MPS, Berlin, Germany

Simulating the interaction of electric fields with matter is fundamental to study dielectric properties and their interplay with structural and vibrational degrees of freedom. Therefore, it is desirable to obtain a general method that is able to deal with static and time-dependent fields, that is scalable to large complex systems, and that retains ab initio accuracy. We describe a machine-learning molecular dynamics method within the electric dipole approximation that describes the coupling of insulating materials to diverse electric fields, spanning liquids, solids, and confined systems [1]. In particular, we also take into account the influence of the electric field on the lattice degrees of freedom. We train equivariant MACE models [2], using density-functional theory data to learn the potential energy and dipole surfaces, including the multi-valued nature of the polarization in periodic systems. The external forces on various degrees of freedom are obtained through automatic differentiation. We present calculations of the dielectric permittivity of water, the temperature and light-driven ferroelectric-paraelectric phase transition of $LiNbO_3$, and simulations of piezoelectric systems. [1] Stocco, E., Carbogno, C. Rossi, M., Npj Comput. Mater. 11, 304 (2025). [2] Batatia, I., et al., Adv. Neural Inf. Proc. Sys. 35, 11423 (2022).

DY 14.9 Mon 17:15 HÜL/S186

Machine-learned Potentials for Vibrational Properties of Acene-based Molecular Crystals — •Shubham Sharma, Burak Gurlek, Paolo Lazzaroni, and Mariana Rossi — MPI for the Structure and Dynamics of Matter, Hamburg, Germany

Machine-learning potentials (MLPs) have enabled efficient modelling of complex atomistic systems with ab-initio accuracy. A major challenge, however, is the construction of sufficiently large and diverse reference datasets using first-principles calculations. To mitigate this, several active-learning strategies have been proposed to improve training efficiency, especially when combined with molecular-dynamics sampling. In this work, we develop protocols for building training sets of MACE potentials [1], targeting an accurate description of the vibrational properties of weakly-bound condensed-phase systems [2]. We assess the performance of MACE against the VASP-ML framework [3], highlighting differences in predictive accuracy for energies, forces, and vibrational properties. We also propagate committee-based uncertainties to estimate errors in dynamical quantities coming from imperfect force predictions. Finally, we demonstrate the generalisation capability of the acene-based potential by applying it to host-guest systems, enabling the identification of distinct vibrational modes within the complex dynamical spectra. [1] I. Batatia et. al., Nat Mach Intell 7, 56-67 (2025); [2] B. Gurlek, S. Sharma et. al., npj Comput Mater 11, 318 (2025); [3] R. Jinnouchi et. al., PRB 100, 014105 (2019).

DY 14.10 Mon 17:30 HÜL/S186

Spin-phonon systems in the age of modern atomistic simulations — •Ilija Srpak[1,2], Michael J. Willatt[2], Stuart C. Althorpe[1], and Ali Alavi[1,2] — [1]Yusuf Hamied Department of Chemistry, University of Cambrige, Cambridge, United Kingdom — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

Spin-phonon systems are molecules or crystals containing open-shell atoms whose spin-spin interaction is significantly affected by lattice displacements, sometimes leading to spin-Peierls phase transition. They typically inherit some of the most challenging aspects of statistical physics where many configurations across the phase space may contribute to its properties, and of "strongly-correlated" physics where mean-field methods such as density functional theory and self-consistent field approaches break down.

Over the years a plethora of Monte Carlo based techniques was developed to tackle this problem with some success, but not without (sometimes significant) limitations. Approaching this problem from atomistic simulations background, we developed a path integral molecular dynamics framework which doesn't require any Monte Carlo during the simulation runtime to sample the phase space, it can take arbitrary system parametrizations or even ab-initio description and simulate the system at an arbitrary temperature as well as include nuclear quantum effect. Using neural networks we have developed this framework further. We achieved a speed up of 2-3 orders of magnitude and are able to treat higher dimensional systems.

DY 14.11 Mon 17:45 HÜL/S186

Self-Consistent Benchmarking of Machine Learning Force Fields via Energy-Landscape Exploration — •Anand Sharma[1,2], Igor Poltavskyi[1], and Alexandre Tkatchenko[1] — [1]Department of Physics and Materials Science, University of Luxembourg, Luxembourg — [2]Indian Institute of Science Education and Research Pune, India

The rapid growth of Machine Learning Force Field (MLFF) models has prompted the development of diverse benchmarks to assess their accuracy and transferability. Most existing approaches rely on predefined test datasets, introducing biases and limiting fair comparison between models.

We introduce a general, system- and model-agnostic benchmarking framework that evaluates MLFFs through self-generated datasets. For each model, molecular structures are obtained by sampling random initial configurations of atoms and relaxing them using the model's predicted forces. The resulting datasets are analyzed through (i) comparison with the model's original training data, (ii) validation against ab-initio reference calculations, and (iii) cross-model dataset comparison. Applied to the SO3LR [1] and MACE-MP-0 [2] models, our framework identifies gaps in their training set coverage and enables unbiased evaluation of models' predictive capabilities. Overall, our approach provides a consistent, extensible foundation for comparing and improving next-generation broadly applicable MLFFs.

[1] A. Kabylda, et. al, J. Am. Chem. Soc. 147, 33723 (2025).
[2] I. Batatia, et. al, J. Chem. Phys. 163, 184110 (2025).

DY 14.12 Mon 18:00 HÜL/S186

Solving Classical and Quantum spin glasses with Deep Boltzman Quantum States — Luca Leone[1], •Arka Dutta[1], Markus Heyl[1], Enrico Prati[2], and Pietro Torta[2] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Augsburg, Germany. — [2]Department of Physics, University of Milan, Milan, Italy.

Variational neural network models achieved remarkable success in preparing the ground state of quantum many-body systems. However, addressing classical and quantum spin glasses remains challenging, as exponential growth of deep local energy minima due to disorder and energy frustration hinder conventional Monte Carlo methods. To bridge this gap, we introduce Deep Boltzmann Quantum States, a class of neural quantum states inspired by deep Boltzmann machines, trained by devising Neural Quantum Annealing, an algorithm incorporating the principles of quantum annealing. It solves large-scale classical and quantum spin glasses, matching the exact solution or the best available estimate for several instances of Ising spin-glass models with infinite-range interactions and hundreds of spins.

DY 14.13 Mon 18:15 HÜL/S186

Optimization and Representability of time-dependent Neural Quantum States: a study of the 1D critical quantum Ising model — •Wladislaw Krinitsin[1,2], Mohammad Abedi[1,2], Jonas Rigo[2], and Markus Schmitt[1,2] — [1]PGI-8, Forschungszentrum Jülich, Jülich, Germany — [2]Faculty for Informatics and Data Science, Regensburg University, Germany

In recent years, neural quantum states have emerged as a competitive and powerful numerical approach for many body systems. While they provide a flexible and scalable ansatz, able to represent any state as suggested by the function-approximation theorem, their practical limitations are still opaque, in particular regarding representability and optimization. In this work we investigate these questions within the framework of variational Monte Carlo on the example of the time evolution of the critical transverse-field Ising model in one dimension. Even for moderate system sizes, the departure from the exact solution occurs very early in the dynamics, allowing us to systematically analyze the representability of the state at each time step as well as the impact of different sampling strategies.

DY 15: Focus Session: Large Deviations and Rare Events II

The modeling and understanding of large deviations and rare events is of crucial importance in a wide range of real-world applications, including climate science, actuarial statistics (insurance statistics), natural disaster management, or the description of financial markets. At the same time, such effects are fundamental for the understanding of many systems in condensed-matter physics. In first-order phase transitions, for instance, the coexisting phases are connected by transition states involving droplet excitations whose probability is suppressed by dozens or hundreds of orders of magnitude as compared to the pure-phase peaks. Likewise, for many disordered systems the behavior of typical cases is incompatible with that of the average sample as the problem is described by very broad, heavy-tailed distributions, where averages are dominated by rare events. For many models, like the Kadar-Parisi-Zhang equation or random-graph properties, there has been considerable analytical progress in the last decade. Likewise, new or improved numerical techniques have been proposed that now allow for the treatment of previously inaccessible problems or regimes. This focus session is devoted to an update on the state of the art in this rapidly evolving area.

Organized by Alexander K. Hartmann (Oldenburg) and Martin Weigel (Chemnitz)

Time: Monday 15:00–18:30 Location: ZEU/0114

Invited Talk DY 15.1 Mon 15:00 ZEU/0114

Monte Carlo Simulation Methods for Rare-Event Sampling — •Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, IPF 231101, 04081 Leipzig, Germany

Large fluctuations and rare events play an important role in many physical systems, with nucleation phenomena, first-order phase transitions and frustrated (disordered) systems being only the most prominent examples. To cope with such processes in Monte Carlo computer simulations, several generalized-ensemble approaches such as parallel and simulated tempering and "flat-histogram" methods have been devised and further improved over the years. After a brief overview of the basic ideas of multicanonical (MuCa), Wang-Landau (WL), and Stochastic Appxoximation Monte Carlo (SAMC) schemes, the talk will focus on more recently proposed "non-flat" variants that put even more emphasis on strongly suppressed rare events, and alternative formulations based on the (real) microcanonical ensemble. As illustrations, performance tests and results will be shown for spin glasses, first-order phase transitions in the q-state Potts and Blume-Capel model, Lennard-Jones particle and polymer clusters, and the density of states of O(n) spin models on triangular and hypercubic lattices spanning many hundreds orders of magnitude.

DY 15.2 Mon 15:30 ZEU/0114

Sampling rare events with neural networks — Moritz Riedel[1], Johannes Zierenberg[2], and •Martin Weigel[1] — [1]Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, 37077 Göttingen, Germany

Neural networks can be trained to generate samples from the Boltzmann distribution of many-particle systems. If suitable architectures such as normalizing flows or variational autoregressive networks are chosen, exact generation weights are known, and hence present biases can be corrected for. Still, such networks typically struggle to learn and reproduce configurations from the full range of configuration space, since effects such as mode collapse occur. For the simulation of rare events and suppressed states accessible in generalized frameworks such as the multicanonical ensemble such broad exploration is crucial. Here, we show how a combination of variational autoregressive network and autoencoder allows for a systematic exploration of configuration space in spin models, during which the network is able to learn the density of states. We demonstrate the efficacy of the approach in the Potts system in the strong first-order regime, and we also propose hybrid algorithms combining the neural network approach with traditional Monte Carlo techniques.

DY 15.3 Mon 15:45 ZEU/0114

Large deviation simulation of the coupling time of an Ising ferromagnet — •Mathis Groenhagen[1], Peter Werner[2], and Alexander K. Hartmann[1] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg — [2]Laboratoire de Météorologie Dynamique - ENS, Paris

Coupling from the past, introduced by Propp and Wilson [1], is a Markov-chain Monte Carlo (MCMC) method capable of generating perfectly independent samples from a finite set of states, following exactly a given distribution. The performance of this algorithm for a given model can be characterized by it's *coupling time* τ_c, which measures the time to perfect statistical independence and depends on the used random numbers.

The algorithm is tested for one and two-dimensional Ising models without external field with the single-spin-update heat-bath algorithm. In order to access the distribution $p(\tau_c)$ over a wide range of the support down to densities as small as 10^{-200}, a large-deviation MCMC algorithm is used. With this, we have obtained $p(\tau_c)$ for different lattice dimensions D, edge lengths L and heat-bath temperatures T.

In particular, we observe a change of the shape of $p(\tau_c)$ at T_c for $D = 2$. For the paramagnetic case of $D = 2$ and $D = 1$, $p(\tau_c)$ follows a Gumbel distribution as predicted for the thermodynamic limit [2]. We have studied the dependency of the distribution parameters on T and L.

[1] J. Propp, D. Willson, Random Struct. Algoritms **9**, 223-252 (1996).
[2] A. Collevechio et al., J. Stat. Phys. **170**, 22-61 (2018).

DY 15.4 Mon 16:00 ZEU/0114

Large deviations in response functions of the two-dimensional bond-diluted Ising model — •Lambert Münster[1], Alexander K. Hartmann[2], and Martin Weigel[1] — [1]Institut für Physik, TU Chemnitz, 09107 Chemnitz, Germany — [2]Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26129 Oldenburg, Germany

Studies in statistical physics are most commonly focused on the typical, average behavior of a system. However, there exist cases in which rare events can have a significant impact on physical properties. The Griffiths phase in systems with quenched disorder is one such example. In this case rare regions in the disorder degrees of freedom cause large tails in response functions of physical observables such as the magnetic susceptibility and the specific heat. In this study rare-region effects are investigated by analyzing the distributions of physical observables in the bond-diluted Ising model. In order to obtain these distributions over a wide range of their support, a special type of Markov chain Monte Carlo algorithm is utilized for sampling rare events [1].

[1] L. Münster, A. K. Hartmann and M. Weigel, Phys. Rev. E **110**, 054112 (2024).

DY 15.5 Mon 16:15 ZEU/0114

Universality of the order-parameter large-deviation function for the critical 2D Ising and Blume-Capel models — Nikolaos G. Fytas[1], Víctor Martín-Mayor[2], Attilio L. Stella[3], Gianluca Teza[4], Alexandros Vasilopoulos[1], and •David Yllanes[5] — [1]University of Essex — [2]Universidad Complutense de Madrid — [3]Università di Padova — [4]MPIPKS, Dresden — [5]Universidad de Zaragoza

We revisit the longstanding question of universality in the probability density function (pdf) of the order parameter at criticality, traditionally assumed to hold only for the central region of the distribution. Focusing on the dimensionless magnetization $u = m/\sqrt{\langle m^2 \rangle}$, whose moments are universally defined in the thermodynamic limit, we hypothesize that universality extends to the full

pdf $p_L(u)$, including its exponentially suppressed large-deviation tails scaling as $u^{1+\delta}$. We test this conjecture with large-scale Tethered Monte Carlo simulations of the 2D Blume-Capel model at criticality for several values of the crystal field Δ, including the Ising limit ($\Delta = -\infty$) and approaching the tricritical point $\Delta_c \approx 1.97$. We simulate lattices up to $L = 4096$ with a tethered cluster algorithm, reaching the asymptotic regime for probability densities as small as 10^{-200}. Our results are strong numerical evidence for universality in the full $p_L(u)$ and settle the debated non-universality of the large-deviation function for m, where system-dependent amplitudes obscure scaling behavior. We consider the universality of the unusual combination of a finite-size amplitude with an amplitude for a scaling law related to the large-deviation function.

DY 15.6 Mon 16:30 ZEU/0114

Ising Model under Stochastic Resetting — •Shashank Kallappara[1], Parbati Saha[2], Varsha Banerjee[2], and Martin Weigel[1] — [1]Institut für Physik, TU Chemnitz, Germany — [2]Department of Physics, Indian Institute of Technology Delhi, India

Stochastic resetting refers to the interruption of a system's natural evolution by randomly returning it to a prescribed initial configuration. In this work, we investigate the effect of stochastic resetting on the Ising model and extend the results of Ref. [1] by examining how the resetting protocol modifies energetic properties of the system. In particular, we analyse the behaviour of the energy under different resetting rates and initial magnetisations. Furthermore, we study the impact of resetting in the case of conserved-order-parameter Ising model using Kawasaki dynamics, revealing qualitatively distinct behaviour compared to the nonconserved Glauber dynamics.

[1] Magoni, M., Majumdar, S. N. & Schehr, G. Ising model with stochastic resetting. Phys. Rev. Research 2, 033182 (2020).

15 min. break

DY 15.7 Mon 17:00 ZEU/0114

Classical nucleation theory for active non-conserved scalar field theories — •Michalis Chatzittofi[1], Noah Ziethen[1], Cesare Nardini[2], and Michael Cates[1] — [1]DAMTP, Centre for Mathematical Sciences, University of Cambridge, Cambridge CB3 0WA, United Kingdom — [2]Service de Physique de l' Etat Condense, CNRS UMR 3680, CEA-Saclay, 91191 Gif-sur-Yvette, France

Classical nucleation theory (CNT) has been successfully used in equilibrium conserved theories to explain the behaviour of growing droplets. However, in non-equilibrium field theories such description is more challenging since the dynamics cannot be derived from a free-energy. In this work, we show that it is possible to generalize CNT for the case of out-of-equilibrium non-conserved field theories. By projecting onto the slow manifold of the dynamics, we propose a systematic recipe for deriving an exact analytical expression for the dynamics of the growing nucleus and the corresponding quasipotential. Our findings allow for analytical progress in the context of large deviations and can compliment numerical/machine learning approaches for finding instanton trajectories.

DY 15.8 Mon 17:15 ZEU/0114

Precise large deviations in statistical field theories with weak noise — •Timo Schorlepp[1], Tobias Grafke[2], Rainer Grauer[3], Georg Stadler[1], and Shanyin Tong[4] — [1]NYU Courant, USA — [2]Warwick, UK — [3]Bochum, Germany — [4]UPenn, USA

Large deviation theory (LDT) provides a common theoretical framework to compute probabilities of rare events in stochastic systems out of equilibrium. The theory consists of a saddlepoint evaluation of the path integral describing the stochastic process under study, and has successfully been used in various systems such as growing interfaces, active matter, lattice gases and macroscopic fluctuation theory, fluid dynamics and turbulence, etc. I will describe recent progress in going beyond leading-order LDT asymptotics, developing tractable methods to evaluate 1-loop (Gaussian) corrections around nontrivial LDT minimizers for weak noise Langevin equations and field theories. This allows for quantitative rare event probability estimates, beyond the usual log-asymptotics. To compute the corresponding LDT prefactors, I will present two complementary approaches based on either matrix Riccati differential equations, or (possibly renormalized) Fredholm determinants. I will illustrate these methods in multiple analytical/numerical examples: extreme growth events in the 1d KPZ equation at short times [1], extreme concentrations of a randomly advected passive scalar [2], and extreme strain events in the stochastically forced incompressible 3d Navier-Stokes equations [3]. References: [1] Schorlepp, Grafke, Grauer, J Stat Phys, 2023; [2] Schorlepp, Grafke, arXiv:2502.20114, 2025; [3] Schorlepp, Tong, Grafke, Stadler, Stat. Comput., 2023.

DY 15.9 Mon 17:30 ZEU/0114

Probability graphons and large deviations for random weighted graphs — •Giulio Zucal — Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — Max Planck Institute for Physics of Complex Systems, Dresden, Germany — Center for Systems Biology Dresden, Dresden, Germany

Graph limit theory studies the convergence of sequences of graphs as the number of vertices grows, providing an effective framework for representing large networks. In this talk, I will give a brief introduction to graph limits and report on recent extensions to weighted graphs and multiplex networks (probability graphons and P-variables). As an application of this theory I will present a large deviation principle (LDP) for random weighted graphs that generalizes the LDP for Erdős–Rényi random graphs by Chatterjee and Varadhan (2011), based on joint work with Pierfrancesco Dionigi.

DY 15.10 Mon 17:45 ZEU/0114

Extreme Value Analysis for Finite, Multivariate and Correlated Systems with Finance as an Example — •Benjamin Köhler, Anton J Heckens, and Thomas Guhr — Universität Duisburg-Essen, Germany

Extreme values and the tail behaviour of probability distributions are essential for quantifying and mitigating risk in complex environmental and socio-economic systems. In multivariate settings, accounting for correlations is crucial. Although extreme value analysis for truly infinite correlated systems remains an open challenge, we propose a practical framework for handling a large but finite number of time series.

We study the extremal behavior of high-frequency stock returns after rotating them into the eigenbasis of the correlation matrix. This separates information on the market as a whole and on sectoral behavior while allowing us to use univariate tools of extreme value analysis, even for high-frequency data where discretization effects normally complicate analysis.

Using a Peaks–over–threshold approach, we estimate the tail shape of the rotated returns while explicitly accounting for non-stationarity, a key feature in finance and many other complex systems. Our framework allows for tail risk estimation relative to larger trends and intraday seasonalities at both market and sectoral levels.

DY 15.11 Mon 18:00 ZEU/0114

On the Reconstruction and Predictability of Ocean Rogue Waves — Christian Behnken, Finn Köhne, Metthias Wächter, and •Joachim Peinke — Institute of Physics, University Oldenburg, Oldenburg

We present a data-driven algorithm which allows to reconstruct rogue wave events from surface elevation measurements of ocean gravity waves. In particular we extract from the data stochastic equations for joint multipoint statistics [1]. Our procedure is applied to measurements from the Sea of Japan and the German North Sea over several days. The estimated stochastic equations allow to generate large ensembles of realistic wave time series to investigate the predictability of rogue waves. Furthermore we use the large deviation algorithm "Trajectory-Adaptive Multilevel Sampling" [2] to predict up to now unkown extreme wave events. While the North Sea equations do not lead to Rogue Waves, we do find those for the Sea of Japan. Averaging over several similar rogue waves, we obtain well-known rogue wave patterns like the "three sisters", proposed by from nonlinear-wave equations. i.e. nonlinear Schrödinger equation [3].

[1] Hadjihoseini, A.; et al: EPL (Europhysics Letters) 120 (2017), Nr. 3, 30008

[2] Lestang, T.; et.al Journal of Statistical Mechanics: Theory and Experiment 2018 (2018), Nr. 4, S. 043213

[3] Akhmediev, N.; et al: Physics Letters A 373 (2009), Nr. 6, S. 675–678

DY 15.12 Mon 18:15 ZEU/0114

Forecasting Extreme Events in Atmospheric Turbulence — •Finn Köhne and Joachim Peinke — Institute of Physics and ForWind, University of Oldenburg, Küpkersweg 70, D-26129 Oldenburg, Germany

Extreme wind speed fluctuations on time scales of seconds to minutes generate potentially significant mechanical loads for example on wind turbines and may lead to strong fluctuations in the power output [1,2]. Reliable short-term forecasts of such turbulent events are therefore of high relevance for many applications.

In this contribution, we use a stochastic framework based on the Fokker-Planck-equation (FPE) to forecast wind speed fluctuations in the atmospheric turbulence. We estimate drift and diffusion from measurement data to derive FPEs that describe the probabilistic evolution of wind speed increments without requiring data normalization [3].

The resulting model is used to perform probabilistic forecasts for extreme wind speed fluctuations. The quality of the forecast is quantified using receiver operating characteristic curves. The results demonstrate that the Fokker-Planck-based approach provides reliable short-term predictions of extreme events in the atmospheric turbulence.

[1] Davenport, A. G.; Proc. Inst. Civ. Eng. 19 (1961), Nr. 4, S. 449-472.

[2] DeMarco, A.; Basu, S.; Wind Energy 21 (2018), Nr. 10, S. 892-905.

[3] Peinke, J.; Tabar, M. R. R.; Wächter, M.; Annu. Rev. Condens. Matter Phys. 10 (2019), S. 107-132.

DY 16: Droplets, Wetting, and Microfluidics (joint session DY/CPP)

Time: Monday 15:00–18:30 Location: ZEU/0118

DY 16.1 Mon 15:00 ZEU/0118

Rayleigh instability in the presence of elastocapillarity — •Niphredil Klint and Andreas Isacsson — Chalmers University of Technology, Gothenburg, Sweden

A liquid jet, such as a stream of water, will disintegrate and form droplets if the length-to-radius ratio exceeds a critical value. This occurs due to propagating surface instabilities, a phenomenon known classically as the Rayleigh instability. At the nanoscale, thermal fluctuations affect the breakup dynamics, which may enter a stochastic regime [1]. Placing an elongated nanoscale liquid drop with a high aspect ratio on top of a highly compliant surface, the breakup process is affected by additional noise from thermally excited flexural phonons [2] as well as effects whereby the wetting causes the underlying surface to deform. We use large scale molecular dynamics (MD) simulations to examine the dynamics of the Rayleigh instability in the presence of elastocapillary effects at ambient temperatures. Specifically, we study the interactions between water and suspended graphene, where wetting induced deformations may occur for nanoscale droplets [3]. We focus on characterising the breakup and instability wavelength and isolate the effects of introducing graphene through a comparison of these results to simulations of only water. We also identify the correlation between out-of-plane fluctuations of the graphene and the concentration of water.

[1] J. Eggers, Phys. Rev. Lett. 89, 084502 (2002).
[2] M. Ma et al., Nature Mater. 15, 66 (2016).
[3] M. Kateb et al, Langmuir 39, 12610 (2023).

DY 16.2 Mon 15:15 ZEU/0118

Air layers and wetting under drops impacting on pre-wetted surfaces — •Kirsten Harth and Shiva Moradimehr — Fachbereich Technik, Technische Hochschule Brandenburg, Germany

Drop impact at low Weber numbers causes the formation of a (temporary) air cushion between the drop liquid and the substrate. On hard, dry substrates, its qualitative thickness profile and the location of the thinnest point are strongly governed by the Weber number. For impact on bulk, soft surfaces, like PDMS gels, it was found that impacts on softer substrates entrap more air [1]. Are there similar effects of thin liquid films?

We address the air layer shapes, entrapped air volume and wetting underneath droplets impacting on a hard substrate pre-wetted by microscopic oil layers. We control the Weber number, the oil layer thickness (in the range of micrometers), the oil viscosity, and in that way the *softness* of the substrate. Despite the thinness of the film, we observe clear effects of the oil layer on the volume and drainage of the air entrapment, its profile shapes, and the wetting behavior.

[1] K.R. Langley et al., Soft Matter 16, 5702 (2020)

We acknowledge funding by DFG within SPP2171 (HA8467/2-1, 2-2).

DY 16.3 Mon 15:30 ZEU/0118

Memory Effects in Contact Line Friction — •Niklas Wolf and Nico van der Vegt — TU Darmstadt, Darmstadt, Germany

When a drop of liquid comes into contact with a solid surface, it relaxes towards an equilibrium configuration, either wetting the surface or remaining in a droplet-like shape with a finite contact angle. The speed of this relaxation strongly depends on a friction force opposing the movement of the three-phase contact line. In analogy to the treatment of hydrodynamic friction we present an exact method, based on the Mori-Zwanzig formalism, to extract this friction from equilibrium data. Within the linear response regime, we obtain the frequency-dependent dissipative and elastic response of the contact line to an external perturbation, including a frequency-dependent friction coefficient. We find that the contact line exhibits long-lasting memory with a power-law decay due to coupling to the systems hydrodynamic modes. As a result the microscopic contact line dynamics are neither Markovian nor determined by the movement of a few molecules in the vicinity of the contact line.

DY 16.4 Mon 15:45 ZEU/0118

Reaction-Mediated Arrest and Gradient-Driven Droplet Transport — •Stefan Köstler[1,2], Yicheng Qiang[1], Malcolm Steen[1,2], Guido Kusters[1], and David Zwicker[1] — [1]Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany — [2]University of Göttingen, Institute for the Dynamics of Complex Systems, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Controlling droplet size and position is central to many biological and engineering processes. Chemical reactions can arrest coarsening and sustain spatial concentration gradients, while hydrodynamic flows generally accelerate coarsening and drive droplets along chemical gradients. Using continuum theory, we show that the competition between reactions, diffusion, and hydrodynamic advection yields rich behavior even in binary systems: Advection dominates the coalescence of small droplets, diffusion leads to Ostwald ripening for intermediate sizes, and reactions finally suppress coarsening. Interestingly, a range of droplet sizes is stable, depending on initial conditions and the strength of advection. Crucially, chemical gradients can actively steer droplets and couple to size-control. Our results demonstrate practical routes to control both the size distribution and spatial organization of droplets by tuning chemical activity and gradient-driven flows.

DY 16.5 Mon 16:00 ZEU/0118

From bipedal to chaotic motion of chemically fueled partially wetting liquid drops — •Florian Voss[1] and Uwe Thiele[1,2] — [1]Institute of Theoretical Physics, University of Münster — [2]Center for Data Science and Complexity (CDSC), University of Münster

Chemomechanical coupling is essential to various phenomena in soft matter systems that are kept permanently out of thermodynamic equilibrium, e.g., in reactive complex liquids. Based on a thermodynamically consistent continuum model, we demonstrate that partially wetting liquid drops covered by chemically reacting surfactants display a variety of biomimetic motility modes like shuttling, bipedal, rotational and quasi-random motion when supplied with chemical fuel from an ambient bath. The dynamics originates from chemomechanical feedback between the reaction network on the drop and the Marangoni effect [1] and becomes increasingly complex as a result of competing length scales. Due to the generic underlying thermodynamic structure, we expect that our results are also relevant for other chemically active mixtures and soft matter systems.

[1] F. Voss and U. Thiele, Phys. Rev. Fluids 10, 94005 (2025).

DY 16.6 Mon 16:15 ZEU/0118

Odd Droplets — •Thomas Appleford — University of Amsterdam, Amsterdam, Netherlands

In chiral systems such as active spinning colloidal matter, time-reversal symmetry-breaking interactions often give rise to a macroscopic continuum description in which the stress tensor contains off-diagonal terms. In fluids, these off-diagonal components lead to so-called "odd-viscous" deformations, in which energy is not dissipated. Odd viscous fluids have been shown to exhibit a rich variety of phenomena, including symmetry-broken flow around translating droplets and asymmetric droplet spreading on superhydrophobic surfaces. Our work investigates the behaviour of droplets in suspension. In particular, we present an analytical solution to the droplet-in-shear problem within the framework of two-dimensional odd Stokes flow, followed by the derivation of a formula for the apparent viscosity of a dilute emulsion. We then explore how chirality can be parametrically varied to tune the bulk rheological properties and control the system's overall energy dissipation.

DY 16.7 Mon 16:30 ZEU/0118

Stretching and Sliding Capillary Bridges — •Lennard Holschuh and Lars Pastewka — University of Freiburg, Department of Microsystems Engineering

Capillary forces play a critical role in the adhesion between two contacting bodies. However, existing theories of macroscopic adhesion on rough surfaces often assume dry conditions, attributing adhesive interactions solely to dispersion forces and overlooking the effects of capillary bridge formation. This study employs molecular dynamics simulations to directly examine the interactions of nanoscale probes with nominally flat surfaces in the presence of liquid bridges, which form due to condensation in humid environments. The objective is to link the thermodynamic understanding of capillary bridges with molecular simulations and atomic-force microscopy experiments. These calculations focus on investigating energy dissipation during adhesion (normal separation of the probe from the surface) and friction (lateral motion of the probe). By quantifying the interplay between relative humidity, adhesion, and friction, this work aims to improve the understanding of macroscopic adhesion in humid conditions and guide the development of materials with tailored properties for high-precision applications, such as microelectronic manufacturing.

15 min. break

DY 16.8 Mon 17:00 ZEU/0118

Hyperuniformity in Ternary Fluid Mixtures: The Role of Wetting and Hydrodynamics — •Nadia Bihari Padhan and Axel Voigt — Institute of Scientific Computing, TU Dresden, 01069 Dresden, Germany

Phase separation in multicomponent fluids underlies the organization of complex materials and biological structures, including biomolecular condensates. The Cahn-Hilliard-Navier-Stokes (CHNS) framework provides a natural description of such systems by coupling diffusive and hydrodynamic processes. In this talk, I will present our study of hyperuniformity–suppressed large-scale density fluctuations–in ternary CHNS mixtures. We show that hydrodynamics systematically drives the system toward less hyperuniform states and generates a rich set of morphologies, such as interconnected droplets and double emulsions reminiscent of biological phase separation. In partial-wetting regimes, all three

components display comparable hyperuniformity, whereas in complete-wetting regimes the preferred wetting component exhibits a marked loss of hyperuniformity. These results identify wetting asymmetry as a key control parameter for spatial order in multiphase fluids and offer a pathway for tuning large-scale organization in soft-matter and biological systems.

References [1] Boyer, F. and Lapuerta, C., Study of a three component Cahn-Hilliard flow model, ESAIM: Mathematical Modelling and Numerical Analysis, 40, 653-687 (2006). [2] Padhan, Nadia Bihari and Voigt, Axel, Hyperuniformity in ternary fluid mixtures: the role of wetting and hydrodynamics, arXiv:2506.22647, (2025).

DY 16.9 Mon 17:15 ZEU/0118

Effect of Flow Coupling on Defect Binding and Unbinding in Nematic Fluids — •Jayeeta Chattopadhyay, Simon Guldager Andersen, Kristian Thijssen, and Amin Doostmohammadi — Niels Bohr Institute, University of Copenhagen, Blegdamsvej 17, Copenhagen, Denmark.

Topological defects play a central role in the ordering and dynamics of nematic fluids. We investigate how coupling to fluid flow modifies defect-mediated phase transitions in two-dimensional nematics using fluctuating nematohydrodynamic simulations. The system is driven by tuning the fluctuation strength, with increasing and decreasing fluctuations defining forward and backward protocols. Without flow coupling, the system undergoes a Berezinskii–Kosterlitz–Thouless (BKT)–like transition via the reversible binding and unbinding of $\pm 1/2$ defect pairs. When hydrodynamics is included, the transition depends on the flow–alignment parameter: non-aligning nematics ($\lambda = 0$) retain BKT-like behavior, whereas strain-rate–aligning nematics ($\lambda \neq 0$) form bend–splay walls, lowering the defect-creation threshold and preventing recombination, leaving defects unbound across all fluctuation strengths. In active nematics, defects remain unbound for all λ, showing that self-generated flows also inhibit bound-pair formation. These results demonstrate that coupling to fluid flow fundamentally alters topological phase behavior, suppressing the equilibrium BKT binding mechanism.

DY 16.10 Mon 17:30 ZEU/0118

Electrophoresis in charged chiral active fluids with odd viscosity — •Reinier van Buel, Bogdan Cichocki, and Jeffrey Everts — Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland

Understanding the motion of colloidal particles dissolved in fluids that exhibit odd viscosity – a specific component of the viscous stress tensor found in e.g. chiral active fluids – is of particular interest for realising nontrivial particle transport and characterising out-of-equilibrium thermodynamic properties. Although three-dimensional odd viscosity has not yet been experimentally observed, charge stabilisation is expected to be vital in enabling such measurements. Therefore, we introduce the notion of a charged chiral active fluid and we investigate some of its non-trivial electrokinetic properties. In particular, we focus on electrophoresis of a charged sphere suspended in such an odd viscous fluid. Here, the peculiar nature of odd viscosity breaks the spherical symmetry of the system, and through coupling with the electric double layer and its screening properties, alters the electrophoretic mobility. Using the Lorentz reciprocal theorem, we derive expressions for the electrophoretic mobility of a spherical particle based on the analytical solution for the uncharged flow. Furthermore, we highlight how the Hückel and Smoluchowski limits of the electrophoretic mobility are affected by odd viscosity. Our results demonstrate that odd viscosity leads to directional asymmetries in the electrophoretic mobility tensor, suggesting mechanisms for active control of charged colloidal motion in systems where odd viscosity is prevalent.

DY 16.11 Mon 17:45 ZEU/0118

Experimentally probing microscale torsional memory in a viscoelastic fluid — •Niloyendu Roy[1], Rupayan Saha[2], Debankur Das[2], Matthias Krüger[2], and Clemens Bechinger[1] — [1]Fachbereich Physik, Universität Konstanz, Konstanz, Germany — [2]Institut für Theoretische Physik, Universität Göttingen, Göttingen, Germany

Motion of a colloid inside viscoelastic fluids follows non-Markovian dynamics, meaning its trajectory is influenced by past motion. Such memory effects are typically attributed to intrinsic material timescales arising from relaxation of the fluid microstructure and are usually probed using translationally driven colloids. Here we show experimentally that rotational driving of a colloid by a controlled torque elicits a far richer form of memory: the relaxation of the resulting torsional stresses spans a broad distribution of timescales, even though the fluid itself possesses a single dominant relaxation time. This behaviour allows time-dependent torsional driving histories to be encoded and subsequently read out through characteristic non-monotonic recoil responses. By mapping the flow field and the spatial distribution of torsional stresses, we demonstrate that the geometry of rotation generates an orthogonality between the propagation of angular momentum and the storage of torsional stresses, producing a spatio-temporal memory field not accessible through translational forcing. These results establish torsional driving as a powerful route to generate, store, and retrieve memory in viscoelastic fluids, opening new possibilities for soft-matter information storage and torque-responsive microdevices.

DY 16.12 Mon 18:00 ZEU/0118

3D Optofluidic Control Using Reconfigurable Thermal Barriers — •Falko Schmidt[1,2], Carlos David Gonzalez[3], Marc Sulliger[1], Emilio Ruiz-Rena[4], Raul A. Rica[3,5], Jaime Ortega-Arroyo[1], and Romain Quidant[1] — [1]Department of Mechanical and Process Engineering, ETH Zurich, Zurich 8092, Switzerland — [2]Peter Debye Insitute for Soft Matter Physics, Leipzig University, 04103 Leipzig, Germany — [3]Universidad de Granada, Department of Applied Physics, Granada 18071, Spain — [4]Department of Applied Physics II, University of Malaga, Malaga 29071, Spain — [5]Universidad de Granada, Research Unit Modeling Nature (MNAT), Granada 18071, Spain

Optothermal manipulation enables precise control of small particles via optical and thermal forces, leveraging thermo-osmotic and convective flows for short- and long-range motion. We present a reconfigurable optofluidic method enabling diverse manipulations such as guiding, sorting, trapping, and separating particles. Using light absorption on plasmonic surfaces of gold nanorods, localized hot spots are generated, creating temperature-driven flows. A near-infrared laser spatially modulates temperature landscapes, monitored by 3D holographic microscopy and optical diffraction tomography. Single and double heat sources produce three-dimensional flow control. This creates an optofluidic barrier that redirects particles within a microfluidic chamber. This approach offers a versatile foundation for advancing microfluidic technologies, enabling applications in sorting, trapping, and adaptive system design.

DY 16.13 Mon 18:15 ZEU/0118

Dynamics and Ordering of Microdroplets in Marangoni Flow Field — •Akshay Kallikkunnath and Frank Cichos — Molecular Nanophotonics, Peter Debye Institute for Soft Matter Physics, Faculty of Physics and Earth System Sciences, Leipzig University, Linnéstraße 5, 04103 Leipzig, Germany

Collective organization and internal dynamics are intimately linked and emerge across biological scales, with ordered structures providing a framework within which individual constituents remain dynamically active. Here, we study a system of water-in-oil microdroplets containing heat-releasing particles that organize under thermally induced flows. A sub-kelvin temperature increase from the heated particle at the air-oil interface generates Marangoni circulation that advects the droplets. Interactions through the flow field lead to robust ordering, while internal particle dynamics reflect coupling between local thermal gradients and microscale hydrodynamics. This provides a controllable platform to probe self-organization and emergent order by generating flows driven by weak, localized thermal fields in a fully fluid-in-fluid environment.

DY 17: Active Matter II (joint session DY/BP/CPP)

Time: Monday 15:00–18:30 Location: ZEU/0160

DY 17.1 Mon 15:00 ZEU/0160

Field-controlled self-organization in an active spin system — Mintu Karmakar[1,2,3], •Matthieu Mangeat[4], Swarnajit Chatterjee[5,4], Heiko Rieger[4], and Raja Paul[3] — [1]WIUCAS, Beijing, China — [2]Universitat de Barcelona, Barcelona, Spain — [3]IACS, Kolkata, India — [4]Saarland University, Saarbrücken, Germany — [5]CY Cergy Paris Université, Cergy-Pontoise, France

We investigate the collective response of active Potts particles to an external magnetic field and uncover three striking nonequilibrium phenomena. We first examine how the flocking transition is reshaped for a homogeneous and unidirectional field: the coexistence regime between an apolar gas and a polar liquid is replaced by a phase separation between two polar-ordered phases, a low-density, weakly polarized background and a high-density, strongly polarized band, both moving along the field. Second, when the particles self-organize into a high-density longitudinal lane whose long axis is perpendicular to the field, the lane slowly treadmills against the field direction, driven by the weakly polarized background. Finally, we identify a field-induced interface pinning regime that arises

when the domain is divided into two regions with opposite field directions, causing particles to accumulate and perform a back-and-forth motion at the interface. This pinning phenomenon also leads to the emergence of a disordered state in the presence of a random field orientation. A coarse-grained hydrodynamic theory supports and confirms the phenomena observed in our microscopic simulations.

DY 17.2 Mon 15:15 ZEU/0160

Nucleation kinetics in two-dimensional polar active fluids — •Yuta Kuroda and Thomas Speck — Institute for Theoretical Physics IV, University of Stuttgart, Germany

Polar active fluids constitute one of the most important classes of active matter. These systems possess alignment interactions that cause the local polarization to align with that of neighboring particles, leading to a flocking transition in which global polar order emerges. Extensive numerical and analytical studies have established that the flocking transition is discontinuous, and consequently, the phase diagram possesses a coexistence region in which propagating polar bands appear. Despite intensive studies on flocking transitions, the nucleation mechanism responsible for the formation of these bands remains poorly understood. In this work, we numerically investigate the nucleation kinetics of polar bands using a particle model, namely active Brownian particles with a Kuramoto-type alignment interaction, and we report the behavior of the nucleation rate over a wide range of parameters.

DY 17.3 Mon 15:30 ZEU/0160

Collision dynamics of active Brownian hard disks — •Jonas Buba — Soft Matter Theory Group, Theoretical Physics: Lab for Emergent Phenomena, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Active matter systems, composed of self-driven agents, display emergent behaviors such as collective motion, clustering, and motility-induced phase separation (MIPS). To better understand the microscopic origin of MIPS, we study collisions of active Brownian hard disks within the framework of dynamical density functional theory (DDFT). The particle interactions are modeled using fundamental measure theory (FMT). Each particle is represented by a Gaussian density peak, which allows us to quantify the mean delay from collisions for different configurations. The post-collision density resulting from the simulation can be described by a convolution of the pre-collision density, enabeling the analysis of different contributions to the delay.

DY 17.4 Mon 15:45 ZEU/0160

Active Ornstein-Uhlenbeck Particles: A Stochastic Path Integral Approach — •Carsten Littek, Mike Brandt, and Falko Ziebert — Institut für Theoretische Physik, Universität Heidelberg, Germany

In a recent publication (arXiv:2509.26296) we have developed a path integral formulation of the stochastic dynamics of a single active Brownian particle (ABP), with or without a constant torque, confined by a harmonic trap. This approach is based on the particle's microscopic degrees of freedom and we have derived exact analytic time-dependent expressions for key observable quantities such as the mean position and mean square displacement without the necessity of solving the Fokker-Planck equation. Here we present the application of this approach to the dynamics of active Ornstein-Uhlenbeck particles (AOUP). In particular, we generalize our formulation to systems of many AOUPs interacting via a suitable two-particle potential and derive the statistical quantities relevant in the context of collective phenomena, such as motility-induced phase separation (MIPS).

DY 17.5 Mon 16:00 ZEU/0160

Self-alignment and chirality in dense active matter: from flocking to circling crystals — •Marco Musacchio[1], Alexander Antonov[1], Hartmut Löwen[1], and Lorenzo Caprini[2] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf, Germany — [2]Physics Department, University of Rome La Sapienza, P.le Aldo Moro 5, IT-00185 Rome, Italy

Several experimental systems in active matter are characterized, at the single-particle level, by an effective torque that aligns particle orientation with their instantaneous velocity. This mechanism, known as self-alignment, appears in both biological and granular active systems. In dense active systems, a sufficiently strong self-alignment can suppress mips and drive the system from a clusterized flocking state to an homogeneous one, where all particles move collectively, with aligned velocities. This flocking transition is approached for a broad range of densities, even close to maximal packing, where the system is in a crystalline configuration. Specifically, in the crystal case, the flocking transition can be predicted analytically since the dynamics can be mapped onto a velocity-dependent Landau*Ginzburg free energy, revealing that this disorder*order transition is second order. The onset of chirality drives the system from collective flocking to a circling crystal phase, characterized by coherent circular motion of all the system. Further increasing chirality suppresses the global rotation, leading to a vortex-like structure in the velocity field. These findings are experimentally testable in systems governed by self-alignment and chirality.

DY 17.6 Mon 16:15 ZEU/0160

Number fluctuations distinguish different self-propelling dynamics — •Tristan Cerdin[1,2], Sophie Marbach[2], and Carine Douarche[1] — [1]Université Paris-Saclay, CNRS, FAST, 91405, Orsay, France — [2]CNRS, Sorbonne Université, Physicochimie des Electrolytes et Nanosystèmes Interfaciaux, F-75005 Paris, France

In nonequilibrium suspensions, static number fluctuations N in virtual observation boxes reveal remarkable structural properties, but the dynamic potential of $N(t)$ signals remains unexplored. Here, we develop a theory to learn the dynamical parameters of self-propelled particle models from $N(t)$ statistics.

Theoretical plots of the mean-squared number difference $\langle \Delta N^2(t) \rangle$ exhibit 3 scaling regimes in time corresponding to the 3 regimes of self-propelled particles: diffusive, advective and effectively diffusive again at long times. By expanding the theory in each of these regimes, we recover limiting laws for the number fluctuations, which can be used in practice to quantify self-propulsion properties.

Additionally, unlike traditional trajectory analysis, $N(t)$ statistics distinguish between models, by sensing subtle differences in reorientation dynamics that govern re-entrance events in boxes. This paves the way for quantifying advanced dynamic features in dense, out-of-equilibrium suspensions.

DY 17.7 Mon 16:30 ZEU/0160

Flocking transitions in dense mixtures of active self-aligning and passive particles — •Weizhen Tang[1], Amir Shee[2], Zhangang Han[1], Pawel Romanczuk[3,4], Yating Zheng[3,4], and Cristián Huepe[1,5,6] — [1]School of Systems Science, Beijing Normal University, Beijing, China — [2]Department of Physics, University of Vermont, USA — [3]Department of Biology, Humboldt Universität zu Berlin, Unter den Linden 6, Berlin, Germany — [4]Research Cluster of Excellence 'Science of Intelligence', Berlin, Germany — [5]Northwestern Institute on Complex Systems and ESAM, Northwestern University, Evanston, USA — [6]CHuepe Labs, 2713 West Augusta Blvd #1, Chicago, USA

We investigate the passivity-driven flocking transition in a dense mixture of self-aligning active particles and passive particles, using a minimal model of active polar disks. We show that anisotropic damping leads to a discontinuous flocking transition as a function of the fraction of passive components, whereas isotropic damping produces a smooth transition where the final ordered state can display sustained oscillations and remain trapped in a metastable state, depending on the exact spatial arrangement of the passive particles. We also explore in detail the emergence of metastable oscillatory ordered states and their relation to the spatial distribution of passive particles and interstitial voids. Our findings demonstrate that heterogeneous activity and mobility anisotropy can result in a rich variety of self-organized states in various biological systems, synthetic active materials, and robotic swarms.

15 min. break

Invited Talk DY 17.8 Mon 17:00 ZEU/0160

Topological transition in filamentous cyanobacteria: from motion to structure — •Marco Mazza — Loughborough University, Loughborough, UK

Many active systems are capable of forming intriguing patterns at scales significantly larger than the size of their individual constituents. Cyanobacteria are one of the most ancient and important phyla of organisms that has allowed the evolution of more complex life forms. Despite its importance, the role of motility on the pattern formation of their colonies is not understood. Here, we investigate the large- scale collective effects and rich dynamics of gliding filamentous cyanobacteria colonies, while still retaining information about the individual constituents' dynamics and their interactions. We investigate both the colony's transient and steady-state dynamics and find good agreement with experiments. We furthermore show that the Péclet number and aligning interaction strength govern the system's topological transition from an isotropic distribution to a state of large-scale reticulate patterns. Although the system is topologically non-trivial, the parallel and perpendicular pair correlation functions provide structural information about the colony, and thus can be used to extract information about the early stages of biofilm formation. Finally, we find that the effects of the filaments' length cannot be reduced to a system of interacting points. Our model proves to reproduce both cyanobacteria colonies and systems of biofilaments where curvature is transported by motility.

DY 17.9 Mon 17:30 ZEU/0160

Novel Phase Coexistence in a Multi-Species Vicsek Model — •Eloise Lardet[1], Letien Chen[1,2], and Thibault Bertrand[1] — [1]Imperial College London, UK — [2]University of Edinburgh, UK

A hallmark in natural systems, self-organization often stems from very simple interaction rules between individual agents. While single-species self-propelled particle (SPP) systems are well understood, the behavior of mixtures of self-propelled particles with general alignment interactions remains largely unexplored with a few scattered results hinting at the existence of a rich emergent phase behavior. Here, we first present a generalization of the two-species Vicsek model with reciprocal intra- and interspecies (anti-)alignment couplings, un-

covering a rich phenomenology of emergent states. Notably, we show that rather than destroying polar order, anti-aligning interactions can promote phase separation and the emergence of global polar order. Secondly, we derive a kinetic theory for the system, finding good agreement between theoretical predictions and particle simulations. This includes a novel mechanism for microphase separation, as predicted by a Turing instability. We finally show that these coexistence patterns can be generalized to multi-species systems with cyclic alignment interactions.

DY 17.10 Mon 17:45 ZEU/0160

Flocking in weakly nonreciprocal mixtures — •Charlotte Myin — Max Planck Institute for Dynamics and Self-Organization (MPI-DS), 37077 Goettingen, Germany

We show that weakly nonreciprocal alignment leads to large-scale structure formation in flocking mixtures. By combining numerical simulations of a binary Vicsek model and the analysis of coarse-grained continuum equations, we demonstrate that nonreciprocity destabilizes the ordered phase formed by mutually aligning or anti-aligning species in a large part of the phase diagram. For aligning populations, this instability results in one species condensing in a single band that travels within a homogeneous liquid of the other species. When interactions are anti-aligning, both species self-assemble into polar clusters with large-scale chaotic dynamics. In both cases, the emergence of structures is accompanied by the demixing of the two species, despite the absence of repulsive interactions. Our theoretical analysis allows us to elucidate the origin of the instability, and show that it is generic to nonreciprocal flocks.

DY 17.11 Mon 18:00 ZEU/0160

Collective behavior in nonreciprocal multi-species Vicsek model with permutation symmetry — •Jae Dong Noh[1], Chul-Ung Woo[2], and Heiko Rieger[2] — [1]Department of Physics, University of Seoul, Seoul 02504, Korea — [2]Department of Theoretical Physics and Center for Biophysics, Saarland University, Saarbrücken, Germany

Nonreciprocal systems are typically built upon asymmetric roles among interacting agents, such as a pursuer-evader relationship. We propose a multi-species nonreciprocal active matter model that is invariant under permutations of the particle species. The nonreciprocal, yet symmetric, interactions emerge from a constant phase shift in the velocity alignment interactions, rather from an asymmetric coupling matrix. This system displays rich collective behaviors, including a species-mixed chiral phase with quasi-long-range polar order and a species-separated vortex cell phase. We present numerical evidence for these phases using particle-based Monte Carlo simulations and analytic evidence using continuum Boltzmann and hydrodynamic equations. Our work demonstrates that multi-species chiral fluids can be realized by a nonreciprocal but symmetric alignment interaction, where the rich collective behavior is a consequence of the interplay between nonreciprocity and permutation symmetry.

DY 17.12 Mon 18:15 ZEU/0160

Flocking with random non-reciprocal interactions — •Jiwon Choi[1], Jae Dong Noh[2], and Heiko Rieger[1] — [1]Department of Physics & Center for Biophysics, Saarland University, Campus E2 6, 66123 Saarbrücken, Germany — [2]Department of Physics, University of Seoul, Seoul, 02504, Korea

Flocking is ubiquitous in nature and emerges from alignment interactions among self-propelled agents. Two species that anti-align or interact non-reciprocally exhibit complex collective phenomena, ranging from parallel and anti-parallel flocking and run-and-chase behavior to chiral phases. Whether such behavior survives in the presence of many species with random non-reciprocal interactions has remained unclear. As a first step, we study a continuous-time Vicsek-like model with fully random non-reciprocal interactions between particles. For infinite-range interactions, flocking emerges once the alignment bias becomes comparable to the non-reciprocal interactions, and deep inside this phase random non-reciprocity can still support slow global chiral and oscillating states. For short-range interactions, even without alignment bias, self-organized cliques form, where medium-sized clusters with predominantly aligning interactions remain stable over long times. We further investigate the robustness of clique formation and the coexistence phase under angular noise using a discrete-time Vicsek model with random non-reciprocal interactions. These results provide a basis for studying multi-species flocking with complex non-reciprocal interactions.

DY 18: Active Matter III (joint session BP/CPP/DY)

Time: Tuesday 9:30–12:45 Location: BAR/SCHÖ

DY 18.1 Tue 9:30 BAR/SCHÖ

inertia-driven re-entrant coil-Globule transition of active ring polymers — •Sunil P Singh[1], Roland G Winkler[2], Rakesh Palariya[1], and Arindam Panda[1] — [1]Indian Institute of Science Education and Research Bhopal, India — [2]Theoretical Physics of Living Matter, Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Germany

The role of inertia in the collective dynamics of active systems has been a subject of increasing interest in recent studies. The present study investigates the inertial effects on active agents. We present the conformational and dynamical characteristics of an active Brownian ring polymer using Langevin dynamics simulations. We show that a long active ring polymer shrinks into globular-like structures even in the absence of attractive interactions. This transition becomes sharper and the structures more compressed as the reduced moment of inertia of the monomers increases, particularly in the intermediate range of activity. We demonstrate that the ring polymer undergoes a coil-globule-coil transition, which is modulated by both activity and rotational inertia. The coil-to-globule transition is mapped in the inertial parameter space (J-M) using the radius of gyration. Additional physical quantities, including bond-bond correlations, scaling behavior in the compressed state, monomer contact probability, geometric distances, coordination number, and effective temperature, further elucidate the physical mechanism driving the collapse. Finally, we show that the effective diffusivity of the ring polymer increases with the reduced moment of inertia as $D_p \sim \sqrt{J}$.

DY 18.2 Tue 9:45 BAR/SCHÖ

Shape selectivity by complex buckling dynamics in poroelastic active gels — •Kinjal Dasbiswas[1], Subhaya Bose[1], Arnab Roy[1], Michael Vennettilli[1], and Anne Bernheim[2] — [1]University of California, Merced, USA — [2]Ben Gurion University, Israel

Shape change in animal cells is prototypically driven by active forces, generated by myosin molecular motors bound to the actin cytoskeleton. Inspired by experiments on disc-shaped extracts of crosslinked actomyosin gels, we aim to show how a family of 3D shapes can arise from buckling caused by non-uniform active stresses. Although synthesized with identical composition of actin, myosin and the crossliker fascin, these gels contract and buckle into different shapes depending on the initial aspect ratio of the disc: thinner gels tend to wrinkle, while thicker gels tend to form domes. By incorporating active stresses, actin alignment, and stress-dependent myosin binding kinetics into a 2D poroelastic gel model, we qualitatively capture trends in gel contraction dynamics observed from quantitative particle image velocimetry (PIV). Next, we carry out numeric simulations of a geometric elastic model for thin sheets to obtain 3D buckled shapes from the strain rates predicted by the poroelastic model. Our results show that the coupling of elasticity to solvent flow, motor binding and fiber alignment play an important role in shape changes in living matter. Our studies have implications for shape changes during tissue morphogenesis and cell migration.

DY 18.3 Tue 10:00 BAR/SCHÖ

The energy cost to build a spindle — •Dongliang Zhang[1], Xingbo Yang[4], Jan Brugués[2,1,3,4], and Frank Jülicher[1,3,4] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [3]Center for Systems Biology Dresden, Dresden, Germany — [4]Physics of Life, Cluster of Excellence, TU Dresden, Dresden, Germany

Spindle is a structure actively build from microtubules (MTs), and plays an important role for chromosome segregation during cell cycle. It's observed in experiments that the spindle size and shape depends on the cell level metabolic rate. In this work, we developed a minimal model that captures the active, energy-consuming processes such as MT turnover and active stress generation, which shows the energy cost for spindle mass maintenance and spindle-shape formation. We show that a spindle can be self-organized through these active processes. We aim to predict how the size and shape of the spindle depends on the energy input, and explain relative experimental phenomena, e.g. spindle shrinkage when the metabolism level is reduced.

DY 18.4 Tue 10:15 BAR/SCHÖ

Cytoskeletal oscillations drive large-scale flows and nuclear organization in early embryonic systems. — •Lara Koehler, Elissavet Sandaltzopoulou, and Jan Brugués — Physics Of Life, TU Dresden

Synchronization drives early embryonic development, enabling simultaneous cell divisions and the spatial organization of nuclei within the embryo. In organisms such as Xenopus, Drosophila, and zebrafish, mitotic waves coordinate cell cycles across distances that exceed diffusion limits, guided by a chemical oscillator. At the same time, global cytoplasmic flows in these syncytial tissues contribute to the large-scale self-organization of nuclei, yet the coupling between biochemical signaling and cytoskeletal mechanics that underlies these directed flows remains poorly understood. Here, we relax the geometric constraints of

the embryo and investigate nuclear dynamics in Xenopus egg extracts and complementary simulations. We show that the periodic polymerization and depolymerization of microtubule asters are sufficient to generate robust large-scale directed flows, even though the asters are intrinsically isotropic. Furthermore, we demonstrate that cell division stabilizes short-range order in a global synchronized system. Together, these findings reveal a minimal physical mechanism by which cytoskeletal dynamics and biochemical oscillations jointly organize flows and patterns, with implications for understanding the emergent principles that shape early development across species.

DY 18.5 Tue 10:30 BAR/SCHÖ

Geometric control of cell migration in disordered porous media — •Laeschkir Würthner[1] and Frederik Graw[2] — [1]European Molecular Biology Laboratory, Heidelberg, Germany — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg and Universitätsklinikum Erlangen, Erlangen, Germany

Cell migration is a dynamic process that plays a central role in development, wound healing, and immune responses. Active cell movement is controlled by several biochemical and mechanical cues, including chemokine gradients and the mechanical properties of the extracellular matrix (ECM). Although the biochemical pathways underlying directed cell motion are increasingly well understood, the influence of the porous structure of the ECM on active cell motion remains largely unexplored. Using a combination of computational modeling and theory, we investigate how active cells move through 3D disordered porous environments. We show that cell migration in disordered porous media can be understood as a generalized random walk among "traps", with the effective diffusivity determined by the geometry of the microenvironment. A key implication of our work is that spatial heterogeneities in porosity effectively direct cell motion, revealing a guidance mechanism that we refer to as porotaxis. Overall, our work connects geometry with cell motility and underscores the microenvironment as a key regulator of cell migration.

DY 18.6 Tue 10:45 BAR/SCHÖ

Motility-induced mixing transition in exponentially growing multicellular spheroids — •Torben Sunkel[1,2], Lukas Hupe[1,2], and Philip Bittihn[1,2] — [1]MPI for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, University of Göttingen, Germany

Growth drives cellular dynamics in various dense aggregates, but its effects on other relevant activities have only received limited attention. Here, we investigate the interplay of unconstrained growth, steric repulsion and motility in a minimal agent-based model of exponentially growing, three-dimensional spheroids. Our results reveal a diverging mixing time scale at a critical motility threshold, below which mixing of cells is completely suppressed. Above the threshold, large-scale mixing is enabled. Using an effective phenomenological model parameterized from full simulations, we identify two fundamental mechanisms governing this transition: On the cell scale, weak motility-induced active motion is locally suppressed by growth-induced steric repulsion, consistent with an Active Brownian Particle type description of single-cell dynamics. Beyond this, the expanding nature of the system inhibits global mixing purely geometrically by limiting the exploration range of diffusive cell motion. Both mechanisms naturally scale with the growth rate, highlighting the nature of the transition as an interplay between proliferation and motility. The results provide a baseline for identifying additional biological mechanisms in experiments and could be relevant for competition, heterogeneous tumor evolution and other manifestations of motile proliferating active matter.

15 min. break

DY 18.7 Tue 11:15 BAR/SCHÖ

Fluctuation-Response Theory of Non-Equilibrium Complex Fluids — •Ryota Takaki[1] and Frank Jülicher[1,2,3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Center for Systems Biology Dresden, Dresden, Germany — [3]Cluster of Excellence Physics of Life, TU Dresden, Dresden, Germany

Active soft materials such as cytoplasm and tissues are constantly driven by chemical reactions and often retain long-lived mechanical memory. In this work, we develop a generalized hydrodynamic framework applicable to non-equilibrium fluids with memory at finite wavevectors and frequencies. Our approach is based on exact correlation-function identities, leading to a fluctuation-response relation for steady states, including non-equilibrium. Applying the theory to chemically driven active fluids, we uncover Active Viscoelastic Memory, in which reaction cycles dynamically renormalize the viscous response and can generate negative storage moduli at finite frequency, absent in conventional viscoelastic materials. Our results provide a first-principles basis for modeling memory-dependent dynamics in a broad class of biological and synthetic active systems, and suggest concrete rheological signatures of chemical driving that can be tested experimentally.

DY 18.8 Tue 11:30 BAR/SCHÖ

Chemically Active Liquid Bridges Generate Repulsive Forces — •Noah Ziethen — DAMTP, University of Cambridge, UK

Intracellular droplets help organize cells by compartmentalizing biomolecules and mediating mechanical interactions. When such droplets bridge two structures, they generate capillary forces that depend on the surface properties and the separation between the structures. While the forces exerted by passive liquid bridges are well understood, the impact of active chemical reactions, ubiquitous in biological condensates, remains unclear.

Here, we investigate a single liquid bridge with continuous chemical turnover, in which the production and degradation of droplet material maintain a non-equilibrium steady state. In this active bridge, the reactions dynamically set the bridge radius, thereby controlling the force-distance relation. In striking contrast to passive systems, we find that activity can generate purely repulsive forces over a broad range of separations. These results show that chemical activity can qualitatively alter capillary forces generated by liquid bridges, suggesting a potential route for cells to actively regulate mechanical coupling via droplets.

DY 18.9 Tue 11:45 BAR/SCHÖ

Shared Laws of Pattern Formation in Reaction-Diffusion and Phase Separation — •Daniel Zhou[1] and Erwin Frey[1,2] — [1]Arnold Sommerfeld Center for Theoretical Physics — [2]Max Planck School Matter to Life

Many nonlinear field theories generate a strikingly similar repertoire of patterns: arrested coarsening, traveling waves, and spatiotemporal chaos appear both in phase-separating systems and in classical reaction-diffusion models. These descriptions have different physical origins, yet recent studies on Turing mixtures and foams in protein systems [1] and on chemotaxis-driven phase separation in cell populations [2] have already highlighted unexpected connections between these ostensibly different mechanisms, linking foam-like, phase-separating, and reaction-diffusion-type patterns. The present work revisits the relation between kinetic and phase-separating descriptions from a more general viewpoint. A unifying perspective is developed that places different modeling frameworks on comparable footing, identifies the conditions under which they yield effectively equivalent patterns, and suggests how stability criteria and design principles can be translated between them. This points toward a more systematic classification of pattern-forming dynamics that cuts across traditional divides between reaction-diffusion, chemotactic, and phase-separating systems.

[1] H. Weyer et. al, Deciphering the Interface Laws of Turing Mixtures and Foams, arXiv:2409.20070 (2024).

[2] H. Weyer et. al, Chemotaxis-Induced Phase Separation, Physical Review Letters 135, 208402 (2025).

DY 18.10 Tue 12:00 BAR/SCHÖ

Spatial self-organization of enzymes in complex reaction networks — •Vincent Ouazan-Reboul[1,2], Ramin Golestanian[2,3], and Jaime Agudo-Canalejo[2,4] — [1]LPTMS, CNRS, Université Paris-Sud, 91400, Orsay, France — [2]Max Planck Institute for Dynamics and Self-Organization, Am Fassberg 17, D-37077, Göttingen, Germany — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, OX1 3PU, Oxford, UK — [4]Department of Physics and Astronomy, University College London, WC1E 6BT, London, UK

Living systems contain intricate biochemical networks whose structure is closely related to their function and allows them to exhibit robust behavior in the presence of external stimuli. Such networks typically involve catalytic enzymes, which can have non-trivial transport properties, in particular chemotaxis-like directed motion along gradients of substrates and products. Here, we find that taking into account enzyme chemotaxis in models of catalyzed reaction networks can lead to their spatial self-organization in a process similar to biomolecular condensate formation. We develop a general theory for arbitrary reaction networks, and systematically study all closed unimolecular reaction networks involving up to six chemicals. Importantly, we find that network-wide propagation of concentration perturbations can be key to enabling self-organization, in a manner which is highly sensitive on the global network structure.

DY 18.11 Tue 12:15 BAR/SCHÖ

Spatial organisation of the cell's metabolic power plant via phase separation — •Kathrin S. Laxhuber[1,2] and Frank Jülicher[1,2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck School Matter to Life

Cell metabolism is the power plant that fuels the active processes essential to life. Recent experimental results show that glycolytic enzymes, central to sugar metabolism, phase-separate to form foci under energetic stress and can localise to sites of demand. To understand this phenomenon, we build and study a minimal theoretical model. We show that droplet formation can act as a metabolic switch that enables the system to maintain energetic homeostasis at higher output power. Notably, the metabolic droplets that emerge from this switch can self-organise to colocalise with demand. We discuss the non-equilibrium features and spatial energetic profiles in this system.

DY 18.12 Tue 12:30 BAR/SCHÖ

Emergent interactions lead to collective frustration in robotic matter — •Onurcan Bektas[1,3], Adolfo Alsina[2,3], and Steffen Rulands[1,3] — [1]Arnold-Sommerfeld-Center for Theoretical Physics and Center for NanoSciences, Ludwig-Maximilians-Universität München, Theresienstr. 37, 80333 München, Germany — [2]GISC, Universidad Rey Juan Carlos, Tulipán, 28933, Móstoles, Spain — [3]Max-Planck-Institute for the Physics of Complex Systems, Noethnitzer Str. 38, 01187 Dresden, Germany

Current artificial intelligence systems show near-human-level capabilities when deployed in isolation. Systems with intelligent agents are deployed to perform tasks collectively. This raises the question of whether robotic matter, where many learning and intelligent agents interact, shows emergence of collective behaviour. And if so, what kind of phenomena would such systems exhibit? Here, we study a paradigmatic model for robotic matter: a system composed of a large collection of stochastic interacting particles where each particle is endowed with a deep neural network that optimizes its transitions based on the particles' environments. For a 1D model, robotic matter exhibits complex phenomena arising from emergent interactions, including transitions between long-lived learning regimes, the emergence of particle species, and frustration. We also find an abrupt, density-dependent change in the behaviour of particles. Using active matter theory, we show that this phenomenon is a reflection of a phase transition with signatures of criticality. Our model captures key phenomena observed in more complex forms of robotic systems.

DY 19: Franco-German Session on Granular Matter I

Granular media exhibit rich collective behavior arising from simple interactions such as friction, collisions, elasticity, and confinement. This session brings together experimental, numerical, and theoretical studies addressing key transitions in granular systems, including jamming, viscous-to-inertial regimes, clustering, gas cooling, and impact dynamics, highlighting the links between microscopic mechanisms and macroscopic responses.

Organized by Baptiste Darbois Texier (Paris) and Franco Antonio Tapia Uribe (Dresden)

Time: Tuesday 9:30–12:45 Location: HÜL/S186

Invited Talk DY 19.1 Tue 9:30 HÜL/S186

Mechanics of entangled fibers — •Olivier Pouliquen[1], Aubin Archambault[1], Ignacio Andrade[2], Jerome Crassous[3], Henri Lhuissier[1], and Joël Marthelot[1] — [1]IUSTI, CNRS-Aix Marseille University, Marseille, France — [2]Departamento de Física, Universidad de Chile, Santiago, Chile — [3]CNRS - ESPCI Université PSL/Sorbonne Université/Université de Paris, paris, France

When long, flexible fibers are densely packed, they form cohesive structures, such as those found in bird*s nests, cotton balls, or fibrous insulation materials. These peculiar granular assemblies exhibit complex mechanical behaviors: they can be compacted and sustain tensile stress, despite the absence of adhesive bonds. Through experiments on model materials and discrete-element simulations, we investigate the interplay between elasticity and friction that governs the mechanics of entangled, non-bonded fiber networks.

DY 19.2 Tue 10:00 HÜL/S186

Rheology of suspensions of non-Brownian spheres across the jamming and viscous-to-inertial transition — •Franco Tapia[1,2], Olivier Pouliquen[2], Chong-Wei Hong[2], Pascale Aussillous[2], and Elisabeth Guazzelli[3] — [1]Institute of Urban and Industrial Water Management, TU Dresden, Dresden, Germany — [2]Aix-Marseille Université, CNRS, IUSTI, Marseille, France — [3]Université Paris Cité, CNRS, Matiére et Systèmes Complexes (MSC) UMR 7057, Paris, France

We study the rheology of suspensions of non-Brownian hard and soft particles across the jamming transition and within both viscous and inertial flow regimes, using a custom-built pressure- and volume-imposed rheometer. Our results, expressed in terms of the effective friction coefficient and packing fraction, demonstrate that suspensions of hard spheres exhibit continuous shear thickening when inertia becomes significant at a transitional Stokes number of 10, independent of the packing fraction. These findings can be extended to a Soft Granular Rheology model by renormalizing the volume fraction and friction coefficient to pressure-dependent values, incorporating both viscous and inertial stress scales. SGranR successfully captures the rheological behavior, showing an approximate collapse into two branches through power-law scaling relative to the distance from the jamming point: (i) above the jamming transition, where the behavior is described by a generalized Herschel-Bulkley law with yield stress and shear thinning, and (ii) below the jamming point, where the behavior follows a critical power law, with shear thinning near the jamming point.

DY 19.3 Tue 10:15 HÜL/S186

granular drag towards zero gravity — •tianhui liao[1], tivadar pongo[1], jinchen zhao[1], simeon vöelkel[2], valentin dichtl[2], raúl c. hidalgo[3], and kai huang[1,2] — [1]Collective Dynamics Lab, Division of Natural and Applied Sciences, Duke Kunshan University, 215306 Kunshan, Jiangsu, China — [2]Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany — [3]Department of Physics and Applied Mathematics, University of Navarra, 31009 Pamplona, Spain

The role of gravity on the drag force F_d acting on a projectile impacting granular media is investigated experimentally using embedded inertial measurement unit (IMU) sensor and numerically with discrete element method (DEM) simulations. As gravity approaches zero, the inertial drag plays a dominating role, leading to qualitatively different scaling laws and cavity dynamics. Similarly to fluid dynamics, we define a dimensionless granular drag coefficient C_{gd}, which yields a constant of $\approx 1.2 \pm 0.2$ under microgravity, and a term inversely proportional to the impact velocity v_0 is added in the presence of gravity. This connection to fluid drag sheds light not only on a wide range of applications of granular media in space exploration, but also on drag force in non-Newtonian fluids from a first principle perspective.

DY 19.4 Tue 10:30 HÜL/S186

Impact of Roughness on Packing Fraction — •Adrien Luyckx and Eric Opsomer — GRASP Institute, Liege University, Belgium

This study investigates the impact of particle rugosity on the mechanical properties of piles using computational methods. We focus on smooth, non-convex particles (rod, cross, and star shapes) approximated via multisphere approach. Our research introduces the concepts of macro-rugosity, which increases as we progress from rod to cross to star shapes, and meso-rugosity, which is adjusted by varying the number of spheres composing the particles. Key findings include: (1) A limited meso-rugosity is sufficient to capture the mechanical properties of a pile, such as its height. (2) As macro-rugosity increases, the required meso-rugosity decreases. These results demonstrate that particle representation can be optimized by balancing meso-rugosity with the imposed macro-rugosity, significantly reducing computational demands. Our findings contribute to the ongoing efforts in enhancing the efficiency and accuracy of discrete element methods (DEM) in modeling complex particle systems.

DY 19.5 Tue 10:45 HÜL/S186

Tangential forces govern viscous-inertial transition in dense frictional granular suspensions — •Sudarshan Konidena[1], Franco Tapia[1], Alireza Khodabakhshi[1], Élisabeth Guazzelli[2], Pascale Aussillous[3], and Bernhard Vowinckel[1] — [1]Institute of Urban and Industrial Water Management, Technische Universität Dresden, 01062 Dresden, Germany — [2]Université Paris Cité, CNRS, Matière et Systèmes Complexes (MSC) UMR 7057, Paris, France — [3]Aix Marseille Université, CNRS, IUSTI, Marseille, France

Using pressure-imposed rheology, we carry out particle-resolved simulations to study dense suspensions of frictional suspensions as they move from a viscous regime into an inertial one. By independently tuning the liquid viscosity, the shear rate, and the confining granular pressure, we determine that the onset of this transition always appears at a Stokes number near 8 and does not depend on the volume fraction. A key outcome is that the shear stress evolves toward its inertial behavior more slowly than the particle pressure. This delayed response arises from the combined influence of tangential contact forces and lubrication interactions, which govern how frictional particles gradually switch from predominantly rolling motions to predominantly sliding ones. Although the Stokes number dictates the overall shift, the degree of proximity to jamming also plays a role. We further explore how stronger inter-particle friction alters the characteristics of the viscous*inertial transition.

15 min. break

DY 19.6 Tue 11:15 HÜL/S186

Rheology of Granular Sediment Beds from Dense to Creeping Regimes — •Bernhard Vowinckel[1], Pascale Aussillous[2], and Élisabeth Guazzelli[3] — [1]Institute of Urban and Industrial Water Management, Technische Universität Dresden, 01062 Dresden, Germany — [2]Aix Marseille Université, CNRS, IUSTI,

Marseille, France — [3]Université de Paris, CNRS, Matière et Systèmes Complexes (MSC) UMR 7057, Paris, France

We investigate the rheology of sheared sediment beds using grain-resolved direct numerical simulations supported by experimental data. Poiseuille and Couette configurations are examined, extending monodisperse systems to polydisperse beds with diameter ratios up to 10. The simulations provide depth-resolved stress profiles, fluid-particle momentum exchange, particle volume fraction, and granular pressure. For monodisperse beds, shear and normal viscosities and the effective friction coefficient follow established correlations, with a critical particle volume fraction of about 0.3 marking the transition from dense to dilute regimes. In the dilute transport layer, hydrodynamic interactions are screened and the effective viscosity approaches the Einstein relation. For polydisperse mixtures, we generalize $\mu(J)$-rheology by linking its parameters to the maximum packing fraction, achieving good agreement with reference data. Access to very low viscous numbers shows that the friction coefficient in the creeping regime tends to a finite quasi-static value, reducing the critical friction coefficient by a factor of three. These findings refine closure relations for two-phase sediment transport models.

DY 19.7 Tue 11:30 HÜL/S186

Elastic Soft-Shell Packings — •Eric Opsomer and Nicolas Vandewalle — University of Liege, Liege, Belgium

The evolution of pressure at the bottom of a two-dimensional pile of thin elastic rings is investigated for increasing filling height of the system. Due to the soft nature of the particles, contact forces are only weakly deviated which causes a delay of the pressure saturation that is commonly observed in hard grain system. More importantly, for large fillings, an abrupt transition within the structure of the granular pile is encountered once the surrounding pressure leads to the buckling of the rings composing the bottom layers of the pile. The latter transition can be predicted based on the mechanical properties of the thin rings and the global evolution of pressure can be modeled by extending Janssen's model to an effective two-phase granular media.

DY 19.8 Tue 11:45 HÜL/S186

Rheology of dense suspension: the effects of wall-boundaries on viscous-inertial transition — •Alireza Khodabakhshi, Sudarshan Konidena, Franco Tapia, and Bernhard Vowinckel — Institute of Urban and Industrial Water Management, TU Dresden, Dresden, Germany

The transition from the viscous to the inertial regime in dense suspensions is still not fully clarified. Volume-imposed rheometers with fixed-gap walls offer valuable information by reporting shear and normal stress as functions of shear rate, yet the influence of confining boundaries, especially in narrow-gap configurations relevant to industrial and natural flows, remains insufficiently explored. In this study, we perform particle-resolved Direct Numerical Simulations (pr-DNS) of dense non-Brownian suspensions sheared between rough walls in a confined volume-imposed rheometer. The simulations capture the overall viscous-inertial trend reported in recent experiments and reproduce the observed weakening of the effective friction coefficient during the transition. We analyze multiple cases by varying wall roughness and rheometer height, showing that both parameters strongly affect stress levels by altering particle layering. All configurations develop pronounced layering, but the case with the roughest wall and weaker confinement enhances inter-layer mixing, producing higher stress levels. After sufficient strain, this configuration evolves toward a more ordered, low-mixing state, reducing stress to values similar to the other cases. Despite variations in stress magnitude, all cases follow a consistent viscous-inertial transition.

DY 19.9 Tue 12:00 HÜL/S186

Two time scales drive the formation of transient networks in a ferrogranular experiment - and how to control them — •Ali Lakkis[1], Matthias Biersack[1], Oksana Bilous[2], Sofia Kantorovich[2], and Richter Reinhard[1] — [1]Experimentalphysik 5, Universität Bayreuth — [2]Fakultät für Physik, Universität Wien

We are reporting experiments on the aggregation dynamics in a horizontally confined granular mixture composed of glass and magnetized steel spheres under vertical vibration. Upon a sudden decrease of the shaking amplitude, magnetized particles undergo a transition from a dispersed to an aggregated state. For deep quenches, a transient, percolating network of magnetized spheres rapidly emerges and gradually coarsens into compact clusters. In contrast, moderate amplitude reductions lead directly to dense cluster formation without intermediate networking. Using structural and network metrics such as coordination number and its mean value, we identify two characteristic timescales: a fast one governing the head-to-tail chaining typical of dipolar hard spheres (DHS), and a slower one corresponding to the restructuring into compact aggregates [1]. This progression is driven by the intrinsic susceptibility of the beads but is challenged by inter-sphere-friction. Thus, the employed susceptible dipolar hard spheres (SDHS) are a minimal model for phase separation with two intrinsic time scales in only one constituent.

[1] A. Lakkis, M. Biersack, O. Bilous, S. S. Kantorovich, R. Richter, *Soft Matter* (2025) doi:10.1039/d5sm00726g

DY 19.10 Tue 12:15 HÜL/S186

CT-resolved flow-induced particle migration in pipe bends during concrete pumping — •Daniil Mikhalev[1], Moritz Kluwe[2], Rüdiger Schwarze[2], and Viktor Mechtcherine[1] — [1]TU Dresden, Institute of Construction Materials, 01187 Dresden — [2]TU Bergakademie Freiberg, Institute for Mechanics and Fluid Dynamics, 09599 Freiberg

In this study, we investigate how the granular microstructure of pumped fresh concrete evolves as the suspension passes through a 90° pipe bend. The material is pumped under realistic operating conditions and allowed to harden in situ. To identify shear-dominated regions, a dyed low-viscosity premix is introduced as a passive tracer. Hardened bend sections are then analysed using high-resolution X-ray computed tomography. Segmentation of individual grains, voids, and tracer regions enables spatial statistics of solid volume fraction, grain-size distributions, air-void patterns, and shear-zone geometry along the inflow-bend-outflow transition.

Preliminary results reveal measurable deviations from the symmetric plug - lubrication-layer structure known from straight pipe flow, including radial and azimuthal segregation and restructuring of both solid and air phases. The combined tracer-based and tomographic approach provides a foundation for linking experimentally resolved microstructure with continuum suspension models and particle-migration theories in complex geometries.

General Discussions

DY 20: Focus Session: Water – from Atmosphere to Space I (joint session CPP/DY)

Water plays a vital role in diverse Earth processes across multiple scales, from atmospheric cycles and aerosol chemistry to geological porous media and nanoscale biological functions of hydrated proteins. Despite its fundamental importance and numerous anomalous properties, such as the diverging heat capacity of supercooled water, pure bulk water remains poorly understood. Key phenomena like evaporation and crystallization are relevant not only on Earth but also in extraterrestrial environments. In Germany, molecular water research is flourishing across prestigious centers, exemplified by the new BlueMat cluster at Hamburg University of Technology, the renewed RESOLV cluster at Ruhr-University Bochum, and the Max Planck Society's expanding Liquid Initiative in Mainz. The 2025 inauguration of the Centre for Molecular Water Science (CMWS) at Hamburg's DESY campus further strengthens a Europe-wide interdisciplinary network, uniting 47 founding members from 12 countries to advance water science across disciplines and methods. Within this focus session the state of molecular water research shall be discussed and interactions between the physical sub-fields shall be fostered.

Organized by Alexander Schlaich, Katrin Amann-Winkel, Mischa Bonn.

Time: Tuesday 9:30–11:00 Location: ZEU/LICH

Topical Talk DY 20.1 Tue 9:30 ZEU/LICH

Surface adsorption and protonation equilibrium of atmospheric organics at the aqueous surface — •Nønne Prisle — Center for Molecular Water Science, Deutsches Elektronen-Synchrotron DESY, Notkestrasse 85, D-22607 Hamburg, Germany — Institute of Inorganic and Applied Chemistry, University of Hamburg, Martin-Luther-King-Platz 6, D-20146 Hamburg, Germany — Center for Atmospheric Research, University of Oulu, P.O. Box 4500, FI-90014, Oulu, Finland

Atmospheric aerosols comprise a significant fraction of organic species which frequently exhibit both surface activity and Brönsted acidity or basicity in aqueous solutions. The high surface area to bulk volume ratios of nano- and microscopic aerosols and droplets further favor surface-specific states, affecting both bulk-phase and heterogeneous chemistry.

We used X-ray Photoelectron Spectroscopy (XPS) in combination with high-brilliance synchrotron radiation to directly observe the protonation state of atmospheric acids and bases at the surfaces of aqueous aerosol and droplet models. We found that for each acid-base pair, the neutral species is enhanced in the surface, consistent with its higher surface activity, compared to the charged conjugate. This introduces a shift in the protonation equilibrium at the aqueous surface corresponding to an apparent change in pKa of 1-2 pH units, depending on the concentration, acidity, and surface activity of the conjugate acidic and basic species.

DY 20.2 Tue 10:00 ZEU/LICH

The Effect of pH on the Structure of Model Sea Spray Aerosol Surfaces — •Clara M. Saak, Lars Höhner, and Ellen H.G. Backus — Institute of Physical Chemistry, Faculty of Chemistry, University of Vienna, Währinger Straße 42, 1090 Vienna, Austria

Aerosols play a key role in the global climate due to their ability to scatter and reflect solar radiation and to act as cloud condensation nuclei (CCN), exerting a pronounced cooling influence on the global climate. In particular, the surface availability of ions and organic compounds is known to affect the hygroscopicity of the particle and thereby its ability to act as a CCN [1]. While the surface propensity of individual compounds has been studied widely, much less is known about more complex systems. Here we focus on the impact of bulk pH on the architecture of mixed aqueous interfaces. In atmospheric systems the pH has been shown to range from roughly pH 8 to 2 [2]. Using sum-frequency-generation (SFG) spectroscopy in conjunction with surface tension data we study the surface composition and structure of short and long chain organic acids at different protonation stages, obtained by varying the pH. Using this approach, we find pronounced changes in the structuring of the aqueous sub-surface layers depending on the specific composition and pH, and in the Gibbs free energy of adsorption of the studied organics. Our results show that it is feasible for subtle environmental changes to considerably affect structure and composition of the aqueous interface, which is known to play a key role in aerosol hygroscopicity. [1] Zieger, Nat. Commun. 2017, 8, 15883. [2] Angle, PNAS, 2021, 118, 2, e2018397118

DY 20.3 Tue 10:15 ZEU/LICH

Crystallization behaviour of nanoparticle suspensions — •Isabell Zick[1,2], Eduard Edel[2], and Katrin Amann-Winkel[1,2] — [1]Institut für Physik, Johannes Gutenberg-Universität, Staudinger Weg 7, 55128 Mainz, Germany — [2]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany

Water is one of the most abundant substances in the world and due to this in close contact with many materials including micro- and nanoplastic particles. Those have been detected not only in sea but also in the atmosphere, where the particles can interact with water and act as cloud condensation nuclei or ice-nucleating particles. Emerging evidence suggests that nanoparticles with increased surface roughness or chemical functionalities may promote heterogeneous ice nucleation through different processes like, e.g., contact- and immersion-freezing. Such a behaviour affects cloud properties with significant implications for Earth*s radiative balance and the hydrological cycle.

We investigate atmospherically relevant nanoparticles dispersed in water to investigate their influence on the ice crystallization. Our experiments include calorimetry (DSC) as well as X-ray diffraction measurements (XRD). Our measurements show that the crystallization temperature depends on the particle size, concentration, and the chemical surface of the particles. Using XRD, we investigate the restructuring of the water molecules during supercooling, observed by a shift in the characteristic main diffraction peak of water and the subsequent crystallization process.

DY 20.4 Tue 10:30 ZEU/LICH

Laser-Excited X-ray Reflectivity of Aqueous SrCl2 at the Air-Water Interface — •Ali Ashtiani Abdi[1,2], Julia Kobus[1,2], Svenja C. Hövelmann[1,2], Philipp Jordt[1,2], Nicolas Hayen[1,2], Prashant Hitaishi[1,2], Ajay Ajay[1,2], Rabia Qamar[1,2], Otto Lippmann[1,2], Chen Shen[3], Florian Bertram[3], and Bridget M. Murphy[1,2] — [1]IEAP, CAU Kiel University, Kiel, Germany — [2]Ruprecht Haensel Laboratory, DESY, Hamburg, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Understanding aqueous interfaces is essential for describing chemical processes in atmospheric, marine, and geochemical environments. While monovalent salts have been widely studied, the interfacial behavior of divalent ions is less understood, despite their relevance in seawater aerosols and reactive brines. SrCl2 is a representative divalent electrolyte whose interfacial structure may show alteration by laser illumination.

We investigate aqueous SrCl2 solutions at different concentrations using X-ray reflectivity (XRR) at the liquid-air interface. Measurements were performed at the LISA setup at beamline P08, PETRA III (DESY), where controlled laser illumination can be applied directly to the X-ray footprint, following the instrumentation concept of Warias and Hovelmann et al. (J. Synchrotron Rad. 2024). Reflectivity curves were recorded with and without laser exposure. The data demonstrate the suitability of SrCl2 surfaces for laser-assisted XRR and the sensitivity of the method to potential changes in interfacial structure, including indications of near-surface layering.

DY 20.5 Tue 10:45 ZEU/LICH

Monitoring Uptake, Release and Reaction of Gases at the Liquid-Vapor Interface — •Tillmann Buttersack[1], Shirin Gholami[1], Clemens Richter[1], Daniela Torres-Diaz[1], Bernd Winter[1], Pavel Jungwirth[2], Stephen Bradforth[3], Markus Ammann[4], Ruth Signorell[5], Ivan Gladich[6], Remi Dupuy[7], Philip Mason[2], and Hendrik Bluhm[1] — [1]Fritz Haber Institute, Max Planck Society, Berlin, GER — [2]IOCB, Czech Academy of Sciences, Prague, CZ — [3]University of Southern California, Los Angeles, USA — [4]Paul Scherrer Institut, Villigen, CH — [5]EZH Zürich, CH — [6]University of Urbino, Urbino, I — [7]Sorbonne Université, Paris, F

Multiphase reactions are omnipresent in nature, industrial applications. The direct observation of reactions at the liquid-vapor interface requires spectroscopic techniques that are surface specific and chemically sensitive to detect low concentrations, e.g., photoelectron spectroscopy (XPS). Furthermore, the sample delivery method must allow sufficient time for an interface reaction to proceed. These complex challenges require individual approaches for each system of interest. One example for a multiphase process is the reaction between liquid alkali metal and water vapor, which is extremely fast. We used a slow droplet train of NaK in a wet atmosphere and observed the formation of golden aqueous solutions with metallic properties with XPS. An example with relevance for atmospheric chemistry is the formation and the release of sulfur dioxide (SO2) from aqueous sulfite solutions due to acidification. We demonstrated that dissolved gases can be detected with XPS even though their concentration is only about 1 mM.

DY 21: Stochastic Thermodynamics

Time: Tuesday 9:30–12:45 Location: ZEU/0114

DY 21.1 Tue 9:30 ZEU/0114

Thermodynamic bounds and error correction for faulty coarse graining — •Jann van der Meer and Keiji Saito — Department of Physics No. 1, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan

At the nanoscale, random effects govern not only the dynamics of a physical system but may also affect its observation. This work introduces a novel paradigm for coarse graining that eschews the assignment of a unique coarse-grained trajectory to a microscopic one. Instead, observations are not only coarse-grained but are also accompanied by a small chance of error. Formulating the problem in terms of path weights, we identify a condition on the structure of errors that ensures that the observed entropy production does not increase. As a result, the framework of stochastic thermodynamics for estimating entropy production can be extended to this broader class of systems. As an application, we consider Markov networks in which individual transitions can be observed but may be mistaken for each other. We motivate, derive, and illustrate thermodynamic bounds that relate the error sensitivity of the observed entropy production to the strength of the driving and are valid for arbitrary network topologies. If sufficiently many transitions in the network can be observed, redundancies in the coarse-grained trajectories can be used to detect and correct errors, which potentially improves naive estimates of entropy production. We conclude with an outlook on subsequent research on thermodynamic bounds for erroneous coarse graining.

DY 21.2 Tue 9:45 ZEU/0114

Between heat engine and information engine, characteristics of the entropy production rate in a Brownian ratchet. — Adrien Meynard, Marc Lagoin, Caroline Crauste-Thibierge, and •Antoine Naert — Univ Lyon, Ens de Lyon, Univ Claude Bernard, CNRS, Laboratoire de Physique, F-69342 Lyon, France

A two-state device such as a Brownian ratchet can be regarded as a *heat engine* or an *information engine*. Our experiment, at the centimeter scale, gives access to long time series of all observables of interest, resolved in time. These are the

heat flux $\dot{q}_1(t)$ supplied by the hot (athermal) bath, at an (effective) temperature kT_1, and the work produced per unit time $\dot{w}(t)$.

Taking advantage of the discreet operation of such 1-bit elementary information device, an example of a Maxwell's demon, we can measure the rate of entropy production. We infer a comprehensive characterization of the rate of entropy produced by this device, in the Boltzmann sense. Our findings are compatible with a Poisson point process.

In steady state operation, this entropy is to be released as heat into the surrounding, at ambient temperature $k_B T_2$. (Note that $\dot{q}_2(t)$ is distinct from the various losses.) The heat over temperature ratios of the exchanges with the hot and cold baths are of the same order of magnitude:

$$\frac{\langle \dot{q}_1 \rangle}{kT_1} \simeq \frac{\langle \dot{q}_2 \rangle}{k_B T_2}. \quad (2)$$

We confirm that, within the limit of experimental uncertainties, entropy is conserved in a lossless heat engine, just like energy is.

DY 21.3 Tue 10:00 ZEU/0114

Minimum Action Principle for Entropy Production Rate of Far-From-Equilibrium Systems — •Atul Tanaji Mohite and Heiko Rieger — Department of Theoretical Physics and Center for Biophysics, Saarland University, Saarbrücken, Germany

The Boltzmann distribution connects the energetics of an equilibrium system with its statistical properties, and it is desirable to have a similar principle for non-equilibrium systems. Here, we derive a variational principle for the entropy production rate (EPR) of far-from-equilibrium discrete state systems, relating it to the action for the transition probability measure of discrete state processes [1,2]. This principle leads to a tighter, non-quadratic formulation of the dissipation function, speed limits, the thermodynamic-kinetic uncertainty relation, the large deviation rate functional, and the fluctuation relation, all within a unified framework of the thermodynamic length [2]. Additionally, the optimal control of non-conservative transition affinities using the underlying geodesic structure is explored, and the corresponding slow-driving and finite-time optimal driving exact protocols are analytically computed [1,3]. We demonstrate that discontinuous endpoint jumps in optimal protocols are a generic, model-independent physical mechanism that reduces entropy production during finite-time driving of far-from-equilibrium systems [3].

[1]A.T. Mohite and H. Riger, arXiv:2511.00967. [2]A.T. Mohite and H. Riger, arXiv:2511.00970. [3]A.T. Mohite and H. Riger, arXiv:2511.00974.

DY 21.4 Tue 10:15 ZEU/0114

Asymptotic limit laws of projected empirical currents — •Felix Tippner and Aljaz Godec — Mathematical Physics and Stochastic Dynamics, Institute of Physics, University of Freiburg (GER)

Most experimental measurements capture only a restricted subset of a system's degrees of freedom at any given time. As a result, the higher-dimensional stochastic process that describes the full physical system, such as the high-dimensional conformational dynamics of proteins, can typically be observed only in terms of low-dimensional projections, which are also subject to experimental and sampling constraints. These projections inevitably give rise to non-Markovian behaviour and typically obscure key features of the underlying dynamics, including irreversible probability currents that distinguish driven from reversible systems. The main result of the present work is an asymptotic limit law, i.e., a sharpening of the central limit theorem, for empirical currents of projected observables.

DY 21.5 Tue 10:30 ZEU/0114

Nonlinear Response Theory for Nonequilibrium Biochemical Networks — Ruicheng Bao[1] and •Shiling Liang[2,3,4] — [1]University of Tokyo, Tokyo, Japan — [2]MPI-PKS, Dresden, Germany — [3]MPI-CBG, Dresden, Germnay — [4]CSBD, Dresden, Germany

Living cells process information through biochemical networks operating far from equilibrium. Understanding how these systems respond to finite perturbations, such as changes in enzyme concentrations or metabolic fluxes, is essential, yet the fluctuation-dissipation theorem applies only near equilibrium.

This talk introduces a framework that fills this gap. We derive an exact identity that links nonlinear responses to linear ones through a physically meaningful scaling factor, based on a connection between steady-state responses and mean first-passage times. This provides bidirectional inference: predicting global responses from local biochemical changes, and inferring metabolic costs from measurable observables. We also establish a universal response-resolution limit, a strong-perturbation analogue of the fluctuation-dissipation theorem, which sets fundamental bounds on signal detectability.

Using transcriptional regulation as an example, we show how these parameter-independent bounds constrain the computational expressibility of gene networks. Reliable detection of transcription factor changes requires fold-changes above a universal threshold. Overall, this framework defines general physical limits on cellular information processing, with implications for metabolic control and signal transduction.

DY 21.6 Tue 10:45 ZEU/0114

Compensating random transition-detection blackouts in Markov networks — •Alexander Maier, Benjamin Häsler, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

In Markov networks, measurement blackouts with unknown frequency compromise observations such that thermodynamic quantities can no longer be inferred reliably. In particular, the observed currents neither discern equilibrium from non-equilibrium nor can they be used in extant estimators of entropy production. Our strategy to eliminate these effects is based on formally attributing the blackouts to a second channel connecting states. The unknown frequency of blackouts and the true underlying transition rates can be determined from the short-time limit of observed waiting-time distributions. A post-modification of observed trajectory data yields a virtual effective dynamics from which the lower bound on entropy production based on thermodynamic uncertainty relations can be recovered fully. Moreover, the post-processed data can be used in waiting-time based estimators. Crucially, our strategy does neither require the blackouts to occur homogeneously nor symmetrically under time-reversal. Reference: Alexander M. Maier, Benjamin Häsler and Udo Seifert, arXiv:2511.14679 (2025)

15 min. break

Invited Talk DY 21.7 Tue 11:15 ZEU/0114

Why Life Is Hot — •Tanja Schilling[1], Patrick Warren[2], and Wilson Poon[3] — [1]Institute of Physics, University of Freiburg, Hermann-Herder-Straße 3, D-79104 Freiburg, Germany — [2]The Hartree Centre, STFC Daresbury Laboratory, Warrington, WA4 4AD, United Kingdom — [3]School of Physics and Astronomy, The University of Edinburgh, Peter Guthrie Tait Road, Edinburgh EH9 3FD, United Kingdom

Biological organisms use strongly driven cycles to optimize the output of chemical reactions. This mechanism is versatile, it is employed to meet a large variety of cost functions such as robustness, precision, or sensitivity to external stimuli. However, the improvements over the equilibrium behaviour come at the cost of increased production of heat. We show that the heat generated by this mechanism constitutes a large part of the total heat produced by living organisms. Further we demonstrate that the effect saturates and that nature operates near saturation. Hence we conclude that the heat production of living organisms is consequence of their need to function accurately and to adapt flexibly to varying demands.

DY 21.8 Tue 11:45 ZEU/0114

Optimal Localisation against a Flow — •Till Welker and Patrick Pietzonka — School of Physics and Astronomy, University of Edinburgh, United Kingdom

How much work does it cost for a propelled particle to stay localised near a stationary target, defying thermal noise and a constant flow that would carry it away? We study the control of such a particle in finite time and find optimal protocols for time-dependent propulsion speed and diffusivity, without feedback. Accuracy, quantified via the mean squared deviation from the target, and energetic cost turn out to be connected by a trade-off relation, which complements the one between precision and cost known in stochastic thermodynamics. We show that accuracy better than a certain threshold requires active driving , which comes at a cost that increases with accuracy. The optimal protocols have discontinuous propulsion speed and diffusivity, switching between a passive drift state with vanishing diffusivity and an active propulsion state. If the initial position is fixed, an initial jump of the particle, enabled by a sudden burst of propulsion, can be optimal. This study highlights how a time-dependent diffusivity enhances optimal control and sets benchmarks for artificial self-propelled particles navigating noisy environments.

DY 21.9 Tue 12:00 ZEU/0114

Thermodynamic optimal control out of equilibrium: insights from active and driven systems — •Kristian Olsen[1], Rémi Goerlich[2,1], Yael Roichman[2,3], and Hartmut Löwen[1] — [1]Institut für Theoretische Physik II - Weiche Materie, Heinrich-Heine-Universität Düsseldorf, D-40225 Düsseldorf, Germany — [2]Raymond & Beverly Sackler School of Chemistry, Tel Aviv University, Tel Aviv 6997801, Israel — [3]Raymond & Beverly Sackler School of Physics & Astronomy, Tel Aviv University, Tel Aviv 6997801, Israel

Optimal control far from equilibrium raises intriguing questions in stochastic thermodynamics and offers a route to design microscopic engines that operate out of equilibrium. We study thermodynamically optimal protocols for a harmonically trapped particle driven by arbitrary time-dependent forces, including those from active matter or external fields [1]. The resulting protocols are able to harness non-equilibrium forces to extract a net work. We provide exact solutions for the optimal protocol and associated work for arbitrary forces and protocol duration. We also derive a quasistatic work bound that splits into three parts: an information-geometric term capturing energy stored in an initial non-equilibrium state, the work extracted from time-averaged forces, and extra work from fast dynamical modes. Finally, we analyze the energetic cost of

adding boundary constraints, giving insights into the cost of precision in these protocols.

1. Harnessing non-equilibrium forces to optimize work extraction, Kristian Stølevik Olsen, Rémi Goerlich, Yael Roichman and Hartmut Löwen, In press Nature Communications, arXiv: 2504.07049, 2025.

DY 21.10 Tue 12:15 ZEU/0114

Searching with Memory: Experiments on Stochastic Resetting in Complex Fluids — •Felix Ginot and Clemens Bechinger — University of Konstanz, 78457 Konstanz, Germany

Many natural and technological search processes, from molecular reactions to robotic exploration, benefit from occasionally resetting and trying again. This mechanism, known as stochastic resetting (SR), is well understood in simple memoryless environments, but real systems often exhibit complex relaxation dynamics that retain information about recent motion.

We experimentally investigate SR in a viscoelastic fluid by tracking a colloidal particle undergoing controlled resets. The fluid's delayed elastic response creates restoring forces that oppose each reset and reduce search efficiency. We show that these memory effects can be tuned: holding the particle at the trap center allows the fluid to relax and erase residual memory. With a target present, this control significantly lowers the mean passage time, with optimal performance at intermediate resetting rates. In this regime, memory induces temporal correlations that bunch target encounters and speed up repeated hits.

These results demonstrate that environmental memory can both hinder and enhance search, and they point to new strategies for optimizing transport in non-Markovian media.

DY 21.11 Tue 12:30 ZEU/0114

Information as a Thermodynamic Resource in Non-Markovian Stochastic Systems — •Lokesh Chinnakanna Muruga, Felix Ginot, and Clemens Bechinger — Fachbereich Physik, Universität Konstanz, Konstanz, Germany

The interplay between information and thermodynamics lies at the core of modern stochastic physics. Classical thermodynamics links quantities such as entropy, temperature, and free energy solely to the physical state of a system. Contemporary developments from Maxwell demon and Szilard engine led to fluctuation theorems which revealed that information itself acts as a thermodynamic resource. The acquisition, storage, and use of information can reshape energy landscapes, enable work extraction, and modulate entropy production without violating the second law. In this work, we explore how information stored in unobserved degrees of freedom affects work extraction and equilibrium dynamics in stochastic systems. Using time-resolved position measurements of an optically trapped Brownian particle in a non-Markovian fluid, we show that correlations in the measurement encode memory effects that reveal multiple hidden configurational states. We introduce a new protocol to distinguish these information-bearing states experimentally and quantify their influence on relaxation and work extraction efficiency. Our results highlight how information, whether explicit or hidden can be leveraged as a functional resource for energy extraction and control at the microscale.

DY 22: Pattern Formation

Time: Tuesday 9:30–12:15 Location: ZEU/0118

DY 22.1 Tue 9:30 ZEU/0118

Unexpected wave patterns observed within an extended parameter range of the Barkley model — Vladimir Zykov and •Eberhard Bodenschatz — Max Planck Institute for Dynamics and Self-Organization, D-37077 Goettingen, Germany,

The Barkley model is a widely accepted example of reaction diffusion systems demonstrating different self-organization processes including a creation of self-sustained spiral waves. Recently the study of the spiral wave dynamics performed within the extending parameter region of the Barkley model allowed us to reveal some unexplored features of these processes [1]. The latest computational results performed under a further expansion of the parameter range demonstrate the existence of spiral wave under completely unexpected conditions in monostable and bistable regions. These spirals exhibit absolutely unusual instability, which should be investigated. In parallel to spiral waves self-supported wave segments remaining critical fingers have been observed, which also demonstrated a similar unusual instability.

[1] V. S. Zykov and E. Bodenschatz, Unexplored aspects of the spiral wave dynamics in the Barkley model within an extended parameter range, Phys. Rev. E. 110, 064209 (2024).

DY 22.2 Tue 9:45 ZEU/0118

Dynamics of localized states in a weakly dissipative Korteweg-de Vries-Kuramoto-Sivashinsky Equation — •Justus Keussen[1], Daniel Greve[1], Julien Javaloyes[2], and Svetlana V. Gurevich[1,2,3] — [1]Institute for Theoretical Physics, University of Münster, Münster, Germany — [2]Universitat de les Illes Balears, Palma, Spain — [3]Center for Data Science, University of Münster, Münster, Germany

We are interested in the dynamics of localized solutions in a weakly dissipative Korteweg de Vries Kuramoto Sivashinsky equation, using a combination of analytical, numerical, and path-continuation methods. We show that a traveling solitary soliton exists and is stable over a certain parameter range, even though the homogeneous state is linearly unstable. Furthermore, we employ a variational ansatz to analytically determine the selected velocity of the localized state. Finally, path continuation in the domain size reveals that the corresponding bifurcation points on both the homogeneous and solitary branches follow a power-law scaling with the system length, implying that each domain size admits a finite interval of parameter values in which a stable solitary wave exists.

DY 22.3 Tue 10:00 ZEU/0118

Pattern formation and route to chaos in a two-species reaction-diffusion model with one conservation law — •Simon Navia Rafide[1] and Uwe Thiele[2] — [1]University of Münster, Münster Germany — [2]University of Münster, Münster Germany

In many intracellular reactions, the total amount of a substance remains constant. For example, in reactions involving proteins that can adopt different conformations, it is possible to observe spatio-temporal concentration patterns that differ in their behaviour from those in systems without such constraints. We explore a relatively simple two-species reaction-diffusion model with a single mass conservation law governing cell polarisation [1, 2]. Here, we investigate the bifurcation behaviour of the model in detail and, using numerical continuation and time simulations, show that time-periodic patterns follow a period-doubling route to chaos, which appear in two different flavours. Moreover, we propose an approximate model based on the first two instability modes that allows us to understand the underlying mechanisms behind the first steps of pattern formation.

[1] Kuwamura, M., Izuhara, H., & Ei, S. I., Oscillations and bifurcation structure of reaction-diffusion model for cell polarity formation. J. Math. Biol., 84, 2022. [2] S. Ishihara, M. Otsuji, A. Mochizuki, Transient and steady state of massconserved reaction-diffusion systems, Phys. Rev. E 75, 015203, 2007.

DY 22.4 Tue 10:15 ZEU/0118

The 3-Components Problem — •Davide Toffenetti[1], Beatrice Nettuno[1], Henrik Weyer[2], and Erwin Frey[1] — [1]Ludwig Maximilian University of Munich (LMU), Munich, Germany — [2]KITP, UC Santa Barbara, USA

Our work develops a general framework that connects reaction-diffusion systems with active-matter theories. Earlier studies showed that two-component mass-conserving reaction-diffusion (2cMcRD) systems can be mapped onto Model-B-type dynamics [1], which leads to the coarsening of patterns. We extend this idea by introducing a minimal three-component mass-conserving reaction-diffusion (3cMcRD) model. Using adiabatic elimination, we derive an effective active description for the total-mass dynamics, reminiscent of the well-known AMB+ theory. We validate the mapping through extensive numerical simulations.

Only 3cMcRD systems and their associated effective active theory produce finite-wavelength patterns such as dots, stripes, and foam-like structures, in contrast to the coarsening dynamics of 2cMcRD models. Employing a local quasi-steady-state approximation, we further determine the thresholds separating distinct pattern-forming regimes. In particular, we analyze how fingering instability emerges from an initially flat interface, marking the transition to foam-like patterns.

Our approach naturally generalizes to systems with more than three components and and to more general active-matter theories.

[1] Weyer, Brauns & Frey (2023). Phys. Rev. E 108, 064202.

DY 22.5 Tue 10:30 ZEU/0118

Coarsening dynamics and interface instabilities in coupled conserved pattern-forming systems — Benjamin Winkler[1], Sergio Alonso[2], and •Markus Bär[3] — [1]RKI and FU Berlin, Germany — [2]UPC Barcelona, Spain — [3]PTB and TU Berlin, Germany

We investigate the coarsening dynamics of non-variationally coupled, mass-conserved pattern-forming systems. Our main example is a model describing multiscale pattern formation via the interaction of membrane binding proteins with a multicomponent lipid membrane. We find that the coupling of a reaction-diffusion system for a protein species to an equation describing the phase composition of a lipid membrane exhibiting active phase separation leads to arrested coarsening for strong enough coupling. In addition, inverse coarsening is found if simulations start from large domains. We show that these phenomena are

closely connected with interface instabilities and an exceptional point in the linear properties of the spatially homogeneous state both of which emerge for strong-enough non-variational coupling. Similar phenomena are also found in a version of the non-reciprocally coupled Cahn-Hilliard equations, which have similar linear behavior and instabilities, and in a qualitative model for a compressible active polar fluid. The nonlinear evolution of the interface instability and the emerging complex patterns depend, however, on the specific form of the chosen model. This is demonstrated with a survey of possible dynamical evolutions in different models.

DY 22.6 Tue 10:45 ZEU/0118

Leading mechanisms of defibrillation: A computational approach to study the differences between monophasic and biphasic waveforms — •Daniel Frühwald[1] and Thomas Lilienkamp[1,2] — [1]Nuremberg Institute of Technology Georg Simon Ohm, Computational Physics for Life Science, Nuernberg, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, Biomedical Physics Group, Goettingen, Germany

Sudden cardiac death caused by, for example, malignant ventricular arrhythmia, results in an estimated 600,000 deaths per year in the European Community alone. In addition, atrial fibrillation is the most common cardiac arrhythmia worldwide, affecting worldwide more and more people with around 33.5 million in 2010 and 59 million people in 2019. In both diseases, the heart can be reset to sinus rhythm by cardioversion: The application of a high-energy defibrillation shock delivered either from an external device, or from implantable cardioverter defibrillators (ICDs). In both cases, patients suffer from significant side effects due to this treatment, including additional tissue damage and post-traumatic stress. The introduction of biphasic waveforms, instead of monophasic ones enabled a significant reduction in energy leading to mitigated side-effects. While many hypotheses for the increased efficiency of biphasic waveforms exist, the underlying mechanisms are not entirely understood. In a statistically driven multi-scale study, we use numericalsimulations to investigate the influence of different cardiovascular structures on the success rate of defibrillation.

15 min. break

DY 22.7 Tue 11:15 ZEU/0118

Travelling waves of invasion in ecological communities with phenotypic variation — •Pierre A. Haas — Max Planck Institute for the Physics of Complex Systems — Max Planck Institute of Molecular Cell Biology and Genetics — Center for Systems Biology Dresden

Bacterial populations can switch to slowly growing "persister" subpopulations that are resilient to competition. Here, I will present a minimal model for the effect of this phenotypic variation on the spatial competition of two species. One of these species switches, both randomly and in response to the other, competitor species, to such a persister phenotype. One would expect this phenotypic switching to slow down the travelling wave by which the competitors invade the first species.

Combining exact results and numerical calculations, I will show that, surprisingly, this expectation does not hold true: phenotypic switching does not affect the speed of this wave. Somewhat conversely, I will demonstrate that phenotypic switching can speed up the reverse wave by which this species invades the competitors. This suggests that, counterintuitively, persisters can be an offensive, rather than defensive ecological strategy.

DY 22.8 Tue 11:30 ZEU/0118

How spatial patterns can lead to less resilient ecosystems — •David Pinto-Ramos and Ricardo Martinez-Garcia — Center for Advanced Systems Understanding (CASUS), Helmholtz-Zentrum Dresden-Rossendorf, Görlitz D-02826, Germany

Several theoretical models predict that spatial patterning increases ecosystem resilience. However, these predictions rely on simplifying assumptions, such as assuming isotropic and infinitely large ecosystems, and empirical evidence directly linking spatial patterning to enhanced resilience remains scarce. We introduce a unifying framework, encompassing existing models for vegetation pattern formation in water-stressed ecosystems, that relaxes these assumptions. This framework incorporates finite vegetated areas surrounded by desert and anisotropic environmental conditions that lead to non-reciprocal plant interactions. Under these more realistic conditions, we identify a novel desertification mechanism, known as nonlinear convective instability in physics but largely overlooked in ecology. These instabilities form when non-reciprocal interactions destabilize the vegetation-desert interface and can trigger desertification fronts even under stress levels where isotropic models predict stability. Importantly, ecosystems exhibiting periodic vegetation patterns are more susceptible to nonlinear convective instabilities than those with homogeneous vegetation, suggesting that spatial patterning may reduce, rather than enhance, resilience. These findings challenge the prevailing view that self-organized patterning enhances ecosystem resilience.

DY 22.9 Tue 11:45 ZEU/0118

Time-crystals in actively mode-locked lasers — Elias Koch[1], Ruiling Weng[2], Jesús Yelo-Sarrión[2], Josep Batle[2], Julien Javaloyes[2], and •Svetlana V. Gurevich[1,3] — [1]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str.9 48149 Münster, Germany — [2]Departament de Física and IAC3, Universitat de les Illes Balears, Campus UIB 07122 Mallorca, Spain — [3]Center for Data Science and Complexity (CDSC), University of Münster, Corrensstrasse 2, Münster, 48149, Germany

We propose a time-delayed model for the study of active mode-locking that is devoid of restriction regarding the values of the round-trip gain and losses. There, we report the occurence of discrete time-crystal phases and crystallites. By tuning either the bias current or the modulation frequency, the system undergoes a spontaneous symmetry-breaking transition from the harmonically mode-locked state towards robust, highly coherent time-crystal states that persist indefinitely. Two equivalent time-crystal configurations, shifted by one driving period, can coexist as domains separated by sharp, long-lived boundaries analogous to domain walls. Additionally, we present recent experimental results that are in good quantitative agreement with the theoretical predictions. Our findings demonstrate that mode-locked semiconductor lasers offer a readily accessible platform to explore and control non-equilibrium phases of light, enabling practical implementations of time-crystal physics in photonic systems.

DY 22.10 Tue 12:00 ZEU/0118

Unified Simulation Framework for Multi-Soliton Dynamics in Femtosecond Lasers — •Julia A. Lang[1], Julien Javaloyes[2], Svetlana V. Gurevich[3], and Georg Herink[1] — [1]University of Bayreuth, Germany — [2]University of the Balearic Islands, Spain — [3]University of Münster, Germany

Ultrafast lasers exhibit a rich variety of multi-pulse dynamics, strongly influenced by the underlying laser architecture and system-specific nonlinear effects.

In this contribution, we present a novel simulation approach that flexibly integrates diverse effects into a single, unified framework. A key feature of our model is the inclusion of full gain dynamics. This enables us to reproduce a wide range of experimentally observed soliton interactions, including harmonic mode-locking in erbium fiber lasers [1], the formation of soliton molecules via delayed feedback [2] or Raman-induced soliton molecules in Ti:sapphire lasers [2].

We introduce a classification of characteristic inter-soliton trajectories by attributing hierarchies of critical weights to nonlinear effects. The resultant classification provides deeper insights into the origins of multi-pulse interactions and enables novel approaches for harnessing multi-soliton applications.

[1] Lang JA et al. Sci Adv. 2024;10(2):eadk2290.
[2] Nimmesgern L et al. Optica. 2021;8(10):1334.
[3] Völkel A et al. Nat Commun. 2022;13(1):2066.

DY 23: Complex Fluids and Soft Matter (joint session DY/CPP)

Time: Tuesday 9:30–12:45 Location: ZEU/0160

DY 23.1 Tue 9:30 ZEU/0160

Process-Directed Self-Assembly of Copolymer Blends: Micro- and Macrophase Separation — •Jiayu Xie and Marcus Müller — Institute for Theoretical Physics, Georg August University Göttingen, 37077 Göttingen, Germany

The equilibrium phase behavior of binary diblock copolymer blends involves a complex interplay between microphase and macrophase separation. We investigate blends of linear diblock copolymers, A_1B_1 (cylinder-forming) and A_2B_2 (cylinder- or lamella-forming), using a combination of self-consistent field theory (SCFT) and single-chain-in-mean-field (SCMF) simulations. When the chain-length asymmetry between the A_1B_1 and A_2B_2 copolymers becomes large, the equilibrium phase diagram exhibits a wide macrophase-separation channel. Strikingly, our simulations reveal a strong pathway dependence within this region: rapid quenching yields a spatially homogeneous structure with narrow cylinder-size distributions and strong hexagonal order, whereas gradual annealing promotes local demixing, resulting in bimodal domain sizes and weaker order. We demonstrate that this process-dependent nonequilibrium behavior can be explained by the distinct evolutions of the system state and free-energy landscape of the blends under quenching or annealing. These findings highlight how different processing conditions can direct nanostructure formation in block copolymer blends, and establish a mechanistic link between processing pathway and the final morphology, thus offering insights into rational design of targeted nanostructured materials.

DY 23.2 Tue 9:45 ZEU/0160

Topological defect engineering enables size and shape control in self- assembly — Lara Koehler[1,3], Markus Eder[2], Vincent Ouzan-Reboul[3], Christoph Karfusehr[2], Andrey Zelenskiy[3], Pierre Ronceray[4], Friedrich Simmel[2], and •Martin Lenz[3] — [1]MIPPKS, Dresden, Germany — [2]TU Munich, Germany — [3]U. Paris-Saclay, Orsay, France — [4]Aix-Marseille-Université, Marseille, France

Equilibrium self-assembly is a powerful way to build nano- and microscale structures out of interacting subunits. The size and shape of such structures must be controlled in many biological and technological functions, posing significant practical challenges as current strategies require multiple subunit types or the precise control of their shape and mechanics. Here we introduce an alternative approach that circumvents these obstacles. Our method uses subunits whose interactions promote crystals, but also favor crystalline defects. We show theoretically that the magnitude of these interactions, which is well controlled in experiments, governs the self-assembly through topological restrictions on the scope of the defects. Using DNA origami, we demonstrate both size and shape control in two-dimensional disk- and fiber-like assemblies. Our basic concept of defect engineering operates well beyond these examples, and provides a broadly applicable framework to control self-assembly.

DY 23.3 Tue 10:00 ZEU/0160

Soft colloidal monolayers under drying conditions — •Kai Luca Spanheimer[1], Maret Ickler[2], Julian Ringling[3], Nicolas Vogel[2], Matthias Karg[4], and Hartmut Löwen[1] — [1]Insitut für Theoretische Physik II, Heinrich-Heine-Universität, 40225 Düsseldorf, Germany — [2]Institute of Interfaces and Particle Technology, Friedrich-Alexander University, Erlangen, Germany — [3]Physikalische Chemie I: Kolloide und Nanooptik Heinrich-Heine-Universität, 40225 Düsseldorf, Germany — [4]Institut für Chemie, Martin-Luther-Universität Halle-Wittenberg, 06099 Halle, Germany

Langmuir-Blodgett deposition is a well established technique in research and industry. Even though, there still are effects in this process that are not yet explored from a theoretical standpoint. It is usually assumed that the deposited pattern is identical with the one appearing at the water-air interface. In recent experimental studies, strong reorganization during the drying of soft colloidal monolayers has been observed [1]. Capillary forces during drying are known to change nanoscopic structures, sometimes even leading to their destruction. To model these processes we propose a combination of overdamped particle dynamics coupled to dewetting dynamics of an evaporating liquid film. The patterns produced by this model fit those observed in experiment. This theoretical approach allows exploration of the drying dynamics. Thereby we gain new insights into the drying process and makes experimental results produced with Langmuir-Blodgett deposition more reliable.

[1] K. Kuk, et al: Adv. Sci., 11, 2406977 (2024).

DY 23.4 Tue 10:15 ZEU/0160

Mechanical assessment of microfluidically-generated poroelastic microgel particles — Aude Sagnimorte[1,2], Anke Lindner[2], and •Joshua McGraw[1] — [1]Gulliver-CNRS, ESPCI-PSL, 10 rue Vaquelin, 75005 Paris — [2]PMMH-CNRS, ESPCI-PSL, 10 rue Vaquelin, 75005 Paris

Soft microgels have numerous applications in diverse fields,such as tissue engineering, drug delivery systems, soft robotics, or as model systems for suspensions or colloids. Among these, photopolymerized hydrogels such as poly(ethylene glycol) diacrylate (PEGDA) are commonly used due to their highly tunable mechanical properties. However, proper characterisation of these properties is challenging, in part due to their small scale, on the order of tens of microns, and in particular the lack of assessment of their time-dependent properties. Here we provide a comprehensive mechanical characterisation of individual photopolymerised microgels particles using atomic force microscopy (AFM) for precise local measurements. In particular, we performed indentation-relaxation tests on PEGDA microdisks immersed in water. By varying indentation depth and probe diameter, we changed the contact area and observed relaxation responses which are indicative of poroelastic behaviour. In particular, larger contact areas resulted in longer relaxation times. Our results also show that increasing the amount of solvent increased the relaxation time. Our collected results are consistent with a simple, Herzian poroelastic model giving good agreement with both the approach and relaxation phases of the experiments.

DY 23.5 Tue 10:30 ZEU/0160

Nonlinear Viscoelastic Response and Stress Shielding in Driven Bistable Spring Chains — •Sven Pattloch[1,2] and Joachim Dzubiella[1,2] — [1]Applied Theoretical Physics-Computational Physics, Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, D-79104 Freiburg, Germany. — [2]Cluster of Excellence livMatS@FIT-Freiburg Center for Interactive Materials and Bioinspired Technologies, Albert-Ludwigs-Universität Freiburg, D-79110 Freiburg, Germany

Bistable micromodules are a promising route to design adaptive mechanical metamaterials with tunable viscoelastic response. Here, a driven one-dimensional chain of bistable springs is studied in which both the mechanical deformation and the internal excitation states evolve dynamically under time-dependent forcing. Their coupling produces rich nonlinear viscoelastic behaviour, including frequency-dependent susceptibilities, delayed deformation, and pronounced hysteresis in cyclic loading.

Using analytical linear response theory complemented by numerical simulations, the model quantifies how microscopic parameters and driving protocols control effective stiffness, loss, and phase lags. A key result is a strong attenuation ('shielding') of stress propagation along the chain that is already present for monostable springs but is markedly amplified by excitation switching in bistable modules. These findings provide simple design principles for tailoring nonlinear viscoelasticity, hysteresis, and stress shielding in driven soft matter and mechanical metamaterial systems.

DY 23.6 Tue 10:45 ZEU/0160

Euler buckling on curved surfaces — •Shiheng Zhao[1,2,3] and Pierre A. Haas[1,2,3] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Max Planck Institute of Molecular Cell Biology and Genetics — [3]Center for Systems Biology Dresden

Nearly three hundred years ago, Euler showed that an inextensible straight elastic line in the plane buckles under compression when the compressive force F reaches a critical value $F_* > 0$. But how does such an elastic line buckle within a general curved surface? Here [1], we reveal that the classical instability changes fundamentally: By weakly nonlinear analysis of the buckling of an asymptotically short elastic line, we show that the critical force for the lowest buckling mode is $F_* = 0$ and discover a new bifurcation structure in which the modes of classical Euler buckling split into pairs. For long elastic lines, we numerically find an additional bifurcation by which the second of these new modes becomes the lowest mode and show that, at sufficiently large F, they undergo discontinuous snap-through to higher end-to-end compression. We explain these bifurcations in terms of the general unfolding of a pitchfork. This constitutes the foundations for a class of mechanical instabilities within curved surfaces from which, for example, biological shape emerges in development.

[1] S. Zhao and P. A. Haas, Phys. Rev. Lett. (in press)

15 min. break

DY 23.7 Tue 11:15 ZEU/0160

Linking molecular dynamics and experimental FORCs in multicore magnetic nanoparticles — Ekaterina Novak[1], •Malika Khelfallah[2], Andrey Kuznetsov[3], Deniz Mostarac[4], Claire Carvallo[2], Amélie Juhin[2], and Sofia Kantorovich[3] — [1]Ekaterinburg, Russia — [2]Sorbonne Université, Paris, France — [3]University of Vienna, Vienna, Austria — [4]University of Edinburgh, Edinburgh, United Kingdom

Multicore magnetic nanoparticles - clusters of several magnetic grains embedded in a nonmagnetic matrix - exhibit collective behaviour distinct from single-core particles and are promising candidates fro drug targeting and magnetic hyperthermia. Their magnetic cores possess finite anisotropy, and the multicore assemblies range from near-spherical to elongated ellipsoids, features that strongly affect their response to external fields. To study these effects, we use molecular dynamics simulations [1] to model internal structure, anisotropy distribution, and collective switching. As a key diagnostic, we employ First Order Reversal Curves [2], which experimentalists routinely measure for immobilised multicore particles, enabling direct comparison between simulations and experiments. FORC diagrams reveal coercivity distributions and magnetic interactions between grains, offering detailed insight into interaction mechanisms and domain processes.

The work was financially supported by the RSF grant No. 25-22-00762.

[1] R. Weeber et al. (2024), Comprehensive Computational Chemistry, 3, 578-601. [2] C. R. Pike et al., J. Appl. Phys., 1999, 85, 6660

DY 23.8 Tue 11:30 ZEU/0160

Hydrodynamics substantially affects induced structure formation in magnetic fluids — •Henning Reinken and Andreas M. Menzel — Otto-von-Guericke-Universität Magdeburg, Germany

Magnetorheological fluids consist of micrometer-sized magnetic particles suspended in a carrier liquid [1]. Sufficiently strong external magnetic fields lead to the formation of string-like particle aggregates, which results in complex magnetorheological behavior. This mechanism can further be used in the production of magnetic elastomers during the polymerization process when the carrier medium is still fluid and particulate structure formation still possible [2]. Using numerical simulations that spatially resolve both fluid flows and magnetization, we demonstrate that hydrodynamic interactions play a substantial role during structure formation. Hydrodynamics supports the emergence of string-like aggregates, while magnetic interactions align them. Considering besides this fundamental insight the enormous technical importance and potential of magnetic fluids, our results are substantial also from an application perspective.

We acknowledge support by the German Research Foundation DFG through Research Unit FOR 5599 on structured magnetic elastomers.

[1] S. Odenbach, Arch. Appl. Mech. **86**, 269 (2016).
[2] D. Günther, D. Yu Borin, S. Günther, S. Odenbach, Smart Mater. Struct. **21**, 015005 (2012).

DY 23.9 Tue 11:45 ZEU/0160

Near-surface colloidal dynamics in jammed and slipping microgel suspensions — •Masoodah Gunny[1], Frédérick Caetano[2], Matilde Bureau[2], Alexandre Vilquin[1], Marie Le Merrer[2], Catherine Barentin[2], and Joshua McGraw[1] — [1]Gulliver - CNRS, ESPCI-PSL 10 Rue Vauquelin 75005 Paris, France — [2]ILM - CNRS, Claude Bernard University, 16 Enrico Fermi 69100 Villeurbanne, France

Jammed suspensions of soft microgel particles exhibit wall slip along smooth boundaries. The direct observation of dynamics within a supposed depletion layer near the wall were difficult to achieve as a result of the layers' supposed sub-micrometric dimensions. We use total internal reflection fluorescence microscopy (TIRFM) to observe colloidal-particle dynamics near the interface between glass and microgel suspensions. Remarkably, microgel suspensions display nanoscale velocity profiles with a slope rupture; particle velocity increases with distance near the wall, and tends to a constant beyond a distance which is characteristic of the ones predicted previously. Beyond velocimetry, we also study the statistical particle altitude distributions near the wall in TIRFM measurements. These distributions are strongly pressure dependent, with nanoparticles more likely found near the solid/liquid interface when the fluid is transported faster near the wall. This high-velocity particle enrichment, not seen for the Newtonian case, is consistent with the development of a depletion layer under such conditions. Taken together, our observations give strong support for the existence of a depletion layer being responsible for wall slip.

DY 23.10 Tue 12:00 ZEU/0160

Random close packing as a conserved directed percolation transition — •Thomas Axmann and Michael Schmiedeberg — Theoretical Physics: Lab for Emergent Phenomena, Soft Matter Theory Group, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

In studying quenches in soft sphere systems O'Hern et al. related the onset of overlaps to isostaticity [1], and consequently to the random close packing scenario. The conditions that lead to the avoidance of overlaps between spheres can be studied with the random organization model [2], which was initially introduced to investigate self organization in sheared colloids. Modifications of this model, which dynamically reduce interparticle overlaps, were used to characterize the random close packing problem as the critical point of a dynamic absorbing state transition in the $d+1$ dimensional conserved directed percolation universality [3,4].

We aim to deepen the understanding of this connection by demonstrating that the configuration change at each time step can be chosen with a fully deterministic strategy while retaining the features of the transition. We clarify difficulties in the treatment of percolating clusters and find that the median overlap depth proves to be a more useful order parameter.

[1] O'Hern et al. PRE 68 (2003)
[2] Corté et al. Nat. Phys. 4 (2008)
[3] Milz et al. PRE 88 (2013)
[4] Wilken et al. PRE 128 (2021)

DY 23.11 Tue 12:15 ZEU/0160

Rescaled mode-coupling scheme for dynamics in binary mixtures of highly charged colloids — •Daniel Weidig and Joachim Wagner — University of Rostock, Rostock, Germany

We investigate dynamic processes in binary mixtures of highly charged colloidal particles by means of Brownian dynamics and multi-component mode-coupling theory (MCT). As input for MCT, thermodynamically consistent, static structure factors from integral equations with Rogers-Young closure are used which are in quantitative agreement to Fourier transforms of static pair correlation functions resulting from simulations.

MCT based on partial structure factors in many-particle systems predicts dynamic properties such as long-time self-diffusion coefficients in qualitative agreement to simulation trajectories. Using instead structure factors from systems with slightly reduced number of effective charges as input, a quantitative agreement of MCT with simulations is achieved. In mixtures of identically charged particles with different short-time mobilities, this rescaled MCT scheme accurately predicts coupling effects in long-time dynamics observed in Brownian dynamics simulations.

DY 23.12 Tue 12:30 ZEU/0160

Electric double layers - the software package capDFT — Fabienne Dressler and •Andreas Härtel — Institute of Physics, University of Freiburg

Electric Double Layers are used to store electric energy, they can be utilized to harvest energy from waste heat or steps in concentrations, and they stabilize colloidal systems. In all cases, mobile ions arrange themselves to screen surface charges, resulting in sometimes densely packed regions of microscopic particles far from bulk states that dominate the macroscopic physical properties of the system. Modeling these complex systems has theoretical and numerical limitations, but good although expensive solutions exist. We present an open-source software package to treat the described modeling utilizing classical density functional theory [1]. The package has been used successfully in studies of underscreening [2] and allows to go beyond the standard mean-field approximation of primitive models [3]. We will demonstrate the package by discussing an example, where we study capacities of structured electrodes.

[1] https://github.com/andreashaertel/capdft
[2] Anomalous Underscreening in the Restricted Primitive Model. A. Härtel, M. Bültmann, and F. Coupette. Phys. Rev. Lett. 130, 108202 (2023)
[3] The primitive model in classical density functional theory: beyond the standard mean-field approximation. M. Bültmann and A. Härtel. J. Phys. Condens. Matter 34, 235101 (2022)

DY 24: Focus Session: Water – from Atmosphere to Space II (joint session CPP/DY)

Time: Tuesday 11:15–12:45 Location: ZEU/LICH

DY 24.1 Tue 11:15 ZEU/LICH

Microscopic diffusion and reactivity in aqueous solutions: photogenerated nascent halogen atoms, solvated electrons and subsequent dihalide formation — •Zhangatay Nurekeyev[1,2], Hyein Hwang[1,2], Fernando Rodriguez Diaz[1], Mei Bai[3], Michael Thorwart[3], Michaela Schäfer[4], Carmen Herrmann[4], and Christian Bressler[1,2,5] — [1]Inst. of Exp. Physics, Universität Hamburg — [2]The Hamburg Centre of Ultrafast Imaging (CUI) — [3]I. Inst. of Theor. Physics, Universität Hamburg — [4]Dept of Chemistry, Universität Hamburg — [5]European XFEL, Schenefeld

The solvent plays an important role in the assembly, stability and reactivity of (bio)chemical molecules. Small changes of the caging solvent can alter the reaction outcome, but little is known about the atomic-scale solvation shell dynamics. Our approach utilizes aqueous mono-atomic halide solutes, which are transformed into nascent neutral halogen atoms upon femtosecond optical excitation together with a separated solvated electron. Combining X-ray absorption with transient optical absorption spectroscopies we monitor the subsequent diffusion-driven atom-electron recombination, each focusing on the halogen atom and on the solvated electron, respectively. We also monitor the appearance of dihalides on the tens of picosecond time scale. Using all x-ray and laser observables we deliver a new picture of the ensuing dynamics, for which the existence of the long-lived (X:e) contact pair is not required. Next steps aim to trace more complex guest-host scenarios towards functional proteins in solution.

DY 24.2 Tue 11:30 ZEU/LICH

Surface Propensity of Halide Ions in Water: New Evidence from LJ-XPS — •Daniela Torres-Díaz[1], Shirin Golami[1], Tillmann Buttersack[1], Qi Zhou[1], Rémi Dupuy[2], Bernd Winter[1], Chistophe Nicolas[3], and Hendrik Bluhm[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Laboratoire de Chimie Physique - Matière et Rayonnement (Sorbonne Université, CNRS), Paris, France — [3]Synchrotron SOLEIL, Saint-Aubin, France

The surface propensity of halide ions in water is still a matter of debate. While the famous Onsager&Samaras model indicates that charged species should avoid the interface, more recent Molecular Dynamics simulations that take into account the polarizability of the ions indicate notably that iodide and bromide prefer the interface while chloride and fluoride avoid it. Different models, however, differ in how strong this effect is, while experimental studies have reported contradictory results. Here I will discuss recent results obtained using Liquid-Jet X-Ray Photoemission Spectroscopy on water interfaces for potassium halide solutions. In particular, the measurement of the photoelectron angular distributions allow for a higher spatial resolution than classic XPS measurements.

DY 24.3 Tue 11:45 ZEU/LICH

Ion Correlations Drive Collective Adsorption of Hydronium Ions at the Air-Electrolyte Interface — •Elena Köhler Ruiz, Maximilian Becker, Louis Lehmann, and Roland Netz — Fachbereich Physik, Freie Universität Berlin, Germany

Acids exhibit distinct interfacial behavior at the air-water interface compared to simple monoatomic salts. While monoatomic ions are largely repelled from the interface, hydronium ions preferentially reside at the interface due to formation of an interfacial hydrogen-bond network. To investigate these contrasting behaviors, we perform molecular-dynamics simulations with thermodynamically optimized force fields, analyzing ionic distributions at the interface as well as resulting surface tensions and potentials. The simulated surface potentials reproduce the concentration-dependent trends observed in SFG experiments: At high concentrations, interfacial hydronium promotes co-adsorption of counterions, which results in a decrease of the surface potential with rising concentration,

consistent with experimental observations. These findings highlight the critical role of ion-ion correlations at interfaces, which are not accounted for by modified Poisson-Boltzmann models.

DY 24.4 Tue 12:00 ZEU/LICH

Calcium-amino acid complexation in water probed by Intermolecular Coulombic Decay — •Michele Pugini, Nicolas Velasquez, Harmanjot Kaur, Florian Trinter, Qi Zhou, Lukas Tomaník, Uwe Hergenhahn, and Bernd Winter — Fritz-Haber-Institut, Berlin

The Ca2+ ion is the most abundant metal ion in the human body, playing essential roles in numerous biological processes, many of which involve interactions with proteins. Gaining molecular-level insight into the nature of the interaction between Ca2+ ions and solvated amino acids is therefore crucial for understanding calcium's biological function. Intermolecular Coulombic decay (ICD), a non-local autoionization process, offers unique sensitivity to the local chemical environment and can selectively probe interactions within the first solvation shell of solvated Ca2+ ions.

Here, we demonstrate the sensitivity of resonant ICD3 to the chemical composition of the solvation shell, enabling the identification of Ca2+ associations with specific amino acids. Our model system is the amino acid proline. The interaction, if present, is revealed via the ICD electrons resulting from the ionization of the biomolecule upon the 2p to 3d excitation of Ca2+.

Our results unequivocally identify Ca2+-proline interactions, indicating substitution of water molecules in the ion's coordination shell by proline. These findings establish ICD as a sensitive probe of metal-biomolecule interactions and highlight its potential as a powerful spectroscopic tool for investigating biomolecular structure in solution.

DY 24.5 Tue 12:15 ZEU/LICH

Distinguishing cavity and non-cavity solvation structures of the hydrated electron — •Sy Dat Ho and Benjamin Philipp Fingerhut — Department of Chemistry and Centre for NanoScience, Ludwig-Maximilians-Universität München, 81377 München, Germany

Solvated electrons in water are prototypical low-dimensional quantum systems that are coupled to a fluctuating, many-body environment. However, their hydration structure is still a matter of debate, with both cavity and non-cavity models having been suggested. First-principles molecular dynamics simulations are performed of excess-electron localization in liquid water, using hybrid-meta-GGA and hybrid-GGA density functionals that accurately reproduce bulk water structure. Perturbations to the local hydrogen bond structure of water due to interaction with the excess charge are identified, giving rise to specific signatures in transient radial distribution functions. These patterns are then compared with preliminary liquid-phase MeV-UED data obtained during an early science campaign at SLAC. In order to distinguish the structural changes induced by excess electrons in the diffraction patterns, long-time simulations at an unprecedented level of theory are required in order to minimise statistical noise. Our results clarify the coupling of hydrated electrons to solvent fluctuations and provide microscopic insight into polaron formation in disordered condensed phases.

DY 24.6 Tue 12:30 ZEU/LICH

Mesoscopic Structures in Water/HFIP based Electrolytes — •Sophie Zeilinger[1,2] and Markus Mezger[1] — [1]Center for Nano Structure Research, Faculty of Physics, University of Vienna, AT-1090 Vienna — [2]Institute of Physical Chemistry, Faculty of Chemistry, University of Vienna, AT-1090 Vienna

Previous studies have shown that binary water/hexafluoroisopropanol (HFIP) mixtures exhibit nanoscale heterogeneties that strongly affect properties such as reaction rates. The complex hydrogen bonding network of the binary mixture together with the amphiphilic character of the HFIP molecule provides a sensitive environment in which subtle changes in interactions can generate nanoscale heterogeneties. Here, we study the structure formation in water/HFIP under the influence of hydrophilic and hydrophobic ions by Small Angle X-Ray Scattering (SAXS). Depending on water content, pH, salt concentration and temperature we observe monotonous and oscillatory density correlations with structural parameter on the nanometer length scale. These structures are explained by the coupling of coulombic interactions between charged hydrophilic and hydrophobic ions vs. local fluctuations in water/HFIP concentrations.

DY 25: Franco-German Session on Granular Matter II

Granular media exhibit rich collective behavior arising from simple interactions such as friction, collisions, elasticity, and confinement. This session brings together experimental, numerical, and theoretical studies addressing key transitions in granular systems, including jamming, viscous-to-inertial regimes, clustering, gas cooling, and impact dynamics, highlighting the links between microscopic mechanisms and macroscopic responses.

Organized by Baptiste Darbois Texier (Paris) and Franco Antonio Tapia Uribe (Dresden)

Time: Tuesday 14:00–15:30 Location: HÜL/S186

DY 25.1 Tue 14:00 HÜL/S186

Avalanches of a granular medium reinforced with flexible fibres — •Baptiste Darbois Texier, Georges Gauthier, and Ladislas Wierzchalek — FAST, CNRS UMR 7608, University Paris-Saclay

Debris flows and landslides are catastrophic geophysical events that typically occur on sloped terrains and involve a large amount of granular materials in motion. At the laboratory scale, such events can be studied by observing avalanches of granular materials flowing down a slope and analyzing the factors that influence their initiation and cessation. In this study, we explore the effect of incorporating flexible fibres into granular media as a strategy to attenuate avalanches and stabilize granular piles. While fibre reinforcement has been shown to enhance the mechanical strength of soils, its influence on avalanche dynamics remains largely unexplored. We perform rotating-drum experiments at low rotation speeds using mixtures of grains and flexible fibres with varying volume fractions and aspect ratios. We measure the angles at which avalanches start and stop, as well as the relaxation dynamics following individual events. Increasing the fibre content or aspect ratio systematically raises both start and stop angles and broadens their distributions, accompanied by a marked rise in the number of small-amplitude avalanches. Analysis of relaxation curves further shows that fibres enhance dissipation, leading to slower, more gradual avalanche decay compared with pure grains. These findings provide quantitative evidence of the stabilizing effects of fibres on granular slopes and their role in dissipating energy during avalanches.

DY 25.2 Tue 14:15 HÜL/S186

Magnetic-Field Controlled Self-Diffusion and Clustering in Ferrogranular Mixtures — •Oksana Bilous[1], Kirill Okrugin[1], Ali Lakkis[2], Richter Reinhard[2], and Sofia Kantorovich[1] — [1]Computational and Soft Matter Physics, University of Vienna, Vienna, Austria — [2]Experimental Physics 5, University of Bayreuth, Bayreuth, Germany

We investigate self-diffusion in ferrogranular mixtures of magnetic and glass beads via Langevin/molecular dynamics of quasi-2D Stockmayer spheres mixed with repulsive non-magnetic ones, complemented by mm-scale experiments. We vary out-of-plane magnetic induction and total area fraction. The field aligns dipoles and reduces in-plane aggregation by inducing repulsion, while dipole-dipole interactions and central attractions (or susceptibility in experiments) drive chain-like and compact clustering. Increasing area fraction counteracts field-induced suppression and stabilizes larger clusters. Single magnetic particles and glass beads remain mostly diffusive, with diffusion only weakly concentration dependent, whereas particles embedded in clusters show persistent subdiffusion. The field also alters diffusion type: cluster-bound particles exhibit robustly non-Gaussian dynamics that amplify with area fraction and field. At sufficiently high induction and crowding, the glass component becomes non-Gaussian, revealing field-driven dynamical freezing of the non-magnetic species. Simulations and experiments consistently show how external fields, dipolar self-assembly, and crowding govern transport in ferrogranular layers.

DY 25.3 Tue 14:30 HÜL/S186

Angular Velocity of Spherical Particles in a Granular Gas under Microgravity during Granular Cooling — •Mahdieh Mohammadi[1], Raúl Cruz Hidalgo[2], Dmitry Puzyrev[3], Ralf Stannarius[1,3], and Kirsten Harth[1,3] — [1]Department of Engineering, Brandenburg University of Applied Sciences, Magdeburger Str. 50, 14770 Brandenburg an der Havel, Germany — [2]Departamento de Física y Matemática Aplicada, Facultad de Ciencias , Universidad de Navarra, Pamplona, Spain — [3]MARS and MTRM, Otto von Guericke University Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

We investigate the rotational dynamics of spherical particles in a granular gas in microgravity, which allows a clean realization and observation of collisional kinetics. The system starts in a highly excited state and undergoes dissipative collisional cooling (loss of mean kinetic energy). Patterned spheres were tracked from video data using two cameras, their 3D trajectories and velocities were extracted. Surface markers enable 3D orientation reconstruction via feature-based and projection-consistent analysis. Continuous angular trajectories are obtained by interpolating missing orientation data. From these, we extract angular veloc-

ities and analyze their evolution across different cooling intervals.

Our studies are funded within by the German Aerospace Center (DLR) projects PARADYSE, KORDYGA and EVA-II (50WM2542, 50WM2242, 50WK2348).

DY 25.4 Tue 14:45 HÜL/S186

Granular gas mixtures: Experiments and numerical simulations — •Dmitry Puzyrev[1], Kirsten Harth[2,1], Torsten Trittel[2,1], Raúl Cruz Hidalgo[3], and Ralf Stannarius[2,1] — [1]Otto von Guericke University, Magdeburg, Germany — [2]Brandenburg University of Applied Sciences, Brandenburg an der Havel, Germany — [3]University of Navarra, Pamplona, Spain

Granular gases are ensembles of free-moving macroscopic particles which collide inelastically, which leads to effects like unusual heating (gain of mechanical energy from external sources) and cooling (dissipative loss of mechanical energy), clustering, and spontaneous collective movement. Such systems can exist in different dynamical regimes depending on filling fraction, particle shapes and material properties, as well as external energy input. Our investigation is focused on 3D microgravity experiments with ensembles of non-spherical, rod-shaped particles [1] and their mixtures [2]. Machine learning-aided software used for particle detection, 3D matching and tracking is available as an open-source package [3] and can be applied to other multiparticle tracking problems. In addition to previously published results for a mixture of thinner and thicker rods [2], we present the initial results for a short/long rods mixture. Our studies are funded within by the German Aerospace Center (DLR) projects EVA-II, VICKI, KORDYGA and PARADYSE (50WK2348, 50WM2252, 50WM2242, 50WM2542). [1] K. Harth et al., Rev. Lett., 120, 214301 (2018) [2] Puzyrev et al., npj Microgravity, 10, 36 (2024) [3] A. Niemann et al., github.com/ANP-Granular/ParticleTracking, JOSS 10(109), 5986 (2025)

DY 25.5 Tue 15:00 HÜL/S186

Granular gases of non-convex particles: Experiments and numerical simulations — Torsten Trittel[1,2], Mohammad Enezz[1], Dmitry Puzyrev[2], Kirsten Harth[1], Raúl Cruz Hidalgo[3], and •Ralf Stannarius[1,2] — [1]Brandenburg University of Applied Sciences, Brandenburg an der Havel, Germany — [2]Otto von Guericke University Magdeburg, Magdeburg, Germany — [3]University of Navarra, Pamplona, Spain

Granular gases are dilute ensembles of macroscopic particles that are not in permanent contact. Owing to the low packing fraction, they interact only by random inelastic collisions. Consequences are permanent dissipative loss of mechanical energy (granular cooling) and spontaneous clustering. Most experiments and numerical simulations so far considered spheres. The present study investigates spatial crosses (hexapods). They add more complexity in the particle interactions, and alter the role of the collisions in the exchange of translational and rotational kinetic energies. We present experiments performed in microgravity on a suborbital rocket flight [1], demonstrate particle tracking from the optical video data [2], and show results of DEM simulations of these systems. The study is funded within by DLR within projects EVA-II and JACKS (50WK2348, 50WM2340).

[1] https://sscspace.com/six-science-projects-to-space-from-sweden/
[2] A. Niemann et al., JOSS 10(109), 5986 (2025)

General Discussion

DY 26: Focus Session: Water – from Atmosphere to Space III (joint session CPP/DY)

Time: Tuesday 14:00–15:30 Location: ZEU/LICH

Topical Talk DY 26.1 Tue 14:00 ZEU/LICH

Why water in plants survives negative pressure — Marin Šako[1,2], Emanuel Schneck[3], Roland Netz[4], and •Matej Kanduč[1] — [1]Jožef Stefan Institute, Ljubljana, Slovenia — [2]University of Ljubljana, Faculty of Mathematics and Physics, Ljubljana, Slovenia — [3]Physics Department, Technische Universität Darmstadt, Darmstadt, Germany — [4]Fachbereich Physik, Freie Universität Berlin, Berlin, Germany

It may seem surprising that we can lower the pressure in a liquid to negative values, far below the saturated vapor pressure at which a vapor phase should form. In water, such deeply metastable states are possible only when it is exceptionally pure and free of nucleation sites. It is therefore even more striking that plants transport water at negative pressures down to −100 atm without cavitation, even though xylem sap is anything but pure: it contains dissolved ions, sugars, lipids, and other organic molecules. How is this possible?

In this talk, I will show how molecular simulations and theory can explain this surprising behavior. We find that amphiphilic molecules such as lipids can adsorb onto hydrophobic surface crevices — places that would normally trap nanobubbles. Once coated, these surface defects can no longer stabilize bubbles, which allows water to stay intact even under strong tension. This mechanism offers a molecular-level explanation for how trees transport water to heights of over 100 meters without cavitation. More broadly, it illustrates how soft-matter physics and interfacial molecular organization can control the mechanical stability of liquids under extreme conditions.

DY 26.2 Tue 14:30 ZEU/LICH

Cholesterol Controlled Photo-Switching Activity of Azobenzene Glycoconjugates in Lipid Membranes — •Prashant Hitaishi[1,2], Svenja C. Hövelmann[1,2], Michael Röhrl[3], Nicolas Hayen[1], Ella Diebell[1], Ali Ashtiani[1], Carlotta Mager[1], Thisbe Lindhorst[3], and Bridget M. Murphy[1,2] — [1]Institute of Experimental and Applied Physics, Kiel University, Leibnizstraße 19, Kiel, 24118, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, Hamburg, 22607, Germany — [3]Otto Diels-Institut für Organische Chemie, University of Kiel, Germany

Reversible photo-switchable molecules enable precise optical control of soft interfaces and are attractive for smart surfaces and light-triggered drug delivery. Azobenzene glycoconjugates (Azo) undergo reversible trans-cis isomerization under alternating UV and visible illumination, thereby modulating their conformation and interactions with lipid membranes. Here, Azo is incorporated into DPPC monolayers containing 0, 15, or 30 mol% cholesterol to mimic biologically relevant membrane compositions. Langmuir monolayer isotherm studies combined with time-resolved illumination cycles and X-ray measurements are used to quantify Azo-induced changes in membrane structure and relaxation kinetics. Increasing cholesterol slows Azo photo-switching, indicating a more constrained, rigid nanoenvironment, and shows that membrane composition can be used to tune light responsiveness in lipid interfaces for designing azobenzene-based responsive biomaterials.

DY 26.3 Tue 14:45 ZEU/LICH

Photoelectron Angular Distributions of Ions Influenced by Surfactants at the Solution-Vapor Interface — •Shirin Gholami[1], Tillmann Buttersack[1], Clemens Richter[2], Rémi Dupuy[3], Daniela Torres-Díaz[1], Christophe Nicolas[4], Uwe Hergenhahn[1], and Hendrik Bluhm[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]SPECS Surface Nano Analysis GmbH, Berlin, Germany — [3]Sorbonne Université, CNRS, Paris, France — [4]Synchrotron SOLEIL, Paris, France

Aqueous liquid-vapor interfaces play key roles in atmospheric and oceanic processes. The ocean-air boundary forms the largest aqueous-vapor interface, covering over 70 % of Earth's surface. In addition to Na^+ and Cl^-, Mg^{2+} and SO_4^{2-} are the most abundant ions in ocean water.

Here, we investigate how Mg^{2+} and SO_4^{2-} ions behave at the aqueous solution-vapor interface in the presence of charged surfactants. Using sub-monolayer coverages of octylamine $-CNH_3^+$ and octanoate $-COO^-$, we examine how these surfactants modify the distance of the ions from the interface. Liquid-jet X-ray photoelectron spectroscopy in combination with photoelectron angular distributions provides Å-scale depth sensitivity, enabling us to quantify ion-surfactant interactions.

Our results show that differently charged surfactants shift the interfacial positioning of Mg^{2+} and SO_4^{2-}, and that specific ion-ion interactions influence their interfacial propensity.These findings reveal how surfactants govern the depth distribution of ions, providing insight into oceanic and atmospheric processes.

DY 26.4 Tue 15:00 ZEU/LICH

Contact line dynamics on moving fibers measured by X-ray holography — •Louisa E. Kraft[1,2], Jens Lucht[3], Fiona Berner[1,2], Hannes P. Hoeppe[3], Tobias Eklund[1,2], Yizhi Liu[1], Markus Osterhoff[3], Tim Salditt[3], Hans-Jürgen Butt[1], and Katrin Amann-Winkel[1,2] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Johannes Gutenberg University, Institute for Physics, Mainz, Germany — [3]Georg-August-University, Institute of X-ray Physics, Göttingen, Germany

The wetting properties of solid surfaces are important for many natural and industrial processes, especially with respect to dynamic wetting. The wetting dynamic of solid surfaces, in particular the quantitative description of the dynamic contact angles, is still under debate. Dynamic contact angle variations connect macroscopically measured quantities with microscopic processes. Most studies rely on optical or confocal microscopy which limits the experimental access to the sub-microscopic region where these processes take place. We present data from X-ray holography experiments, imaging the three-phase contact line on moving glass fibers with an improved spatial resolution of about 450 nm combined with a temporal resolution of 10 Hz. We used the GINIX nanofocus-

ing setup at the P10 beamline at PETRA III (DESY, Hamburg). The used glass fibers were pulled out of a liquid bath filled with varying aqueous solutions while changing the lateral velocity. We could clearly observe a decrease of the receding dynamic contact angle with increasing fiber velocity confirming the predictions of dynamic wetting theory.

DY 26.5 Tue 15:15 ZEU/LICH

Properties of micrometre-sized supercooled water droplets — Claudia Goy[1], •Frédéric Caupin[2], Felix Lehmkühler[1], and Robert E. Grisenti[3,4] — [1]Deutsches Elektronen Synchrotron DESY, Hamburg, Germany — [2]Université Claude Bernard Lyon 1, Villeurbanne, France — [3]GSI, Darmstadt, Germany — [4]J. W. Goethe-Universität, Frankfurt am Main, Germany

Water displays a wide range of anomalous behaviors, many of which become particularly pronounced in the supercooled state, where its properties deviate strongly from those of other liquids. A prevailing hypothesis suggests that, at low temperatures, water may locally adopt two distinct structural motifs. This presentation will discuss results from temperature-dependent experiments that probe the physical and chemical properties of liquid water. The studies employ evaporatively cooled liquid jets in vacuum, investigated with techniques such as Raman spectroscopy and X-ray spectroscopy. These approaches enable a detailed examination of inter- and intramolecular vibrational modes, providing insight into the molecular dynamics of cooling water and optical properties, including the refractive index. Together, these experimental methods offer a comprehensive view of the temperature-dependent behavior of water, shedding light on the complex interactions that drive its anomalies. Through these studies, we aim to elucidate the mechanisms governing water's unique behavior in the supercooled regime and contribute to a deeper understanding of its structural transformations and physical properties.

DY 27: Statistical Physics far from Thermal Equilibrium II

Time: Tuesday 14:00–15:30 Location: ZEU/0114

DY 27.1 Tue 14:00 ZEU/0114

Efficiency of Carnot-like engine for intracellular diffusivity fluctuations and diffusing diffusivity — •Yuichi Itto — Aichi Institute of Technology, Japan — ICP, Universität Stuttgart, Germany

In contemporary physics of intracellular diffusion, much attention is paid to understanding how environmental conditions affect the diffusivity [1], the change of which is crucial, e.g., for tuning the rates of biochemical reactions. Recently, the heat-like engine for local diffusivity fluctuations, which slowly vary and obey a universal exponential law, has been constructed to extract the diffusivity change in a cycle realized by compression/expansion of cells and temperature change [2]: it has the Carnot-like efficiency determined by the average diffusivity.

Here, the effect of slowly varying fluctuation on the efficiency [3] is discussed based on "diffusing diffusivity" [4] that describes the dynamics of the fluctuation distribution by an advection-diffusion equation, the stationary solution of which is of the exponential type. The entropy of the fluctuations, which gives the exponential law at its maximum, takes positive production rate under the dynamics. The tendency to approach the (stationary) average diffusivity is dominantly governed by the factor characterizing the diffusion term in its square root, showing its peculiar role in view of the fact that the exponential law is due to the advection term.

[1] N. Bellotto, J. Agudo-Canalejo, R. Colin, R. Golestanian, G. Malengo, V. Sourjik, eLife 11, e82654 (2022). [2] Y. Itto, Eur. Phys. J. B 98, 183 (2025). [3] Y. Itto, arXiv:2511.06851 (2025). [4] M. V. Chubynsky, G. W. Slater, Phys. Rev. Lett. 113, 098302 (2014).

DY 27.2 Tue 14:15 ZEU/0114

Relaxation speed in quenched-random force fields — •Jan Meibohm and Sabine H.L. Klapp — Technische Universität Berlin, Institut für Physik und Astronomie, Fachgruppe Theoretische Physik, Hardenbergstraße 36, 10623 Berlin, Germany

We determine the asymptotic relaxation speed of a Brownian particle in quenched-random force fields with a harmonic background in dimensions $d \geq 2$. For random forces derived from a potential, we show that relaxation is generally slower than in the unperturbed case when the background is isotropic. By contrast, for strongly anisotropic backgrounds, where the background is stiffer in all directions except one, we find a crossover between slow and fast relaxation, similar to the one-dimensional case discussed in [1]. Allowing for non-potential forces changes this picture and leads to generally faster relaxation. In the limits of small and large correlation length of the random force, we identify universal regimes in which the relaxation speed becomes independent of of the details of the random forces. Finally, we analyse a scaling limit for quasi-isotropic backgrounds at weak disorder, where the change in relaxation speed becomes anomalously large.

[1] Meibohm & Klapp, Phys. Rev. Lett., 134.8, 087101 (2025)

DY 27.3 Tue 14:30 ZEU/0114

Mpemba effect for a particle in a bistable potential: classical versus quantum — •Jannis Michael Melles[1], Hartmut Löwen[1], Benno Liebchen[2], and Alexander Antonov[1] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Düsseldorf, Germany — [2]Institut für Physik der kondensierten Materie, Technische Universität Darmstadt, Darmstadt, Germany

An anomalous cooling behavior where initially hot systems cool faster than initially warm ones is referred to as the Mpemba effect and clearly goes beyond quasi-static thermodynamics. For classical particles, such a cooling behavior has been thoroughly studied for a simple paradigmatic set up involving a single classical colloidal particle in a bistable optical potential [1]. We quantize this model and consider a quantum particle coupled to an external bath with the Lindblad damping [2]. The Mpemba effect does occur during the cooling of this quantum system; however, the origin of the anomalous cooling is qualitatively massively different from that of its classical counterpart for temperatures close to or at zero. Additionally, we identify a doubled inverse quantum Mpemba effect when the system is heated instead. Our results are amenable for an experimental verification with an ultracold atom in a suitable laser-optical trap potential.

[1] A. Kumar and J. Bechhoefer, Nature **584**, 64 (2020)
[2] J. Melles, H. Löwen, B. Liebchen and A. Antonov, to be published

DY 27.4 Tue 14:45 ZEU/0114

Brownian gyrators: from mono- to quadrupolar gyration — •Iman Abdoli and Hartmut Löwen — Institut für Theoretische Physik II - Soft Matter, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, D-40225 Düsseldorf, Germany

Thermally anisotropic Brownian systems-where different spatial directions are coupled to different effective temperatures-break detailed balance and generate circulating probability currents, exemplified by the Brownian gyrator. Such systems provide a minimal framework for studying nonequilibrium energy conversion and the emergence of directed motion and torques driven purely by fluctuations. We demonstrate how these anisotropic fluctuations can be harnessed as a microscopic heat engine, whose efficiency can approach Carnot performance at maximum power when appropriately loaded with external mechanical forces [1]. Furthermore, we show that confining a thermally anisotropic particle to a narrow ring produces quadrupolar steady-state gyration, a symmetry-protected circulation pattern arising solely from anisotropic noise [2]. These results highlight the rich flux structures and energetic functionalities enabled by thermal anisotropy.

[1] I Abdoli, A Sharma, H Löwen, Phys. Fluids. 37 (4)
[2] I Abdoli, H Löwen, arXiv preprint arXiv:2508.08792

DY 27.5 Tue 15:00 ZEU/0114

Role of kinetics in mesoscopic dynamics of a driven Potts model — •Maciej Chudak[1], Massimiliano Esposito[2], and Krzysztof Ptaszyński[1] — [1]Institute of Molecular Physics, Polish Academy of Sciences, Mariana Smoluchowskiego 17, 60-179 Poznań, Poland — [2]Department of Physics and Materials Science, University of Luxembourg, 30 Avenue des Hauts-Fourneaux, L-4362 Esch-sur-Alzette, Luxembourg

The Potts model is a generalization of the Ising model, where spins can take more than two states. We study a driven three-state non-equilibrium Potts model with homogeneous all-to-all coupling. At a macroscopic level, this model exhibits complex behavior such as synchronization and persistent oscillations (limit cycles). In the mean-field limit the model dynamics is described via deterministic equations of motion. Choice of the transition rate function can reshape the phase diagram of the model. We identified seven distinct dynamical phases separated by seven bifurcation types. Beyond the mean-field analysis, we characterize the effect of rare fluctuations on the model behavior. We determine the coherence lifetime of the oscillations and compare it to a thermodynamic bound given by the entropy production per cycle. The trade-off between coherence lifetime and entropy production can be fine-tuned. We characterize the rare stochastic transitions among the coexisting mean-field attractors using the instanton approach. Such transitions tend to relax the system to a single attractor that determines the macroscopic behavior of the model. In case of multistability, the ordered state is usually the most likely.

DY 27.6 Tue 15:15 ZEU/0114

Continuous-time multifarious systems — •Jakob Metson[1], Saeed Osat[1,2], and Ramin Golestanian[1,3] — [1]Max Planck Institute for Dynamics and Self-Organization (MPI-DS), 37077 Göttingen, Germany — [2]Institute for Theoretical Physics IV, University of Stuttgart, 70569 Stuttgart, Germany — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

Multifarious assembly models consider multiple structures assembled from a shared set of components. We explore Gillespie simulations of lattice-based assembly models, comparing these to Monte Carlo simulations. We start with an equilibrium model, in which detailed balance is obeyed. However, due to the rough energy landscape, the systems often end up in long-lived metastable states. Despite this, the Gillespie and Monte Carlo simulations are largely consistent. We present physical arguments to predict the state boundaries, which also reconciles a small discrepancy between the two simulation methods. We furthermore study an explicitly non-equilibrium model, the non-reciprocal multifarious self-organisation model. Here, non-reciprocal interactions between the building blocks break detailed balance. Also in this case, the Gillespie and Monte Carlo simulations demonstrate the same range of behaviours. Additionally, we explore the timescales of shape-shifting present in this model, developing analytical calculations to compare with simulations. Overall, these results demonstrate that both Gillespie and Monte Carlo simulations can be relied on to explore such systems, even when the dynamics are far from equilibrium.

DY 28: Fluid Physics and Turbulence

Time: Tuesday 14:00–15:15 Location: ZEU/0118

Invited Talk DY 28.1 Tue 14:00 ZEU/0118

Geometry of turbulent mixing in thermal convection — •Jörg Schumacher — Institut für Thermo- und Fluiddynamik, TU Ilmenau, Germany

Thermal convection flows, which are driven by buoyancy forces, are ubiquitous in nature and technology ranging from atmospheric dynamics to heat transfer in blankets of nuclear fusion devices. They are mostly connected to further physical processes, such as phase changes, radiation or magnetic fields, but the paradigm to all these turbulent flows is the plane Rayleigh-Bénard convection layer that is uniformly heated from below and cooled from above. In my talk, I will review some recent numerical investigations, both in the Eulerian and Lagrangian frames of reference, which shed new light on geometric aspects of these flows. This comprises the organization of thermal plumes in hierarchical and self-affine near-wall networks, the large-scale organization of the flow structures, and the organization of tracer particle tracks to extreme swirling events. Consequences for the turbulent transport of heat and momentum across the convection layer and their necessary modeling will be discussed.

DY 28.2 Tue 14:30 ZEU/0118

Compression, simulation, and synthesis of turbulent flows — •Stefano Pisoni[1,2], Raghavendra Peddinti[2], Siddhartha Morales[2], Egor Tiunov[2], and Leandro Aolita[2] — [1]TUHH, Hamburg, Germany — [2]TII Abu, Dhabi, UAE

Numerical simulations of turbulent fluids are paramount to real-life applications. However, they are also computationally challenging due to the intrinsically nonlinear dynamics, which requires a very high spatial resolution to accurately describe them. A promising idea is to represent flows on a discrete mesh using tensor trains (TTs), where the values of the velocity field are encoded as a product of matrices (also known as Matrix Product States). This representation features an exponential compression of the number of parameters, under the assumption of low inter-scale correlations. However, it is yet not clear how the achieved compression of TTs is affected by the complexity of the flows. In fact, no TT fluid solver has been extensively validated in a fully developed turbulent regime yet. We fill this gap by analyzing TTs as an Ansatz to compress, simulate, and generate 3D snapshots with turbulent-like features. We first investigate the effect of TT compression on key turbulence statistical signatures. Second, we present a TT solver to time evolve a 3D fluid fields according to the incompressible Navier-Stokes equations. Third, we develop a memory-efficient TT algorithm to generate artificial snapshots displaying turbulent-like features. In all three cases we observe that the memory-efficient TT representation captures the relevant features of turbulent flows, offering a powerful quantum-inspired toolkit for their computational treatment.

DY 28.3 Tue 14:45 ZEU/0118

Physics-based reduced order modeling of complex chemical reactors — •Lisanne Gossel[1], Leon L. Berkel[2], Maira Gauges[2], Paul Brand[1], Mathis Fricke[1], Christian Hasse[2], Alessandro Stagni[3], Hendrik Nicolai[2], Dieter Bothe[1], and Tiziano Faravelli[3] — [1]Mathematical Modeling and Analysis, Technical University of Darmstadt, Darmstadt, Germany — [2]Simulation of Reactive Thermo-Fluid Systems, Technical University of Darmstadt, Darmstadt, Germany — [3]CRECK Modeling Group, Politecnico di Milano, Milan, Italy

Understanding and predicting observables in complex reacting flows is crucial for many applications related to the clean energy transition. We are interested in describing chemical reactors with detailed, often multiphase chemistry including thousands of reactions. While detailed understanding of the fluid physics can be gained by highly-resolved numerical models of the reactors, i.e., different types of Computational Fluid Dynamics (CFD) simulations, these usually rely on strongly simplified chemistry models to retain computational tractability. On the other hand, we use a physics-based reduced order method that allows to complement CFD by detailed chemistry computations. This is achieved by describing the reactor by a network of modeling components representing certain states of the reactor. The talk will focus on recent achievements in the development of algorithms for creating these network models based on prior CFD results. We discuss the roles of model consistency and defining proper trade-offs between model ac- curacy and complexity.

DY 28.4 Tue 15:00 ZEU/0118

Numerical investigation of surface wind veer in a transitional Atmospheric Boundary Layer — •Maharun Nesa Shampa, Heiko Schmidt, and Marten Klein — Brandenburgische Technische Universität Cottbus-Senftenberg, Cottbus, Germany

The Atmospheric Boundary Layer (ABL) is defined as the lower part of the atmosphere that dynamically couples the free atmosphere and Earth's surface. Transitional features and strong variability in boundary layer thickness due to surface heating and cooling pose a challenge for modeling atmospheric dynamics, placing a burden on flow profile and surface-flux parameterizations. This study addresses the mentioned challenge by investigating an idealized ABL, the so-called Ekman Boundary Layer (EBL) using a stochastic One-dimensional Turbulence (ODT) model as standalone tool. The EBL is characterized by absence of stratification such that a statistically stationary force balance between the pressure-gradient, Coriolis and drag forces is reached asymptotically for a prescribed synoptic pressure gradient. A single non-dimensional parameter, the Reynolds number, characterizes the flow regime and reflects the range of the turbulent scales participating in the flow. It is demonstrated that ODT is capable of capturing surface properties (like friction velocity, wind-turning angle) compatible with reference data and appropriate parameterization for transitional Reynolds numbers. In addition, the model offers additional insight into the boundary layer structure and statistical flow properties, which are likewise discussed. By constraining the stochastic sampling of turbulent length scales, an outlook to cut-off mechanisms is given.

DY 29: Active Matter IV (joint session DY/BP/CPP)

Time: Tuesday 14:00–15:30 Location: ZEU/0160

DY 29.1 Tue 14:00 ZEU/0160

Automated decision-making by chemical echolocation in active droplets — •Aritra K. Mukhopadhyay[1], Ran Niu[2], Linhui Fu[2], Kai Feng[2], Christopher Fujta[1], Qiang Zhao[2], Jinping Qu[2], and Benno Liebchen[1] — [1]Technische Universität Darmstadt, Darmstadt, Germany. — [2]Huazhong University of Science and Technology, Wuhan, China.

Motile microorganisms like bacteria and algae combine self-propulsion, cooperation, and decision-making at the micron scale. Inspired by these biological systems, synthetic microswimmers are emerging as human-made counterparts capable of self-propulsion. Recent breakthroughs provide a platform to integrate additional functionalities, bridging the gap between biology and synthetic systems. We propose and experimentally demonstrate a mechanism that enables synthetic microswimmers, including autophoretic colloids, droplet swimmers, and ion-exchange-driven modular swimmers, to make autonomous navigational decisions. These swimmers generate chemo-hydrodynamic signals that interact with boundaries, producing echoes that encode structural information about

the environment. These echoes trigger automatic responses, such as synthetic chemotaxis, allowing swimmers to avoid dead ends and autonomously find paths through complex mazes. We show the mechanism remains robust across different maze geometries, ensuring reliable navigation without external cues. Our findings illustrate how simple physical principles can endow synthetic systems with advanced navigation functionalities.

DY 29.2 Tue 14:15 ZEU/0160

Dead or alive?—Probing scale-dependent liveliness in multiscale active matter — •Joscha Mecke[1] and Klaus Kroy[2] — [1]Institute for Advanced Study, Shenzhen University, Shenzhen, China — [2]Institut für Theoretische Physik, Universität Leipzig, Leipzig, Germany

If you have ever watched live and dead trouts swimming upstream, side by side, you may have wondered how closer inspection of their mesoscale activity might help to tell them apart. But probing spatially heterogeneous activity in living matter is a major challenge. We demonstrate the emergence of multiple effective ("active") temperatures in nonequilibrium molecular- and Brownian-dynamics simulations of an active polymer. Energy injection at different length scales leads to mode coupling, inter-modal energy transfer, and entropy production. We put forward a generalised Langevin equation for a labelled monomer, which, by application of a harmonic potential, can serve as a spectroscopic device. Upon varying the trap stiffness, we can selectively scan through the emergent effective temperatures and thereby resolve the scale-dependent activity. Our approach thus provides a minimally invasive spectroscopic tool to generate quantitative maps of liveliness, across multiple scales.

DY 29.3 Tue 14:30 ZEU/0160

Tuning the velocity of thermophoretic microswimmers with thermo-sensitive polymers — Franziska M. Braun, Aritra K. Mukhopadhyay, Samad Mahmoudi, Benno Liebchen, and •Regine von Klitzing — Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstrasse 8, 64289 Darmstadt

Understanding and controlling the motion of self-propelled particles in complex fluids is crucial for applications in targeted drug delivery, microfluidic transport, and the broader field of active matter. Here, we investigate the thermophoretic self-propulsion of partially gold-coated polystyrene Janus particles (Au-PS) in temperature-responsive linear Poly(N-isopropyl acrylamide) (PNIPAM) solutions across various PNIPAM concentrations and temperatures. Particle velocities are examined at three representative temperatures: far below, near but below and above the LCST. In pure water, Au-PS Janus particles propel with the PS hemisphere leading, driven by their intrinsic thermophoretic response. Conversely, the positive Soret coefficient of PNIPAM results in depletion forces that induce motion of the Janus particle towards the hot Au side. The experiments reveal a non-monotonic dependence of particle velocity on temperature, with a maximum near the LCST. Interfacial processes like ion movement in the electric double layer and PNIPAM adsorption at the Au-PS particles are separated from processes that are coupled to the bulk solution. Theoretical calculations are in good agreement with the experimental findings and are essential for the understanding of the complex interplay of microswimmers with thermoresponsive polymers.

DY 29.4 Tue 14:45 ZEU/0160

Non-reciprocal multifarious self-organization — •Saeed Osat[1] and Ramin Golestanian[2] — [1]Institute for Theoretical Physics IV, University of Stuttgart, Heisenbergstraße 3, 70569 Stuttgart, Germany — [2]Max Planck Institute for Dynamics and Self-Organization (MPI-DS), 37077 Goettingen, Germany

Biological systems exhibit a unique ability to design diverse structures from a shared set of building blocks, with a plethora of proteins made from a limited set of amino acids as a prime example. Furthermore, these systems often use building blocks efficiently by introducing transformations between different structures. A structure might undergo structural transformations to form a new structure with different functional purposes, without the need to discard the current structure and start anew. To unravel this mystery, one must examine the underlying non-equilibrium processes that make this shape-shifting behavior feasible.

Here, we leverage non-reciprocal interactions between building blocks to provide a foundation for designing dynamic structures. We used a multifarious self-assembly (MSA) model, which is the molecular counterpart of the Hopfield associative memory. By upgrading the MSA model to its non-equilibrium counterpart with non-reciprocal interactions, we introduce the ability to not only self-assemble different structures on demand but also facilitate shifts and transformations that lead to shape-shifting behavior.

Invited Talk DY 29.5 Tue 15:00 ZEU/0160

Designing topological edge states in bacterial active matter — Yoshihito Uchida[1], Daiki Nishiguchi[2,1], and •Kazumasa A. Takeuchi[1] — [1]The University of Tokyo, Tokyo, Japan — [2]Institute of Science Tokyo, Tokyo, Japan

Besides its potential relevance to the life sciences, active matter also manifests as a novel, intrinsically non-equilibrium kind of matter, endowed with characteristic transport properties distinguished from conventional matter. A challenge is how to control and design transport in active matter. A potentially useful, emerging concept here is topological transport developed in condensed matter physics, which was extended to active matter successfully, but experimental realizations have thus far relied on the chirality of the active particles, which limits design capabilities.

Here we report a controlled realization of topological edge states in dense bacterial suspension, induced by microfabricated geometry instead of the bacteria's chirality. First we demonstrate that we can rectify bacterial collective motion by a channel with asymmetric shape. Then we construct networks made of asymmetric channels and show that we can control the emergence of topological edge states through the network design. Through modelling and experiments, we discuss what properties of the network and the bacterial flow are crucial to the observed topological phenomenon. We expect our results may pave the way for establishing a control and design principle of topological transport in such active matter systems.

Ref) Y. Uchida, D. Nishiguchi, and K. A. Takeuchi, to appear.

DY 30: Nonequilibrium Quantum Systems I (joint session TT/DY)

Time: Wednesday 9:30–12:45 Location: CHE/0091

See TT 44 for details of this session.

DY 31: Networks, From Topology to Dynamics – Part I (joint session SOE/DY)

Time: Wednesday 9:30–11:00 Location: GÖR/0226

See SOE 8 for details of this session.

DY 32: Many-body Systems: Equilibration, Chaos, and Localization (joint session DY/TT)

Time: Wednesday 9:30–12:45 Location: HÜL/S186

DY 32.1 Wed 9:30 HÜL/S186

Compression of Floquet random circuits — •Francesca De Franco[1,2], David Luitz[3], Dante Kennes[4], Matteo Rizzi[1,5], and Markus Schmitt[1,2] — [1]FZ Juelich, Institute of Quantum Control (PGI-8) — [2]University of Regensburg — [3]University of Bonn — [4]RWTH Aachen University — [5]University of Cologne

Current quantum computing hardware suffers from significant dissipation due to the coupling to the environment. This limits the depth of unitary quantum circuits which can be applied with high fidelity and hence the physical timescales reachable by digital quantum simulation. Here, we show that the reachable timescale in practice depends strongly on the physics of the many-body system under investigation: For systems deep in a many-body localized phase, we can find shallow circuit representations of the evolution operator U to late times, while in a chaotic regime this is not possible. The associated compressibility of the late time evolution operator is hence associated with the accessibility of long times on noisy quantum hardware. Moreover, we compare the performance of these compressed, variationally obtained circuits to tensor-network simulations, which allow us to compute quantum-information-spreading diagnostics such as entanglement entropy and out-of-time-ordered correlators.

DY 32.2 Wed 9:45 HÜL/S186

Spectral pairing statistics in Floquet time crystals — Alexander-Georg Penner[1], •Harald Schmid[1,2,3], Leonid I. Glazman[4], and Felix von Oppen[1] — [1]Dahlem Center for Complex Quantum and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — [2]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany — [4]Department of Physics, Yale University, New Haven, Connecticut 06520, USA

Floquet time crystals are characterized by the subharmonic behavior of temporal correlation functions. Studying the paradigmatic time crystal based on the disordered Floquet quantum Ising model, we show that its temporal spin correlations are directly related to spectral characteristics and that this relation provides analytical expressions for the correlation function of finite chains, which compare favorably with numerical simulations. Specifically, we show that the disorder-averaged temporal spin correlations are proportional to the Fourier transform of the splitting distribution of the pairs of eigenvalues of the Floquet operator, which differ by pi to exponential accuracy in the chain length. We find that the splittings are well described by a log-normal distribution, implying that the temporal spin correlations are characterized by two parameters. We discuss possible implications for the phase diagram of Floquet time crystals.

DY 32.3 Wed 10:00 HÜL/S186

Spin-Spin Correlations and Multifractality in 1D disordered $SU(2)$-Invariant Heisenberg Spin Chains — •Debasmita Giri, Julian Siegl, and John Schliemann — Institute for Theoretical Physics, University of Regensburg, Regensburg, Germany

Disorder and interactions in one-dimensional quantum spin chains give rise to rich non-ergodic phenomena that lie beyond the conventional eigenstate thermalization hypothesis (ETH). In the presence of sufficiently strong quenched disorder, many-body localization (MBL) can emerge: transport is frozen, entanglement growth is logarithmically slow, and local operators retain memory of their initial conditions even at infinite temperature. On the contrary, studies on models with non-Abelian symmetries have demonstrated that continuous symmetries, such as $SU(2)$, can obstruct the construction of local integrals of motion and thus hinder full localization. We investigate spin correlations in one-dimensional $SU(2)$-invariant Heisenberg chains with exchange disorder for spin lengths $S = 1/2$ and $S = 1$. In the weak-disorder regime, the eigenmodes of the spin-spin correlation matrix are delocalized, consistent with ergodic behavior. Under strong disorder, the system enters a quasi-localized multifractal phase characterized by exponentially decaying, dimer-like spin correlations. Finite-size scaling of the inverse participation ratios of the correlation-matrix eigenmodes yields a correlation dimension, $D_2 \approx 0.37-0.39$, confirming the presence of a multifractal regime that is distinct from both the ergodic limit ($D_2 = 1$) and the fully localized limit ($D_2 = 0$).

DY 32.4 Wed 10:15 HÜL/S186

Timescales for Deep and Full Thermalization — •Tabea Herrmann[1], Felix Fritzsch[2], and Arnd Bäcker[1] — [1]TU Dresden, Institut für Theoretische Physik, Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Isolated quantum systems typically approach thermal equilibrium as described by the Eigenstate Thermalization Hypothesis (ETH). Going beyond this involves either higher order correlators (full ETH) or the approach of moments of the reduced density matrix towards thermal equilibrium (deep thermalization). In this talk we compare these two types of thermalization using extensive numerical studies within a paradigmatic model for chaotic many-body quantum dynamics. For this we find exponential relaxation for both types: For deep thermalization all moments relax with the same rate, which approximately equals the relaxation rate of two-point correlation functions within full ETH. In contrast, all higher order correlation functions approach equilibrium twice as fast.

DY 32.5 Wed 10:30 HÜL/S186

Free Cumulants and Full Eigenstate Thermalization from Boundary Scrambling — •Felix Fritzsch, Gabriel O. Alves, Michael A. Rampp, and Pieter W. Claeys — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Out-of-time-order correlation functions (OTOCs) represent important probes of quantum information dynamics and scrambling. We introduce a solvable many-body quantum circuit model, which we term boundary scrambling, for which the full dynamics of OTOCs is analytically tractable. These dynamics support a decomposition into free cumulants and unify recent extensions of the eigenstate thermalization hypothesis (full ETH) with predictions from random quantum circuit models. We moreover obtain exact expressions for higher-order correlations between matrix elements as predicted by the full ETH. The solvability is enabled by the identification of a higher-order Markovian influence matrix, capturing the effect of the full system on a local subsystem.

DY 32.6 Wed 10:45 HÜL/S186

Mechanism of Eigenstate Thermalization Breakdown — •Rafał Świetek[1,2,3] and Lev Vidmar[2,3] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany — [2]Department of Theoretical Physics, J. Stefan Institute, SI-1000 Ljubljana, Slovenia — [3]Department of Physics, Faculty of Mathematics and Physics, University of Ljubljana, SI-1000 Ljubljana, Slovenia

Establishing a common framework for ergodicity-breaking transitions has many potential applications and provides insight into the nature of non-ergodic phases. In this work, we show that the softening of fluctuations within the recently established fading ergodicity framework can be derived directly from the emergence of the Fermi Golden Rule (FGR), ultimately classifying fading ergodicity as manifestation of FGR physics in quantum many-body systems. We show that this framework identifies the width of the local density of states and the fractal nature of eigenstates in the unperturbed basis as building blocks for fading ergodicity. Furthermore, we argue that our theory can be also applied to integrability-breaking transitions, where the critical point drifts exponentially with system size to a singular point, providing a common framework for ergodicity breaking in RMT models and integrability-breaking in local Hamiltonians.

15 min. break

DY 32.7 Wed 11:15 HÜL/S186

Entanglement in bipartite systems with symmetry: coupled chaotic kicked Bose-Hubbard systems — •Jan Himmelsbach[1], Maximilian F.I. Kieler[1,2], and Arnd Bäcker[1] — [1]TU Dresden, Institut für Theoretische Physik, Dresden, Germany — [2]CESAM research unit, University of Liège, B-4000 Liège, Belgium

We study the eigenstate entanglement of a time-periodically driven Bose-Hubbard system in a bipartite setting with a tunable coupling between two subsystems. By incorporating the symmetry of the particle conservation and employing perturbation theory we find that the entanglement transition for varying coupling strength is described by a universal transition parameter. It turns out that the entanglement transition is governed by localization for the particle conservation symmetry and a thermalizing process between the subsystems.

DY 32.8 Wed 11:30 HÜL/S186

Dynamical Pictures for Growth of Entanglement and Decay of Correlators in U(1) Conserving Random Circuits — •Marco Lastres[1,2], Olexei I. Motrunich[3], and Sanjay Moudgalya[1,2] — [1]Technical University of Munich, School of Natural Sciences, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany — [3]Department of Physics, Caltech, Pasadena, CA, USA

We study the dynamics of random circuit models with a global $U(1)$ charge conservation law. Prior work showed that systems without conservation laws exhibit linear growth of entanglement, linked to domain wall dynamics in an effective ferromagnetic model. In contrast, rigorous upper bounds for $U(1)$-conserving systems indicate that diffusive charge transport constrains Rényi entropies to grow only diffusively as $\sqrt{t}$. We study the second Rényi entropy in $U(1)$-conserving random circuits by mapping its dynamics onto the low-energy physics of an effective interacting Hamiltonian. This approach explicitly demonstrates the microscopic mechanism which produces diffusive growth of entanglement in the effective replica model. We also show that the same effective model naturally captures the recently discovered subexponential decay of non-hydrodynamic correlations through a closely related mechanism. Further, we demonstrate that in a different regime this model can also describe the dynamics of entanglement in noisy free-fermion systems, which also exhibit diffusive entanglement growth, but through a different mechanism. Finally, we discuss extensions to other continuous symmetries and to higher Rényi entropies.

DY 32.9 Wed 11:45 HÜL/S186

Correspondence principle, dissipation, and Ginibre ensemble — •David Villaseñor, Hua Yan, Matic Orel, and Marko Robnik — CAMTP - Center for Applied Mathematics and Theoretical Physics, University of Maribor, Mladinska 3, SI-2000 Maribor, Slovenia, European Union

The correspondence between quantum and classical behavior has been essential since the advent of quantum mechanics. This principle serves as a cornerstone for understanding quantum chaos, which has garnered increased attention due to its strong impact in various theoretical and experimental fields. When dissipation is considered, quantum chaos takes concepts from isolated quantum chaos to link classical chaotic motion with spectral correlations of Ginibre ensembles. This correspondence was first identified in periodically kicked systems with damping, but it has been shown to break down in dissipative atom-photon systems [Phys. Rev. Lett. 133, 240404 (2024)]. In this contribution, we revisit the original kicked model and perform a systematic exploration across a broad parameter space, reaching a genuine semiclassical limit. Our results demonstrate that the correspondence principle, as defined through this spectral connection, fails even in this prototypical system. These findings provide conclusive evidence that Ginibre spectral correlations are neither a robust nor a universal diagnostic of dissipative quantum chaos.

DY 32.10 Wed 12:00 HÜL/S186

Quantum Mpemba effect from Stark localization — •Nico Albert[1], Masudul Haque[1], and Shovan Dutta[2] — [1]TU Dresden, Dresden, Germany — [2]Raman Research Institute, Bangalore, India

In the Mpemba effect a system prepared at a higher temperature cools down faster to a target equilibrium state than the same system prepared at a lower temperature. We investigate how quantum effects can influence the occurence of such an effect. As an example we consider a bosonic chain subject to a suitable onsite potential that is dissipatively cooled to its ground state, and find that Stark localization significantly enhances the Mpemba effect compared to analogous classical systems.

DY 32.11 Wed 12:15 HÜL/S186

Robustness of interference-caged QMBS under real-space local perturbations: analysis through the Fock-space local interference pattern — •Tao-Lin Tan[1] and Yi-Ping Huang[1,2,3] — [1]Department of Physics, National Tsing Hua University, Hsinchu 30013, Taiwan — [2]Physics Division, National Center for Theoretical Sciences, Taipei 10617, Taiwan — [3]Institute of Physics, Academia Sinica, Taipei 115, Taiwan

Quantum many-body scars (QMBS) represent a notable violation of the eigenstate thermalization hypothesis (ETH), hosting non-thermal eigenstates embedded in an otherwise thermal spectrum. Despite recent progress, a systematic understanding of their stability under real-space local (r-local) perturbations remains lacking. Building on recent insights of interference-caged quantum many-body scars (ICQMBS), protected by exact many-body destructive interference on Fock-space graphs, we develop an interference-based diagnostic to assess the robustness of ICQMBS in various lattice Hamiltonians. Applying this framework to quantum link models (QLM) and quantum dimer models (QDM), we analyze how r-local perturbations deform the underlying Fock-space local (f-local) interference structure, thereby identifying heuristic mechanisms that stabilize or destabilize ICQMBS. Our results broaden the applicability of the interference-based perspective beyond previously studied models and provide practical criteria for evaluating the persistence of ICQMBS in experimentally relevant Hamiltonians.

DY 32.12 Wed 12:30 HÜL/S186

Scrambling and Scarring in Topological Materials — •Nicholas Sedlmayr, Dominik Szpara, and Szczepan Głodzik — Institute of Physics, M. Curie-Skłodowska University, 20-031 Lublin, Poland

Topological insulators and superconductors have recently attracted considerable attention, and many different theoretical tools have been used to gain insight into their properties. Here we investigate how perturbations can spread through exemplary one-dimensional topological insulators and superconductors using out-of-time ordered correlators. Out-of-time ordered correlators are often used to consider how information becomes scrambled during quantum dynamics. The wavefront of the out-of-time ordered correlator can be ballistic regardless of the underlying system dynamics, and here we confirm that for topological free fermion systems the wavefront spreads linearly at a characteristic butterfly velocity. We pay special attention to the topologically protected edge states, finding that information can become trapped in the edge states and essentially decoupled from the bulk, surviving for relatively long times - a form of scarring. We further investigate what happens due to the chiral and helical edge modes of two dimensional topological models. The information travels around the edge, carried by the edge mode, but again is not scrambled over very long time scales.

DY 33: Statistical Physics of Biological Systems I (joint session DY/BP)

Time: Wednesday 9:30–12:45 Location: ZEU/0114

DY 33.1 Wed 9:30 ZEU/0114

Metastability in the mixing/demixing of two species with reciprocally concentration-dependent diffusivity — •Benjamin Lindner[1,2], Alexander B. Neiman[3,4], and Xiaochen Dong[2] — [1]Department of Physics, Humboldt University Berlin, Berlin, Germany — [2]Bernstein Center for Computational Neuroscience Berlin — [3]Department of Physics and Astronomy, Ohio University, Athens, OH, United States — [4]Neuroscience Program, Ohio University, Athens, OH, United States

It is known that two species of diffusing particles can separate from each other by a reciprocally concentration-dependent diffusivity: the presence of one species at a certain location amplifies the diffusion coefficient of the respective other one in this location, causing the two densities of particles to separate spontaneously. In a minimal model, Schimansky-Geier et al. (2021) observed this with a quadratic dependence of the diffusion coefficient on the density of the other species. Here, we consider a sigmoidal dependence in the form of a logistic function on the other particle's density averaged over a finite sensing radius. The sigmoidal dependence leads to a new regime in which a homogeneous disordered (well-mixed) state and a spontaneously separated ordered (demixed) state coexist, forming two long-lived metastable configurations. In systems with a finite number of particles, random fluctuations induce repeated transitions between these two states. By tracking an order parameter that distinguishes mixed from demixed phases, we measure the corresponding mean residence in each state.

DY 33.2 Wed 9:45 ZEU/0114

Phase separation in a mixture of proliferating and motile active matter — Lukas Hupe[1], Joanna M. Materska[2], David Zwicker[1], Ramin Golestanian[1,3], Bartlomiej Waclaw[2,4], and •Philip Bittihn[1] — [1]MPI for Dynamics and Self-Organization, Göttingen, Germany — [2]Dioscuri Centre for Physics and Chemistry of Bacteria, Institute of Physical Chemistry, Warsaw, Poland — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, United Kingdom — [4]School of Physics and Astronomy, The University of Edinburgh, United Kingdom

Proliferation and motility are ubiquitous drivers of activity in biological systems. Here, we study a dense binary mixture of motile and proliferating particles with exclusively repulsive interactions, where homeostasis in the proliferating subpopulation is maintained by pressure-induced removal. Using large-scale simulations, we show that this heterogeneous active matter undergoes spontaneous phase separation at high density and weak enough self-propulsion. We recapitulate this behavior using an effective Active Brownian Particle model that incorporates the emergent effects of the proliferating matrix on motile particles: enhanced diffusion, renormalized self-propulsion, reduced persistence, and an effective attraction between motile particles. Our results establish a new type of phase transition and reveal how mechanical activity from growth can mediate non-equilibrium interactions and fluctuations. This mechanism provides a conceptual framework to reinterpret the physics of dense pattern-forming cellular populations, such as bacterial colonies or tumors, as systems of mixed active matter.

DY 33.3 Wed 10:00 ZEU/0114

Reentrant phase separation and critical behaviour in cellular aggregates — •Subhadip Chakraborti[1,2] and Vasily Zaburdaev[1,2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Max-Planck-Zentrum für Physik und Medizin, Erlangen, Germany

We study pili-mediated bacterial colonies as a paradigm for attractive cellular aggregates. The interplay between inherent motility and intercellular attraction leads to a reentrant phase separation between attraction-induced and motility-induced phase separation separated by a homogenous state. Using finite-size scaling of the largest cluster we characterise these two transitions and thereby determine the associated critical lines in terms of the control parameters - density, pili lifetime and attraction strength. We further evaluate critical exponents corresponding to two transitions in the parameter space and from their relations determine the respective universality classes.

DY 33.4 Wed 10:15 ZEU/0114

Phase separation with non-local interactions — Filipe C. Thewes, Yicheng Qiang, Oliver W. Paulin, and •David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Phase separation takes place in many complex systems, notably biological cells. While simple theories predict coarsening until only macroscopically large phases remain, concrete models often exhibit patterns with finite length scales, e.g., caused by chemical reactions, elasticity, membrane interactions, or charge. To unify such models, we here propose a field theory that combines phase separation with non-local interactions. If these interactions are long-ranged, they generally suppress coarsening, whereas systems with non-local short-range interactions additionally exhibit a continuous phase transition to patterned phases. Only the latter system allows for the coexistence of homogeneous and patterned phases, which we explain by mapping to the conserved Swift–Hohenberg model. Taken together, our generic model provides a framework that unifies similar phenomena observed in many complex phase-separating systems.

DY 33.5 Wed 10:30 ZEU/0114

Motile response of bacterial swimmers towards competing chemical signals — •Agniva Datta[1], Robert Grossmann[1], and Carsten Beta[1,2] — [1]Institute of Physics and Astronomy, University of Potsdam, Germany — [2]Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kakuma-machi, Kanazawa 920-1192, Japan

Understanding how bacteria navigate in bulk fluid has gained significant interest in the field of active matter and random transport processes in the last few decades. We use the soil bacterium *Pseudomonas putida* as our model organism, the motility pattern of which is characterized by persistent runs, interrupted by

random reorientation events (turns). In addition to this, bacteria sense chemical signals and adapt their motility pattern accordingly. Recent experiments show that bacteria can change the frequency of turns (duration of runs) depending on the concentration of nutrients as well as auto-inducer molecules that they themselves produce in the medium. This complex interplay of the dynamics of nutrients, auto-inducers and bacterial density may lead to dynamic instabilities. Combining experiments and theory, we are elucidating the dynamics of bacteria in the presence of these two competing signaling factors.

DY 33.6 Wed 10:45 ZEU/0114

Anisotropic hierarchy decides the fate of an amorphous droplet — •Andrey Zelenskiy, Pietro Caracciolo di Torella, and Martin Lenz — LPTMS, CNRS, Orsay, France

The classical description of ordering, from theories of phase transitions to classical nucleation, typically emphasizes a direct transition from disorder to order. Yet, the majority of systems in nature deviate from this simple description, and often choose indirect pathways to ordering. In particular, complex structures often form via disordered or partially ordered intermediates – the amorphous precursors.

We present a model of self-assembling patchy particles, where the interactions are characterized by a hierarchy of geometric competitions. By tuning the anisotropy, we can stabilize a variety of aggregate morphologies, including crystals, gels, lamellar sheets, and fibers. However, due to geometric frustration, self-assembly proceeds via a dense amorphous intermediate, where the anisotropic interactions are largely averaged out. Our simple framework based on an anisotropic hierarchy sheds light on this non-classical mechanism of particle assembly, and provides a platform for new experimental principles of complex structure design.

15 min. break

DY 33.7 Wed 11:15 ZEU/0114

Improving neuronal information transmission with pathway splitting — •Kolja Klett[1,2] and Benjamin Lindner[1,2] — [1]Humboldt University, Berlin — [2]Bernstein Center for Computational Neuroscience, Berlin

In many organisms sensory information can take different neuronal paths from sensory cells to destinations in the brain. These paths can be made up of neurons serving distinct functions. Often, pathways consisting of neurons coding the increase (ON) or decrease (OFF) of a signal are observed which have be found to improve the transmission static signals. Here, we consider a simple network of spiking ON and OFF neurons to study the effects of pathway splitting on the transmission of dynamic signals. To that end, we use the coherence function as a frequency-resolved measure of informations transmission. We relate the information transmission of the whole network to that of the constituting neurons by employing response theory leading to approximate relations for the coherence function. For a simple white noise driven integrate-and-fire model of spiking neurons, we find an optimal mixture of ON and OFF neurons which maximizes the coherence function over a broad frequency range. The effect can be attributed to the nonlinear response of the neurons that only becomes relevant for sufficiently strong stimuli.

DY 33.8 Wed 11:30 ZEU/0114

Population sparseness in recurrent spiking neural networks — •Jakob Stubenrauch[1,2], Naomi Auer[3], Richard Kempter[2,3,4], and Benjamin Lindner[1,2] — [1]Physics Department HU Berlin — [2]Bernstein Center for Computational Neuroscience Berlin — [3]Institute for Theoretical Biology HU Berlin — [4]Einstein Center for Neurosciences Berlin

It is long known that in association tasks for neural networks, the fraction of active neurons in patterns to be associated plays an important role. Specifically, the number of patterns that can be simultaneously remembered grows when the information content per pattern is decreased. In binary networks, this content can be constrained by the population sparseness (one minus fraction of active neurons). For neurons with graded activity, population sparseness can be quantified by the Treves-Rolls measure or by the Gini coefficient. Here, we present results on the spontaneous and evoked population sparseness in different variants of recurrent neural networks of integrate-and-fire neurons. We find that the type of competition between neurons plays an important role and discuss that neurons in fully disordered networks can, in a mean field limit, only compete across a low-dimensional effective inhibition hub. We showcase the relevance of our findings for association tasks in spiking neural networks.

DY 33.9 Wed 11:45 ZEU/0114

Minority-triggered reorientation yields macrocscopic cascades and maximal responsiveness in a Vicsek swarm — •Simon Syga[1], Chandraniva Guha Ray[2,3,4], Josué Manik Nava Sedeño[5], Fernando Peruani[6], and Andreas Deutsch[1] — [1]Technische Universität Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany — [4]Center for Systems Biology Dresden, Germany — [5]Universidad Nacional Autónoma de México, Mexico City, Mexico — [6]CY Cergy Paris Université, Paris, France

Collective motion in animals and cells often exhibits bursty reorientations and scale-free velocity correlations associated with criticality. This ensures that information, like the presence of predators, quickly spreads through a group, ensuring an adequate response. To explain this phenomenon, we introduce a simple, biologically plausible mechanism, a minority-triggered reorientation rule: when local order is high, agents sometimes follow a strongly deviating neighbor instead of the majority. This generates heavy-tailed cascades of reorientations and macroscopic spatial correlations over broad parameter ranges, without fine-tuning. Our mechanism preserves cohesion while markedly enhancing collective responsiveness: localized directional cues elicit amplified, group-level reorientation. Our results provide a parsimonious, biologically interpretable route to critical-like fluctuations and high susceptibility in collective motion.

DY 33.10 Wed 12:00 ZEU/0114

Noise structure shapes transitions in cell differentiation processes — •Sara Oliver-Bonafoux[1], Javier Aguilar[1,2], Tobias Galla[1], and Raúl Toral[1] — [1]Institute for Cross-Disciplinary Physics and Complex Systems IFISC (CSIC-UIB), Campus UIB, Palma de Mallorca, Spain — [2]Laboratory of Interdisciplinary Physics, Department of Physics and Astronomy "G. Galilei", University of Padova, Padova, Italy

Stochastic differential equations provide a natural framework to describe dynamical systems influenced by random fluctuations, but they require specifying the structure of the noise term (e.g., additive, demographic, or environmental). In biological systems, the choice of an appropriate noise description remains a matter of debate. Understanding how stochastic fluctuations shape biological dynamics is a central challenge in biophysics and systems biology.

We address this question in the context of a model of cell differentiation, the process by which an unspecialised cell commits to a specialised cell type with a specific structure and function. Both the undifferentiated state and differentiated states are stable, and transitions between them are induced by noise. A recent study has provided theoretical evidence that different noise structures can give rise to substantially distinct differentiation paths. Here, we use stochastic bridges to sample differentiation paths under different types of noise and for varying noise intensity.

DY 33.11 Wed 12:15 ZEU/0114

Darwin's paradox of the peacock tail: a stochastic perspective on sexual selection — •Ian Magalhaes Braga — CASUS, Gorlitz, Germany

Many species show male traits that are extravagant, costly, and seemingly disadvantageous, yet they evolve and persist. Classical explanations especially deterministic versions of Fisher's runaway struggle to fully account for this pattern, mostly because they ignore the inherent randomness of evolutionary processes. In this work, I propose that stochasticity is not a secondary detail but the key element that reshapes the dynamics of trait preference coevolution. Treating sexual selection at the microscopic, probabilistic level reveals a simple but unexpected idea: in finite populations, a costly trait can actually support the evolution of female preference. I refer to this effect as the cost advantage. The basic picture is that stochastic fluctuations change the timing of fixation events, creating conditions under which preference benefits from the very cost that penalizes the trait. Using large-scale simulations across multiple evolutionary architectures, I show that this behavior is general and does not depend on specific modelling choices. The results suggest that costly ornaments are not paradoxical after all they may simply reflect the true stochastic nature of evolutionary change.

DY 33.12 Wed 12:30 ZEU/0114

Local equations for the generalized Lotka-Volterra model on sparse asymmetric graphs — •David Machado Pérez[1,2,3], Pietro Valigi[1], Tommaso Tonolo[4,5], and Maria Chiara Angelini[6] — [1]Physics Department, Sapienza University of Rome, Rome I-00185, Italy — [2]Department of Theoretical Physics, Physics Faculty, University of Havana. CP10400, Havana, Cuba — [3]CNR-NANOTEC, Rome Unit, Rome I-00185, Italy — [4]Gran Sasso Science Institute, 67100 L'Aquila, Italy — [5]INFN-Laboratori Nazionali del Gran Sasso, 67100 Assergi (AQ), Italy — [6]INFN, Sezione di Roma I, 00185 Rome, Italy

Real ecosystems are characterized by sparse and asymmetric interactions, posing a major challenge to theoretical analysis. We introduce a new method to study the generalized Lotka-Volterra model with stochastic dynamics on sparse graphs. By deriving local Fokker-Planck equations and employing a mean-field closure, we can efficiently compute stationary states for both symmetric and asymmetric interactions. We validate our approach by comparing the results with the direct integration of the dynamical equations and by reproducing known results and, for the first time, we map the phase diagram for sparse asymmetric networks. Our framework provides a versatile tool for exploring stability in realistic ecological communities and can be generalized to applications in different contexts, such as economics and evolutionary game theory.

DY 34: Focus Session: Fluids with Broken Time-Reversal Symmetry – Odd/Hall Viscosity Between Active Matter and Electron Flows

Viscosity is a fundamental property of fluids and an important physical quantity characterizing resistance to flow and energy dissipation. While time-reversal symmetry holds in conventional fluids, its violation can lead to striking phenomena, one of which is the emergence of a dissipationless transport coefficient called odd viscosity. Odd viscosity, also known as Hall viscosity, was originally proposed by Avron et al., as a quantized observable in electron fluids with a magnetic field. Since this seminal work, odd viscosity has been studied in various systems, such as 2D electron fluids, fractional Hall fluids, and ionic crystals. Although odd viscosity was also known in plasma physics, it was largely overlooked in fluid dynamics, mainly due to the technical challenges involved in its experimental realization. In recent years, however experiments in driven colloidal systems led to a surge of interest in odd viscosity in the active matter community. In parallel, our understanding of odd phenomena was advanced by continuum theories with many novel exact solutions. Major open questions in the field include the microscopic mechanisms that lead to odd viscosity, its experimental manifestations, the transition from two- to three-dimensional systems, and the effect of odd viscosity on hydrodynamic phenomena at different length scales, ranging from microrheology to turbulent flows. This Focus Session will connect the wider condensed matter and active matter physics communities with recent theoretical advances in odd viscosity. It is organized along with a Symposium on the same topic.

Organized by Yuto Hosaka (Göttingen) and Ewelina M. Hankiewicz (Würzburg)

Time: Wednesday 9:30–12:30 Location: ZEU/0160

Invited Talk DY 34.1 Wed 9:30 ZEU/0160

Active turbulence and odd viscosity in a colloidal chiral active system in bulk and in patterned environments — Joscha Mecke[1,2], Yongxiang Gao[1], and •Marisol Ripoll[2] — [1]Institute for Advanced Study, Shenzhen University, Shenzhen, China — [2]Institute for Advanced Simulation, Forschungszentrum Jülich, Jülich, Germany

Experiments for a chiral active fluid composed of a carpet of standing and spinning colloidal rods are compared with simulations for synchronously rotating hard discs in a hydrodynamic explicit solvent [1]. The emergence of multi-scale eddies, with features of self-similar dynamics, indicates the existence of active turbulence, while the particles accumulation in the centre of the vortices allows the quantification of the system odd viscosity. The existence of a non-negligible substrate friction can be shown to be responsible of the truncation of the energy spectra and the related reduction of the vortex size [2], and the interaction with fixed obstacles shows to originate a flow opposite to the rotation direction which induces a pinning vortex effect [3].

[1] J. Mecke, Y. Gao, C. Ramirez-Medina, D. Aarts, G. Gompper and M. Ripoll, Comm. Phys. 6 (2023), 324 [2] J. Mecke, Y. Gao, G. Gompper and M. Ripoll, Comm. Phys. 7 (2024), 332 [3] J. Mecke, Y. Gao and M. Ripoll, Phys. Fluids 37 (2025), 112016

DY 34.2 Wed 10:00 ZEU/0160

From Gels to Rotors: Tunable Chiral Phases in Odd Colloidal Fluids — •Dennis Schorn[1], Stijn van der Ham[2], Suvendu Mandal[1], Benno Liebchen[1], and Hanumantha Rao Vutukuri[2] — [1]Institute for Condensed Matter Physics, Technische Universität Darmstadt, 64289 Darmstadt, Germany — [2]MESA+ Institute, University of Twente, 7500 AE Enschede, The Netherlands

Starfish embryos aggregate into chiral crystals exhibiting odd elasticity (Tan *et al.* Nature **607**, 287 (2022)). Similar structures have been recently observed in externally driven magnetic colloids. In this talk, I present experiments and simulations of binary mixtures of magnetic spinners and passive colloids. We develop a model to predict the phase diagram of the system, which comprises four distinct phases that can be systematically reproduced in experiments. In particular, our simulations and experiments reveal a phase in which the passive particles form a gel-like network, with significant holes filled with self-organized, rotating chiral clusters composed of spinners. This phase can be reversed by changing the system's composition and magnetic field strength, resulting in a spanning spinner phase with embedded counter-rotating chiral clusters made of passive colloids. Both phases exhibit odd viscosity and diffusivity, whose magnitudes depend sensitively on spinner fraction and magnetic field strength. Our system may open the route towards a new type of viscoelastic active chiral matter involving nonreciprocal interactions between both species.

DY 34.3 Wed 10:15 ZEU/0160

Odd Droplets: Fluids with Odd Viscosity and Highly Deformable Interfaces — •Hugo França and Maziyar Jalaal — Van der Waals-Zeeman Institute, Institute of Physics, University of Amsterdam, Science Park 904, Amsterdam, 1098XH, The Netherlands

Flows with deformable interfaces are commonly controlled by applying an external field or modifying the boundaries that interact with the fluid, but realizing such solutions can be demanding or impractical in various scenarios. Here, we demonstrate that fluids with broken symmetries can self-control their mechanics. We present a continuum model of a viscous fluid with highly deformable interfaces subject to capillary stresses. Our model features odd viscosity, a parity-violating property that emerges in chiral fluids. Using direct numerical simulations, we focus on the impact of an odd droplet on a superhydrophobic surface. By numerically solving the full conservation equations, we are able to study this highly non-linear problem hardly accesible through analytical methods. We demonstrate that odd viscosity dramatically disrupts conventional symmetric spreading by inducing asymmetric deformations and chiral flow patterns. Our analysis reveals a variety of dynamic regimes, including leftward and rightward bouncing, as well as rolling, depending on the relative strength of the odd viscosity. Our work illustrates that regulating odd viscosity provides a promising framework for controlling multiphase flows and designing functional metamaterials with tailored fluidic properties.

DY 34.4 Wed 10:30 ZEU/0160

The notion of dissipation in three-dimensional fluids with odd viscosity — •Jeffrey Everts[1,2], Laura Meissner-Oszer[1], and Bogdan Cichocki[1] — [1]Institute of Theoretical Physics, Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland — [2]Institute of Physical Chemistry, Polish Academy of Sciences, 01-224 Warsaw, Poland

Odd viscosity is a transport coefficient that occurs in fluids where the constituent particles carry a non-trivial spin angular momentum. Exemplary realisations in this context are chiral active fluids and electronic systems in an external magnetic field. Due to the symmetry properties of the resulting viscosity tensor it is often stated in the literature that odd viscosity does not contribute to viscous dissipation. In this talk, I will explicitly demonstrate that this statement is incorrect for incompressible odd viscous fluids in three spatial dimensions. In this case, the fluid flow velocity can be affected by odd viscosity, which gives a non-trivial contribution to the dissipated power. As an example, we will show by explicit calculation how odd viscosity contributes to viscous dissipation for a spherical (colloidal) particle immersed in an odd viscous fluid. Furthermore, we will make general statements for viscous dissipation by generalising the Helmholtz minimum dissipation theorem -which is well known for ordinary Stokesian fluids - to fluids with odd viscosity.

DY 34.5 Wed 10:45 ZEU/0160

Exact flow patterns in systems with odd viscosity — •Laura Meissner-Oszer[1], Bogdan Cichocki[1], and Jeffrey Everts[1,2] — [1]nstitute of Theoretical Physics, Faculty of Physics, University of Warsaw, Pasteura 5, 02-093 Warsaw, Poland — [2]Institute of Physical Chemistry, Polish Academy of Sciences, 01-224 Warsaw, Poland

Chiral active fluids are composed of self-spinning particles with a non-trivial spin-angular momentum that is maintained through a continuous injection of energy at the microscopic scale. Due to this property, there are antisymmetric contributions in the viscosity tensor, which are called odd viscosity. In the low Reynolds-number regime we show that there is a uniqueness theorem for such flows akin to ordinary Stokesian fluids. In order to analyse the effect of odd viscosity on flow patterns of a three-dimensional incompressible fluid in the creeping flow regime, we focus on a simple model of a chiral active fluid described by one shear viscosity and one odd viscosity. By considering the Green's function of the linear momentum-balance equation in the presence of a point force, we derive exact closed-form analytical expressions for the velocity and pressure field of the fluid around a translating and rotating spherical particle. Furthermore, we highlight specific features of such flows due to the presence of odd viscosity

and we demonstrate how the direction of spin momentum affects the qualitative features of the streamlines.

15 min. break

DY 34.6 Wed 11:15 ZEU/0160

Resonances in Odd Viscoelastic Materials — •Julius Kiln and Alexander Mietke — Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford, United Kingdom

Active matter describes materials that are powered by microscopic sources of energy. This injection of energy can lead to a wide variety of phenomena and unconventional material properties, including odd elasticity and odd viscosity. Despite recent analytical examination of these systems, a widely applicable method for solving force balance equations for odd materials on finite domains was so far not available.

The Papkovich-Neuber (PN) ansatz, introduced almost a hundred years ago, has proved an invaluable method for solving the force balance equation of a Stokes fluid and of a passive linearly elastic solid. We generalise this idea and find an ansatz for odd solids and fluids that reduces to the known PN solutions in the limit of vanishing odd material parameters. Altogether, this provides a new and versatile method for finding analytical solutions to this class of problems. Using this result, we construct the displacement field for an odd elastic material in circular domain under both displacement and stress boundary conditions. Further extending this method to write displacement and flow solutions of an odd viscoelastic material explicitly, we study the response to oscillatory forcing at the boundary, finding resonances at certain forcing frequencies even in an overdamped system. Finally, based on these new PN solutions, we propose rheological protocols for measuring odd material properties.

DY 34.7 Wed 11:30 ZEU/0160

Edge currents shape condensates in chiral active matter — •Boyi Wang[1,2], Patrick Pietzonka[4], and Frank Jülicher[1,2,3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Center for Systems Biology Dresden, Dresden, Germany — [3]Cluster of Excellence Physics of Life, TU Dresden, Germany — [4]SUPA, School of Physics and Astronomy, University of Edinburgh, Edinburgh, United Kingdom

Chiral active matter, which breaks both parity symmetry and detailed balance, is widespread in living systems. Here, we introduce a minimal two-dimensional chiral active Ising model by incorporating stochastic, biased local rotations. At low temperatures, the system coarsens into condensates with chiral orientations and faceted, crystal-like shapes rather than circular ones observed under Kawasaki dynamics. The interfaces align at characteristic angles to the lattice axes and support persistent, unidirectional, angle-dependent edge currents.

To generalise these results, we develop a continuum theory by adding an active edge-current term to Model B. An edge current with n-fold symmetry produces condensates with corresponding n-fold polygonal shapes. In the sharp-interface limit, we construct an effective active surface potential that predicts the steady-state condensate geometry, consistent across both the lattice model and the continuum description.

Our results reveal how local chiral activity generates global edge currents and demonstrate their fundamental role in governing phase separation and interfacial dynamics in chiral active systems.

DY 34.8 Wed 11:45 ZEU/0160

A mobility based approach to self diffusion in odd-mobile systems — •Filippo Faedi and Abhinav Sharma — University of Augsburg

Odd-diffusive systems, defined by antisymmetric diffusion tensors, display unusual dynamics including enhanced self-diffusion due to interactions, oscillatory force autocorrelation functions in over-damped systems, and reversal of particle mobility. This work introduces a mobility-based approach by externally driving particles with constant forces, uncovering profound transport anomalies. We demonstrate an inverted density wake around a driven tracer, where increasing oddness reverses collision effects, reducing effective friction and enhancing mobility. Using fluctuation-dissipation, mobility-derived self-diffusion confirms prior findings, providing a unified view of interaction-induced anomalous dynamics in chiral media.

DY 34.9 Wed 12:00 ZEU/0160

Exceptional points, chirality and entropy production in nonreciprocal polar active matter — Kim L. Kreienkamp and •Sabine H. L. Klapp — Institut für Physik, Technische Universität Berlin, Germany

Non-reciprocal couplings significantly impact the collective dynamics of mixtures. A particularly striking consequence of such couplings is the spontaneous emergence of time-dependent phases that break parity-time symmetry. Here, we study a paradigmatic model of a non-reciprocal polar active mixture by combining field-theoretical analyses and particle-based simulations. When different species have opposing alignment tendencies, flocking states with spontaneously broken rotational symmetry transform into chiral states characterized by a rotating polarization direction. At the field-theoretical level, the transition to these parity-time-symmetry-breaking chiral states is indicated by so-called exceptional points. We demonstrate that these theoretical concepts have clear counterparts in particle-based systems [1]: we observe chimera-like states with coexisting locally synchronized and disordered regions, and find that both the spontaneous chirality and the entropy production rate [2] peak at coupling strengths corresponding to the exceptional points. Our results highlight the diverse effects of non-reciprocity across different scales.

[1] K. L. Kreienkamp and S. H. L. Klapp, Communications Physics **8**, 307 (2025)

[2] K. L. Kreienkamp and S. H. L. Klapp, arXiv:2508.05209 (2025)

DY 34.10 Wed 12:15 ZEU/0160

The chiral random walk: A model for odd transport on the lattice — Jan Wójcik[1] and •Erik Kalz[2] — [1]Institute of Theoretical Physics and Astrophysics, University of Gdánsk, 80-308 Gdánsk, Poland — [2]Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam, Germany

We present a model for an isotropic chiral random walk on a lattice. Inspired by the quantum random walk framework, we equip the walker with an internal degree of freedom representing chirality and show, both numerically and analytically, that this model resembles odd transport properties on the continuum level. Chirality further acts as a control parameter, and the model resembles unitary transport in the strong-chirality regime. Building on established results from Quantum Random Walk theory, we analyse features such as topologically protected transport in this limit. We find that this qualitative persists also into the dissipative regime, allowing us to theoretically ground edge-transport phenomena, characteristics of dissipative odd systems. We illustrate our approach in spatially confined geometries and in systems with random chirality.

DY 35: Focus Session: Water – from Atmosphere to Space IV (joint session CPP/DY)

Time: Wednesday 9:30–10:45 Location: ZEU/0260

Topical Talk DY 35.1 Wed 9:30 ZEU/0260

Synchrotron X-Ray Studies on Structural Transitions in Water and Alcohol containing Ice Analogues — •Christina M. Tonauer — Institute of Physical Chemistry, University of Innsbruck, Austria — Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany

To this date, 21 different crystalline and at least 3 distinct amorphous forms of water ice have been discovered. In addition to the structural versatility of pure water ice phases, water forms solid guest-host systems, so-called 'clathrate hydrates' where water builds cage-like structures around guest molecules of various sizes (e.g., Ar, CO2, methane, ethanol).

Ices in space are exposed to various forms of (external) stress, e.g., impacts, cosmic rays, UV/Vis radiation as well as endogenous thermal fluctuations, thereby undergoing structural changes. By studying such structural transitions in ice analogues upon heating (and/or radiation), conclusions can be drawn about the conditions at various extraterrestrial environments.

Therefore, we here present temperature-resolved wide- and small-angle synchrotron X-ray scattering data of vapor-deposited water-ethanol mixtures of various concentrations, collected at PETRA 3/DESY. While the SAXS data allows for monitoring of changes of the morphology of the microporous sample, the WAXS data reveals the formation sequence of two different hydrates, offering new insights into the crystallisation of astrophysical ices.

DY 35.2 Wed 10:00 ZEU/0260

Water in exoplanetary atmospheres: from molecular spectra to Water Worlds — •Sergey Yurchenko — Department of Physics and Astronomy, University College London, Gower Street, WC1E 6BT London, United Kingdom

Water vapour is one of the key tracers of atmospheric physics and chemistry on exoplanets, from hot Jupiters to temperate sub-Neptunes and so-called Water Worlds. In this contribution I will give an overview of the role of H_2O across this diversity of atmospheres, focusing on how we infer its presence from transmission and emission spectra. I will review both low-resolution transit spectroscopy and high-resolution cross-correlation techniques, and show how they are applied to data from space- and ground-based facilities, including JWST, Hubble and VLT, as well as future observations with the ELT and ESA's Ariel mission. Special emphasis will be placed on the way clouds and hazes imprint themselves on the observed spectra.

I will summarise the current observational status of water detections and non-detections – including recent and sometimes controversial claims for habitable-

zone planets. A central theme of the talk will be the importance of accurate laboratory and theoretical data for water and related species. I will highlight how comprehensive molecular line lists and cross sections from the ExoMol and HITRAN databases, together with other laboratory measurements, underpin the modelling and retrieval of exoplanet spectra over a wide range of temperatures, pressures and compositions, thereby linking detailed molecular physics to the emerging picture of water in exoplanetary atmospheres.

DY 35.3 Wed 10:15 ZEU/0260

Structures of Ices by Quantum Crystallography and PDF — Krzysztof Wozniak[1], •W. Sławiński[1], G. Łach[2], R. Gajda[1], M. Chodkiewicz[1], P. Rejnhardt[1], M. Arhangelskis[1], Ch. Ridley[3,4], and C. L. Bull[3,5] — [1]Deptm. of Chem., Univ. of Warsaw,Poland — [2]Deptm. of Phys., Univ. of Warsaw, Poland — [3]ISIS Neutron and Muon Source, STFC, RAL, Harwell Campus, UK. — [4]Spallation Neutron Source, Oak Ridge Nat. Lab., Oak Ridge, Tennessee 37830, USA — [5]Univ. of Edinburgh, UK.

Ice is the solid form of water (H*O). The most familiar form of ice is the hexagonally structured ice Ih. However, water can crystallize into at least 21 distinct phases, unique in structure, depending on T and P and route of formation. In this contribution, will present details of structures of ices (VI[3], VII[1,2], Ih [4]) obtained with quantum-crystallographic Hirshfeld Atom Refinement against single crystal X-ray and electron diffraction data. We will also present the first quantitative characterisation of disorder in D2O ice VII and VI obtained through a combination of Pair Distribution Function (PDF) analysis, Reverse Monte Carlo (RMC) modelling, and high-pressure neutron scattering. Our results provide a detailed decomposition of both the average and local atomic structures of Ice VII, revealing a previously unquantified level of structural disorder. References [1] R. Gajda et al., IUCRJ, 12(3) (2025) 288-294; [2] W. A. Sławiński et al., Hidden complexity in D2O Ice VII, Acta Mat., (2025) submitted; [3] M. L. Chodkiewicz et al., IUCRJ, 9 (2022) 573-579; [4] M. L. Chodkiewicz et al., IUCRJ, 11(5) (2024) 730-736.

DY 35.4 Wed 10:30 ZEU/0260

Water dynamics in conductive PEDOT:PSS/cellulose nanocomposite films in dependence of relative humidity and temperature — •Lucas Kreuzer[1], Marie Betker[2], Marcell Wolf[1], Jacques Ollivier[3], Daniel Söderberg[4], and Stephan V. Roth[2,4] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), TUM, Garching, Germany — [2]Deutsches Elektronen Synchrotron, Hamburg, Germany — [3]Institut Laue-Langevin, Grenoble, France — [4]Department of Engineering Mechanics, Royal Institute of Technology KTH, Stockholm, Sweden

PEDOT:PSS is a conductive and water-soluble polymer blend widely used in organic electronics. However, pure PEDOT:PSS films absorb significant amounts of water, causing swelling, degradation, and eventually a decrease in conductivity. Integrating PEDOT:PSS with cellulose nanofibrils (CNFs) overcomes these issues by limiting water absorption and enhancing mechanical stability. However, a minor amount of water is still absorbed, leading to a change in film morphology: high humidity induces de-wetting of PEDOT:PSS from the CNFs, reducing conductivity, whereas drying generally leads to a re-wetting of PEDOT:PSS, thereby restoring conductivity. To investigate further the role of water, quasi-elastic neutron scattering is applied, which reveals two water species in the films: mobile bulk water and slower hydration water. Upon drying, bulk water is released completely, while hydration water remains in the films, supporting the re-wetting of PEDOT:PSS. Moreover, at higher temperatures, different diffusive behavior was found for bulk and hydration water.

DY 36: Focus Session: Water – from Atmosphere to Space V (joint session CPP/DY)

Time: Wednesday 11:00–12:00 Location: ZEU/0260

DY 36.1 Wed 11:00 ZEU/0260

Scalable Machine Learning Model for Energy Decomposition Analysis in Aqueous Systems — •Thomas Kühne — CASUS/HZDR, Görlitz, Germany

Energy decomposition analysis (EDA) based on absolutely localized molecular orbitals provides detailed insights into intermolecular bonding by decomposing the total molecular binding energy into physically meaningful components. Here, we develop a neural network EDA model capable of predicting the electron delocalization energy component of water molecules, which captures the stabilization arising from charge transfer between occupied absolutely localized molecular orbitals of one molecule and the virtual orbitals of another. Exploiting the locality assumption of the electronic structure, our model enables accurate prediction of electron delocalization energies for molecular systems far beyond the size accessible to conventional density functional theory calculations, while maintaining its accuracy. We demonstrate the applicability of our approach by modeling hydration effects in large molecular complexes, specifically in metal-organic frameworks.

DY 36.2 Wed 11:15 ZEU/0260

Advances in absolute-scale electronic structure measurements of liquid water and aqueous solutions — •Florian Trinter — FHI Berlin, Germany

Recent advances in liquid-jet photoelectron spectroscopy (LJ-PES) have enabled the precise determination of absolute electronic energetics of liquid water and aqueous solutions, both in the bulk and at interfaces. By implementing refined vacuum and Fermi-level referencing procedures, rooted in condensed-matter concepts, vertical ionization energies (VIEs) and solution work functions can now be measured with high accuracy. We show that binding energy determinations near the ionization threshold are strongly influenced by quasi elastic electron scattering and indirect ionization processes. Vibrational excitation and autoionization via super-excited states lead to spectral distortions at electron kinetic energies below ~14 eV, necessitating careful data interpretation to extract intrinsic properties. Applying these methods to neat water and aqueous solutions of sodium iodide (NaI) and tetrabutylammonium iodide (TBAI), we reveal solute-specific effects: NaI primarily alters water's bulk structure, increasing the $1b_1$ binding energy with concentration, while TBAI affects surface potentials through interfacial dipole formation, leading to an apparent binding energy decrease. Additionally, we determine the work function of neat water as 4.73 ± 0.09 eV and quantify its reduction in TBAI solutions. These findings establish a framework for quantitative studies of molecular interactions and electronic-structure modifications in aqueous systems, with implications for electrochemical and interfacial science.

DY 36.3 Wed 11:30 ZEU/0260

Liquid-vapor critical behavior of the TIP4P/2005 water model: Effects of NaCl solutes and hydrophobic confinement — •Mayank Sharma and Peter Virnau — Institute of Physics, Johannes Gutenberg University Mainz, Germany

The liquid-vapor critical behavior of water is strongly influenced by both ionic solutes and confinement. Molecular dynamics simulations of aqueous NaCl solutions using the TIP4P/2005 water model and the Madrid-2019 ion parameters reveal a systematic increase in the liquid-vapor critical temperature and pressure with salt concentration, consistent with experimental trends. In contrast, confinement between parallel hydrophobic plates leads to a depression of the critical point. The critical temperature was determined using the Binder cumulant crossing in the NVT ensemble, based on a recently developed method originally applied to an active Brownian particle system [1]. The reliability of this approach was verified through complementary NPT simulations using histogram reweighting. We further demonstrate the pronounced sensitivity of the estimated critical point to the van der Waals cutoff distance, underscoring the importance of properly accounting for long-range interactions. The present results capture qualitative shifts in the critical point of water arising from ionic interactions and confinement, and the Binder-cumulant framework used here is readily extendable to other critical phenomena, including the putative liquid-liquid critical point of water.

[1] J.T Siebert et al., Phys. Rev. E 98, 030601 (2018).

DY 36.4 Wed 11:45 ZEU/0260

Cooperative molecular dynamics and nuclear quantum effects in bulk water — •Margarita Russina — Helmholtz-Zentrum Berlin for Materials and Energy, Berlin, Germany

The cooperative dynamics in water remain difficult to access due to the lack of long-range order and the short lifetimes of molecular correlations. Neutron scattering is well suited to probe such phenomena on the nanoscale but has been hindered by the weak coherent signal of H2O. Using a novel neutron polarization-analysis approach, we directly measure the coherent scattering in H2O and D2O with high accuracy [1]. Beyond self-diffusion and molecular rotation, we identify a picosecond cooperative process in liquid water, likely associated with rearrangements of several neighboring molecules and the reorganization of hydrogen bonds. This process may act as a precursor to large-scale molecular transport. In the intermediate wave-vector range Q < 1 1/Å, the coherent signal in H2O is enhanced compared to the expectation for rigid, noninteracting, randomly oriented molecules. Since this Q-range corresponds to distances of several molecular spacings, our results provide evidence that intermolecular correlations in water extend beyond short-range correlations and involve more distant neighbors, giving rise to cooperative dynamical fluctuations. Such an enhancement can be rationalized by correlated preferential molecular orientations, hydrogen-bond rearrangements, and nuclear quantum effects. In contrast, D2O follows a more hydrodynamic behavior consistent with reported differences in the molecular bonding and symmetry of H2O and D2O. [1] M. Russina et al., J. Phys. Chem. Lett. (2025).

DY 37: Glasses and Glass Transition (joint session DY/CPP)

Time: Wednesday 11:15–12:45 Location: ZEU/0118

Invited Talk DY 37.1 Wed 11:15 ZEU/0118

Topological defects in 2D amorphous ensembles — •Peter Keim — Heinrich-Heine-Universität Düsseldorf

Topological defects are key to understand melting of crystals in two dimensions. A dilute gas of bound thus virtual pairs of dislocations cause the softening of a crystal in the vicinity of melting. If thermal energy is high enough to unbind dislocation pairs, translational order is destroyed and the crystal to melts due to the lack of shear resistance. In an amorphous solid, the concept of topology seems useless for the first glance due to the absence of order. Here, we discuss, how the definition of virtual dislocations can be generalized for a two-dimensional glass. Based on positional data of a binary colloidal monolayer we determine the fugazity of generalized virtual dislocations and measure elasticity close to the glass transition: Youngs modulus gets 16π at melting in surprisingly close analogy to Kosterlitz-Thouless-Halperin-Nelson-Young (KTHNY) - theory for melting of 2D crystals.

DY 37.2 Wed 11:45 ZEU/0118

Glass transition and universal scaling in ultra-low crosslinked microgels — Alessandro Martinelli[1], Rajam Elancheliyan[1], Andrea Scotti[2], Alexander V. Petrunin[3], •Domenico Truzzolillo[1], and Luca Cipelletti[1,4] — [1]Laboratoire Charles Coulomb (L2C), UMR 5221 CNRS-Universitè de Montpellier, F-34095 Montpellier,France — [2]Division of Physical Chemistry, Lund University, SE-22100 Lund, Sweden — [3]Institute of Physical Chemistry, RWTH Aachen University, Landoltweg 2, 52074 Aachen,Germany — [4]Institut Universitaire de France, F-75231 Paris, France

We investigate the glassy dynamics of Ultra-Low Crosslinked (ULC) poly(N-isopropylacrylamide) (PNIPAM) microgels. The glass transition is reached by varying either the temperature (modulating microgel swelling) or the colloidal number density. Our Dynamic Light Scattering (DLS) measurements confirm that the dynamic slowdown is solely governed by the effective volume fraction (φ), with ULC microgels behaving as fragile glass formers. Small-Angle X-ray Scattering data further indicates that the center-to-center inter-microgel distance is insensitive to temperature, scaling geometrically with mass fraction, while the height of the first peak of the static structure factor decreases with increasing concentration, suggesting structural melting above glass transition. We finally we report on the striking emergence of a universal dynamic behavior for the relaxation time (τ_α) dependence on the scattering vector (q) across the entire supercooled and glass regimes, allowing the data to collapse onto a master curve, whose features will be discussed.

DY 37.3 Wed 12:00 ZEU/0118

Strain-rate dependent rheological memory in a model glass former — •Monoj Adhikari and Jürgen Horbach — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany

We investigate the shear response of deeply supercooled liquids far below the mode coupling critical temperature of a model glass former. Our system is based on the Kob-Andersen binary Lennard-Jones mixture (KABLJM) model but incorporates polydispersity, allowing us to combine SWAP Monte Carlo (MC) with Molecular Dynamics (MD) simulations. This hybrid approach enables equilibration at temperatures far below the Mode-Coupling critical temperature, T_{MCT}, while maintaining an equation of state similar to the original binary KABLJM model. We examine the response of these equilibrated samples to shear deformation at finite temperature and strain rate. By combining MD with SWAP MC during shear, we demonstrate that states with stress far below the yield stress can be accessed, making Newtonian fluid behavior observable even at temperatures well below T_{MCT}. To characterize the Newtonian fluid states obtained from this hybrid approach, as well as the solid-like states from standard MD, we employ a strain-rate switching protocol on the steady states. When applying this protocol to the stationary states, we observe intriguing memory effects. In the transient regime, stress overshoots appear when increasing the strain rate, whereas a striking stress undershoot emerges when decreasing it, mirroring recent experimental observations in polymer glasses.

DY 37.4 Wed 12:15 ZEU/0118

An Analytical Relation between Thermodynamics and Dynamics in a Trap-like Model of Supercooled Liquids — •Simon G. Kellers, Anshul D. S. Parmar, and Andreas Heuer — Institute of Physical Chemistry, University of Münster, Corrensstraße 28/30, 48149 Münster, Germany

Recent studies on 2D non-network glass formers, enabled by the million-fold acceleration of Swap Monte Carlo, have revealed clear deviations from Gaussian behavior in the inherent-structure (IS) density of states and linked these features to the fragile-to-strong crossover (FSC) and the emergence of a low-energy depletion regime.

Here, we establish such a connection by introducing a direct analytical relation between thermodynamic PEL statistics and dynamical properties within a trap-like description of supercooled liquids. We illustrate this relation using a binomial distribution of IS states and show that it naturally yields a characteristic trap size for polydisperse systems. This trap size reflects the effective number of degrees of freedom that collectively determine the depth and barrier of a metabasin participating in an activated relaxation event, thereby offering a physically transparent measure of cooperativity.

By combining this analytical framework with simulation data for a polydisperse 2D glass former, we obtain a coherent and quantitatively consistent landscape-based interpretation of the FSC.

[1] Andreas Heuer, J. Condens. Matter Phys. 2008, 20, 373101

[2] Anshul D. S. Parmar, Andreas Heuer, 2023 arXiv preprint arXiv:2307.10143

DY 37.5 Wed 12:30 ZEU/0118

Single particle vs. collective diffusion dynamics in a glassforming ternary Lennard-Jones mixture — •Anna Pini and Jürgen Horbach — Institut für Theoretische Physik II: Soft Matter, Heinrich Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf

Ternary fluid mixtures exhibit a rather complicated diffusion dynamics compared to their binary counterparts. Apart from three self-diffusion coefficient, there are three interdiffusion coefficients. In this work, we study a ternary ABC Lennard-Jones mixture using molecular dynamics computer simulation. It is based on the Kob Andersen binary Lennard-Jones mixture (KABLJM) [1] to which we have added a third C component. While C-C and A-C interactions are respectively identical to A-A and A-B interactions, B-C interactions are different from those between A and B particles. We study the glassy dynamics of this system at a high density of $\rho = 1.2$ and compare it to that of the original KABLM. While the self-diffusion coefficient show a similar temperature dependence for the binary and the ternary system, the behavior of the interdiffusion coefficients in the ternary system is significantly different from that in the binary one; in particular, unlike the binary system, the Darken equation does not hold in the ternary one. [1] W. Kob and H. C. Andersen, Phys. Rev. Lett. **73**, 1376 (1994).

DY 38: Nonequilibrium Quantum Systems II (joint session TT/DY)

Time: Wednesday 15:00–17:30 Location: HSZ/0105

See TT 53 for details of this session.

DY 39: Networks, From Topology to Dynamics – Part II (joint session SOE/DY)

Time: Wednesday 15:00–15:45 Location: GÖR/0226

See SOE 10 for details of this session.

DY 40: Statistical Physics of Biological Systems II (joint session DY/BP)

Time: Wednesday 15:00–16:30 Location: ZEU/0114

Invited Talk DY 40.1 Wed 15:00 ZEU/0114

Learning the statistical folding of bacterial chromosomes — •Chase Broedersz — Vrije Universiteit, Amsterdam, Nertherlands

The physical organization of bacterial chromosomes is inherently variable, with large conformational fluctuations both from cell to cell and over time. Yet, chromosomes must also be structured to facilitate processes such as transcription, replication, and segregation. A physical description of this dynamic statistical folding of bacterial chromosomes remains largely elusive. Hi-C experiments probe chromosome organization by measuring average contact frequencies of chromosomal loci pairs. I will present a principled approach to infer and analyze the dynamic and statistical organization of chromosomes. In particular, we developed a rigorous and fully data-driven 4D Maximum Entropy approach to extract a generative model for the dynamic organization of a replicating bacterial chromosome directly from time-course Hi-C and microscopy data. This data-driven approach aims to unravel the dynamic statistical folding of chromosomes - and its impact on functional processes - in growing and replicating bacteria. Finally, I will discuss how these data-driven inferences can be used to develop mechanistic insights into the contributions of various chromosome segregation mechanisms, including ParABS and loop-extruding SMC complexes. Together, our results illustrate how changes in the geometry and topology of the polymer, induced by DNA-replication and loop-extrusion, impact the organization and segregation of bacterial chromosomes.

DY 40.2 Wed 15:30 ZEU/0114

A freely jointed chain with two-state hinges — •Minsu Yi and Panayotis Benetatos — Department of Physics, Kyungpook National University, Daegu, South Korea

We discuss aspects of the stretching and bending elasticity of a freely jointed chain, where the hinges can be open or closed in a random fashion. This two-state-hinge model captures a specific degree of freedom associated with the local bending stiffness of the polymer, and its variation can be due to internal changes or to the attachment of ligands from the environment. In this presentation, we focus on comparing the effects of two different types of disorder on the hinges: annealed (reversible Freely Jointed Chain, rFJC) or quenched (quenched Freely Jointed Chain, qFJC). It turns out that, as expected, those different types of disorder yield qualitatively different behaviors. For finite-size systems, we obtain a recurrence relation, which allows us to calculate the exact force-extension relation numerically for an arbitrary size of the system for both systems. In the thermodynamic limit, when the contour length is much larger than the persistence length, we obtain an exact expression for the force-extension relation. The difference between the two systems still exists in the thermodynamic limit.

[1] M. Yi, D. Lee and P. Benetatos, J. Chem. Phys. 161 (23): 234908 (2024)
[2] M. Yi and P. Benetatos, J. Stat. Mech. 073501 (2025)

DY 40.3 Wed 15:45 ZEU/0114

Impact of cytosine methylation on the diffusion of charges along DNA: a quantum perspective — •Mirko Rossini, Dennis Herb, Paul Raschke, and Joachim Ankerhold — Institute for Complex Quantum Systems, University of Ulm, Ulm, Germany

We develop a coarse-grained tight-binding (TB) framework that treats electrons and holes on equal footing. TB parameters, required to characterize the model, are derived from an ab-initio molecular scheme (linear-combination-of-atomicorbitals (LCAO)) that includes all valence orbitals. Simulations address unmethylated vs. methylated CpG-rich and regulatory sequences sensible to DNA methylation, enabling us to investigate the impact methylation has on the charge diffusion along models of critical relevance in epigenetics and shedding new light on possible undiscovered mechanisms for epigenetic regulation in cells.

Methylation substantially lowers cytosine charge energies (~150 meV) while leaving the opposite guanine nearly unchanged (<20 meV), thereby introducing site-selective energetic shifts that redesign diffusion pathways. Statistical investigations, such as time-averaged populations and Inverse Partecipation Ratio (IPR) analyses, show enhanced electron localization at methylated cytosines, contrasted by increased hole delocalization: these dual trends suppress electron-hole co-localization (localization at same sites) and reduce recombination probability, leading to higher trapping times of excess charges along the DNA. Consistently, modelled excitations lifetimes increase upon cytosine methylation.

DY 40.4 Wed 16:00 ZEU/0114

Efficient control of F_1 molecular motor — •Deepak Gupta — Institut für Physik und Astronomie, Technische Universität Berlin, Germany

Designing low-dissipation control driving protocols for small-scale systems is an active field of research. In this talk, I will specifically discuss designing efficient driving procedures for a biomolecular motor-the F_1ATPase. In general, designing such protocols is challenging due to the spatial nonlinearity of the systems and the presence of environmental thermal fluctuations. Nonetheless, a near-equilibrium (linear response) framework is found to apply to a broad class of small-scale systems. We follow this framework to design non-trivial protocols to drive the F_1's γ-shaft to synthesize ATP at low-dissipation cost. Our analysis reveals that the designed protocols, based on the linear response approach, dissipate lower energy as compared to the constant velocity driving protocol for a wide range of protocol durations[1]. In the second part of my talk, I will show our recent experimental results on the F_1 ATPase motor, where we compared the dissipation of driving this motor using two experimentally viable protocols: angle clamp and torque clamp. Our experimental results (supported by analytical findings) suggest that angle clamp driving requires less work than that of the torque clamp[2].

[1] J. Phys. Chem. Lett. 13 (51), 11844-11849 (2022). [2] Phys. Rev. Lett. 135 (14), 148402 (2025).

DY 40.5 Wed 16:15 ZEU/0114

Elementary spectrum for the dissonance curve: from biophysics to number theory of musical harmony — •Alexandre Guillet — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Musical harmony, as the ancient problem of finding tunings and scales based on the commensurability of sound waves, has been approached by Helmholtz in terms of a dissonance curve in the frequency domain. This model is here recast in an elementary form related to number theory and a thermodynamical formalism for musical intervals and frequency ratios. The idea of the pioneer of biophysics connects with Riemann's zeta function along the critical line, and Minkowski's question mark measure. The former models rational relationships resulting from the acoustics of a harmonic timbre, while the latter models the probability distribution of the neurocognitive effort to assess the commensurability of frequency pairs. The spectrum of the resulting fractal curve predicts the quasi-periods of widely used musical scales, from the pentatonic division of the octave to microtonal ones, thus constituting a biophysical and mathemusical common ground to harmony across musical genres and cultures.

DY 41: Poster: Nonlinear Dynamics, Granular Matter, and Machine Learning

Time: Wednesday 15:00–18:00 Location: P5

DY 41.1 Wed 15:00 P5

Dynamics of Root Growth in Granular Media — Tianhui Liao[1,3], Jiayun Huang[1], Shihe Pan[1], Matthias Schroeter[1,4], and •Kai Huang[1,2] — [1]Collective Dynamics Lab, Division of Natural and Applied Sciences, Duke Kunshan University, 215306 Kunshan, Jiangsu, China — [2]Experimentalphysik V, Universität Bayreuth, 95440 Bayreuth, Germany — [3]Department of Physics, School of Science, Westlake University, Hangzhou, China — [4]Max-Planck-Institut für Dynamik und Selbstorganisation, Am Faßberg 17, 37077 Göttingen, Germany

Since the pioneering work of C. Darwin, the dynamics of growing plants and its interactions with the surrounding environment have been a topic of interest over centuries. As more frequent flooding and drought arise along with global climate change, it is essential to develop ecological models based on first principle understanding of the 'microscopic' interactions between plant roots and surrounding environment. Given the complex rheological behavior of granular media, it is intuitive to understand how plant roots navigate through granular media with heterogeneous stress distributions. By means of X-ray computer tomography, we measure the local packing density of individual 'soil' particles using (Set-)Voronoi tessellation, along with the morphological changes of plant roots. Our goal is to map temporal changes in packing fraction, displacement fields, and strain fields to reveal how roots actively adapt to the surrounding environment.

DY 41.2 Wed 15:00 P5

Diffusion in a Ferrogranular Pinball Machine — Ali Lakkis[1], Matthias Biersack[1], Oksana Bilous[2], Sofia Kantorovich[2], and •Richter Reinhard[1] — [1]Experimentalphysik 5, Universität Bayreuth — [2]Fakultät für Physik, Universität Wien

We experimentally investigate the diffusion of millimeter-sized glass and steel beads in a vessel under vertical vibration. At high amplitudes of an applied vertically oriented magnetic induction B, the magnetization of the steel beads aligns with the field direction. This causes the magnetized steel spheres to become nearly pinned in a hexagonal lattice due to dipole-dipole repulsion. As a result, they act as obstacles that hinder the diffusion of the glass beads, similar to the pins in a pinball machine. When B is reduced, the hexatic lattice of steel spheres becomes more fluid-like. We track both the glass and steel beads and estimate their mean square displacement (MSD) for different values of B. These results are compared to Molecular Dynamics simulations of a quasi-2D thermalized Stockmayer-glass mixture [1].

[1] O. Bilous, K. A. Okrugin, A. Lakkis, R. Richter, S. S. Kantorovich, *Self-diffusion in Ferrogranulates: Stockmayer Model Revisited*, J. Moll. Liquids, submitted (2025)

DY 41.3 Wed 15:00 P5

Analysis and optimization of power grid stability for rising feed-in of wind energy — •Jean-Luc Schnipper and Philipp Maass — Universität Osnabrück, Institut für Physik, Germany

On the basis of the swing equations for power flow in electricity grids and heterogeneous test grid structures, we analyse the impact of wind-power feed on grid stability. The stability is quantified by the exceedance, that is the fraction of time the network frequency exceeds thresholds triggering primary control measures. Wind farms are incorporated into test grids by replacing conventional generators. They are represented by stochastically driven single turbines with mean power output equal to that of the replaced conventional generator. We find that that the exceedance per unit of installed wind power can vary substantially depending on which generators are substituted and to which extent wind fluctuations are correlated at different locations of wind power injection. This offers strategies for maintaining best power grid stability by optimized spatial allocation of wind farms.

DY 41.4 Wed 15:00 P5

On Uncertainty Quantification in Parameter Estimation of Ordinary Differential Equation Initial Value Problems — •Oliver Strebel — Angelstr. 17, 75392 Deckenpfronn

Parameter estimation tasks for ordinary differential equation initial value problems (ODE-IVP) arise, when solution data for the ODE-IVP are given and for a given model the parameters and initial values are estimated. From the mathematical definition of the ODE-IVP it follows that uncertainty due to noise in the data and from a misfit of the model is reflected in the parameters and initial values alone. This uncertainty determines the uncertainty in the solution curves of the ODE-IVP. It is shown that simple Monte Carlo simulations, using the standard nonlinear regression measure, are well-suited for uncertainty quantification (UQ) in ODE-IVPs. This approach also uncovers practical identifiability issues related to the parameters and initial conditions. Additionally, the limitations of the method, such as its sensitivity to initial conditions and computational feasibility, are discussed.

DY 41.5 Wed 15:00 P5

Transition to Turbulence via Synchronization and Interacting Wakes — •Urantuya Batsuuri[1,2], Michael Hölling[1,2], Matthias Wächter[1,2], and Joachim Peinke[1,2] — [1]School of Mathematics and Science, Institute of Physics, Carl von Ossietzky Universität Oldenburg, 26129 Oldenburg, Germany — [2]ForWind - Center for Wind Energy Research, Küpkersweg 70, 26129 Oldenburg, Germany

The study investigates the dynamics of wake interactions under periodic perturbations using an active grid with two independently driven shafts, which are excited with different frequencies. Downstream velocity field is measured with constant-temperature anemometry to resolve the flow response.

For the single-shaft excitation case, a nonlinear synchronization effect is observed: the wake meandering synchronizes to the small-amplitude shaft motion, and this synchronized behavior grows downstream until it collapses into turbulence. Through this synchronization mechanism, the transition to turbulence appears to be accelerated.

For the two-shaft excitation case, an incipient interaction of the vortices leads to a low-dimensional quasi-periodic state. Further downstream, increasing nonlinear dynamics generate enhanced higher harmonics and interharmonics (mixing components). Eventually, the spectrum broadens into a fully turbulent state that follows the classical -5/3 power-law decay.

DY 41.6 Wed 15:00 P5

BHD In semi-chaotic phasespace — •Nico Fink — RPTU Kaiserslautern Landau; Kaiserslautern; Erwin Schrödinger Straße 46, Germany

The previous project showed a realisation of breaking of time reversal symmetry in a system with one degree of freedom, leading to the "rediscovery" of what was coined the Krystal-Neistadt-henrard-Theorem. This project extends the system to a nonlinear System with 1,5 degrees of freedom, displaying the rise of chaos around the separatrix widening and splitting of ensembles. Tje aim is to explore the macroscopic behaviour of ensembles by a bottom up approach.

DY 41.7 Wed 15:00 P5

Laminar chaos in systems with state-dependent delay — •David Müller-Bender — Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany

Laminar chaos, an extremely low-dimensional form of chaotic dynamics, was originally discovered in time-delay systems with large, periodically time-varying delays [Phys. Rev. Lett. 120, 084102 (2018)]. In contrast, the same systems with constant delay exhibit high-dimensional turbulent chaos. Laminar chaos therefore provides a clear example of how temporal modulation of the delay can drastically change the dynamics of a time-delay system. While turbulent chaos is characterized by strong high-frequency oscillations, laminar chaos shows nearly constant laminar phases, whose intensity levels follow the dynamics of a chaotic one-dimensional iterated map.

Following a bottom-up approach, we subsequently investigated systems with quasiperiodic [Phys. Rev. E 107, 014205 (2023)], random, and chaotically time-varying delays [Phys. Rev. E 112, 064203 (2025)], thereby stepwise increasing the generality of the delay variation and building on insights from the preceding cases. In the present work, we consider the case of state-dependent delays and present first results, demonstrating that laminar chaos can also be observed in such systems.

DY 41.8 Wed 15:00 P5

Mesoscopic interface laws in patterns formed by non-equilibrium cell polarity models — •Tobias Alexander Roth[1], Henrik Weyer[2], and Erwin Frey[1,3] — [1]Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität München — [2]Kavli Institute for Theoretical Physics, UCSB — [3]Max Planck School Matter to Life

Inspired by minimal models for protein-based polarization of living cells, we investigate the dynamics of interfaces in quasi-stationary patterns generated by two-component mass-conserving reaction-diffusion systems. These models describe two density fields that diffuse and interconvert through chemical reactions. Simulations reveal that for fast reactions sharp interfaces emerge, that separate high- and low density regions, which coarsen over time and eventually become a single patch. To quantitatively describe this process, we derive reduced descriptions for the motion of these interfaces, which are strikingly similar to what is found in crystal growth processes with dynamic heat deposition. Our derivation allows for a diffusio-chemical version of surface tension and kinetic drag and explains a cross-over in coarsening exponents. Taken together, we put non-equilibrium two-component models in context to classical thermodynamic models and give insight into biological self organization.

DY 41.9 Wed 15:00 P5

Nonlinear pulse dynamics in harmonic active mode-locking — •Shakiba Khajenooriranjbar[1], Elias R. Koch[1], Julien Javaloyes[2], and Svetlana V. Gurevich[1,2,3] — [1]Institute for Theoretical Physics, University of Münster, Wilhelm-Klemm-Str. 9, Münster 48149, Germany — [2]Departament de Física & IAC-3, Universitat de les Illes Balears, Cra. de Valldemossa, km 7.5. E-07122 Palma, Spain — [3]Center for Data Science and Complexity, Corrensstr. 2, 48149 Münster, Germany

Active mode-locking (AML) is a prominent technique for generating ultra-short laser pulses and frequency combs, finding applications in fields such as medicine and laser metrology. We employ a time-delayed model to study the multipulse dynamics in AML that is valid for large values of the round trip gain and losses. It allows us to access the typical regimes encountered in semiconductor lasers and to perform an extended bifurcation analysis. Close to the harmonic resonances and to the lasing threshold, we recover the Hermite-Gauss solutions. However, we also discover a global bifurcation scenario in which a single pulse can jump, over a slow time scale, between the different minima of the modulation potential. There, a periodic orbit terminates at an homoclinic limit point of the solution branch, where not all potential slots occupied with the pulses, forming a so-called time-crystal state. Next, we analyzed the interaction between pulses by analyzing their phase relations. Numerical path continuation reveals the existence of multistable splay states and the laser may wander between them under the influence of stochastic forces.

DY 41.10 Wed 15:00 P5

Dynamic Models for Two Nonreciprocally Coupled Fields: A Microscopic Derivation for Zero, One, and Two Conservation Laws — Kristian Blom[1], •Uwe Thiele[1], and Aljaz Godec[2] — [1]Institute of Theoretical Physics, University of Münster, Wilhelm-Klemm-Strasse 9, 48149 Münster, Germany — [2]Mathematical bioPhysics group, Max Planck Institute for Multidisciplinary Sciences, Am Faßberg 11, 37077 Göttingen, Germany

Dynamical field theories form a cornerstone of statistical and soft matter physics, providing continuum descriptions of complex systems through a coarse-grained order parameter field. These theories can be derived either by explicit coarse-graining of microscopic dynamics or by top-down symmetry and conservation arguments.

An intriguing class of such models are nonreciprocal field theories, including the nonreciprocal Allen-Cahn and Cahn-Hilliard models, which describe the

spatiotemporal evolution of two fields coupled through interactions that violate Newton's third law. Depending on the underlying microscopic dynamics, two interacting fields may exhibit zero, one, or two conservation laws associated.

In this poster, we demonstrate how the evolution equations for each of these scenarios can be systematically derived from a single microscopic framework: the nonreciprocal Ising model. After obtaining the corresponding field-theoretic descriptions, we briefly discuss their linear and nonlinear behavior, and finally show how distinct combinations of kinetic modes give rise to a set of sixteen different nonreciprocal field theories.

DY 41.11 Wed 15:00 P5

Competing instabilities in electroferrofluids via non-variationally coupled Swift-Hohenberg equations — •Emil Stråka[1], Max Phillip Holl[1], Maria Sammalkorpi[1], and Mikko Haataja[2] — [1]Aalto University, Finland — [2]Princeton University, USA

Recent experiments in charged ferrofluids, so called electroferrofluids, have shown that they can exhibit Rosensweig-like patterns with non-equilibrium activity [1]. The observed activity rises from the competition of an magnetic and electric field induced instabilities. In this work, we study the phenomenon via two non-reciprocally coupled Swift-Hohenberg equations analytically and numerically [1,2]. In addition to the propagating patterns predicted by theory, the model equations reveal a wide range of dynamics, including irregular, active motions [2].

Our findings demonstrate how competing instabilities in a simplified model system can generate new, nontrivial pattern dynamics. These results suggest that similar active dynamics may arise broadly in complex fluids with competing instability mechanisms.

[1] Rigoni, C., Holl, M. P., Scacchi, A., Stråka, E., Sohrabi, F., Haataja, M. P., Sammalkorpi, M., & Timonen, J. V. I. (2025). Active Rosensweig Patterns. arXiv:2510.09099. https://arxiv.org/abs/2510.09099

[2] Stråka, E., Holl, M. P., Sammalkorpi, M. & Haataja, M. P., under preparation (2025). Competing instabilities in complex fluids via Swift-Hohenberg equations with non-variational coupling.

DY 41.12 Wed 15:00 P5

Mitigating Degradation in Anion Exchange Membrane Water Electrolysis: Repurposing Shutdowns to Probe Cell Health — •Limei Jin[1], Violeta Karyofylli[2], Karsten Reuter[1], and Christoph Scheurer[1,2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]IET-1, Forschungszentrum Jülich

The reliable integration of Anion Exchange Membrane Water Electrolysis (AEMWE) into renewable energy systems is hampered by rapid cell degradation, a challenge exacerbated by variable loads and frequent, safety-mandated shutdowns. This performance loss has been attributed to cell reversal: when the cell's potential drops below a critical inflection point, an acute negative current excursion occurs.

To address this challenge, we present an effect analysis of key shutdown parameters on the inflection point of the potential, using this operational signature as a critical indicator to correlate with long-term aging. We base the analysis on our comprehensive COMSOL multiphysics model to accurately simulate dynamical processes governing the shutdown and reversal phenomena in detail. Data generated from these simulations are integrated into an AI-driven optimization framework to identify ideal operating parameters. It will be used to design an optimal pulse sequence for an active online control to suppress reversal events and mitigate degradation.

DY 41.13 Wed 15:00 P5

TANGO and Machine Learning Enhanced Experimentation for Real Time Tracking of Actively Steered Magnetic Particles. — •Nikita Popkov[2,3], Nikolai Weidt[1,2], Yahya Shubbak[1,2], Rico Huhnstock[1,2], Kristina Dingel[2,3], Bernhard Sick[2,3], and Arno Ehresmann[1,2] — [1]Institute for Physics and CINSaT, University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany — [2]AIM-ED, Joint Lab of Helmholtzzentrum für Materialien und Energie, Berlin (HZB) and University of Kassel, Hahn-Meitner-Platz 1, 14109, Berlin, Germany — [3]Intelligent Embedded Systems, University of Kassel, Wilhelmshöher Allee 71-73, 34121, Kassel, Germany

This work presents an AI-driven closed-loop framework for automating experimental tasks, demonstrated for the remote-controlled on-chip transport of magnetic particles. The system integrates machine learning models for particle detection, tracking, and classification, enabling dynamic feedback control during experiments. It autonomously adjusts experimental parameters to improve data quality and align outcomes with research objectives. The TANGO controls modular design allows adaptation to different experimental setups and hypotheses. Overall, it emphasizes how autonomous systems could iteratively optimize experiments, advancing the field of next-generation laboratory automation and, specifically for our experiments, the development of novel lab-on-a-chip devices.

DY 41.14 Wed 15:00 P5

Machine Learning of a Classical Density Functional for 2D Hard Rods — •Paul Bitzer, Jens Weimar, and Martin Oettel — Eberhard Karls University of Tübingen, Tübingen, Germany

Obtaining phase diagrams and density distributions via Grand canonical Monte Carlo simulations (GCMC) for classical fluids still requires substantial computational resources. Here, classical density functional theory (cDFT) is more efficient if the excess functional for the free energy is known. Recently, machine learning (ML) methods have become popular to learn such functionals (which are broadly applicable) from a limited amount of training data obtained in random, inhomogeneous external potentials [1]. We discuss an extension of an ML scheme to lattice fluids and apply it to the case of hard rods in two dimensions (2D). This model shows demixing between majority phases of vertically resp. horizontally oriented rods. This is typical of demixing in a binary, continumm fluid whose phase diagram has been learned recently in [2] employing only training data inhomogeneous in 1D. The use of explicit 2D training data allows applications to more general inhomogeneous situations [3].

[1] A. Simon and M. Oettel, Machine learning approaches to classical density functional theory (review), arXiv:2406.07345

[2] S. Robitschko et al, J. Chem. Phys. 163, 161101 (2025)

[3] F. Glitsch, J. Weimar and M. Oettel, Phys. Rev. E 111, 055305 (2025)

DY 41.15 Wed 15:00 P5

Neural-Network-Driven Sequential Quasi Monte Carlo Sampling for Bayesian Inference with Complex Posteriors — •Andreas Panagiotopoulos[1], Javed Mudassar[2], Jens-Uwe Repke[2], Georg Brösigke[2], and Sebastian Matera[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Technische Universität Berlin

Bayesian inference has seen an increasing popularity in recent years, because it overcomes some of the limitations of classical parameter fitting. The price is the need to sample the potentially high-dimensional parameter space, which can become computationally demanding for complex forward models. This is enhanced when faced with uninformative priors but accurate data in conjunction with highly sensitive and nonlinear models. Posteriors will be sharply localized and of complex nature resulting in challenging sampling problems. To address this, we have developed a sequential importance sampling approach which utilizes neural network normalizing flows to exploit the superior sampling properties of Quasi Monte Carlo (MC) techniques. An initial sampling from a simple distribution is employed to learn the first layer of the normalizing flow, i.e. a first coarse approximation of the posterior distribution. Using this flow to quasi MC sample from that distribution provides the data to learn the next layer and so on. As at early stages appropriate sampling of the posterior is intractable, a tempering strategy is employed to make this strategy more robust. We demonstrate the approach on a realistic problem with complex posteriors stemming from the field of chemical kinetics.

DY 41.16 Wed 15:00 P5

Computational modeling and design of self-stratifying colloidal materials — •Mayukh Kundu and Michael Howard — Auburn University, Auburn, United States

Mixtures of colloidal particles suspended in a solvent can spontaneously form layered structures during fast solvent drying. This process, called self-stratification, can be leveraged to fabricate multilayered colloidal materials in a single processing step. Existing models for simulating self-stratification are computationally expensive or inaccurate. I have developed a better model for simulating the phenomena using dynamic density functional theory (DDFT). DDFT is a continuum model that is systematically formulated from particle-level interactions and dynamics. As such, it incorporates physics that would be present in particle-based simulations but can access much larger length scales and longer time scales. DDFT has two key inputs: a thermodynamic model (free-energy functional) and a dynamics model (mobility tensor). DDFT model can be made faster using the simplest approximations of these inputs that give the desired accuracy. I systematically investigated approximations of both inputs to develop an accurate, efficient DDFT model for drying suspensions. I also coupled these drying simulations to an optimization strategy based on surrogate modeling to inverse design self-stratified coatings with targeted thickness and particle distribution. This work has the potential to reduce the time and resources required to create these novel materials in the laboratory.

DY 42: Poster: Quantum Dynamics and Many-body Systems (joint session DY/TT)

Time: Wednesday 15:00–18:00 Location: P5

DY 42.1 Wed 15:00 P5

Operator spreading through the lens of the information lattice — •Luca Gawalleck[1,2], Maxime Debertolis[1], Jens H. Bardarson[3], and David J. Luitz[1] — [1]Institut of Physics, University of Bonn, Nußallee 12, 53115 Bonn, Germany — [2]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — [3]Department of Physics, KTH Royal Insititute of Technology, Stockholm, 106 91 Sweden

We study the entanglement growth during Heisenberg time evolution by extending the framework of the information lattice to operators using the operator entanglement entropy. We focus on one-dimensional quantum spin chains and work in the tensor network formalism. The generalization of the information lattice to matrix product operators allows us to observe the spreading of initially local operators in a way that is not biased by the choice of a probing operator. We demonstrate that the operator information lattice we introduce contains all information typically provided by the out-of-time-order correlator with the additional ability to resolve the correlations on different scales. This method provides a good way to analyze systematically the time dependence of entanglement and can seamlessly be integrated into existing information-lattice-based algorithms.

DY 42.2 Wed 15:00 P5

Non-Perturbative Out-Of-Equilibrium Dynamics with Initial Four-Point-Correlations — Jürgen Berges, Louis Jussios, and •Cosima Schmitt — ITP Heidelberg

We investigate how initial correlations affect the equilibration dynamics of closed systems in quantum field theory. For interacting scalar fields with N components, we derive nonequilibrium evolution equations from a self-consistent large-N expansion to next-to-leading-order. By going beyond conventional Gaussian initial conditions, we point out the role of initial four-point correlations for the propagator evolution at early times and in the late-time approach to thermal equilibrium.

DY 42.3 Wed 15:00 P5

Nonequilibrium Green Function Simulations for Large Systems — •Erik Schroedter, Jan-Philip Joost, and Michael Bonitz — Christian-Albrechts-Universität zu Kiel, Kiel, Germany

Nonequilibrium Green Functions (NEGF) provide a powerful framework for accurately simulating the dynamics of correlated many-body systems. A major limitation of standard NEGF approaches is the cubic scaling of computational cost with the number of time steps. Recently, the G1-G2 scheme [1] overcame this limitation, achieving linear scaling. However, it introduces its own challenges, such as numerical instabilities at strong coupling and large memory requirements, which have so far restricted simulations to small systems with fewer than 150 basis states. Here, we introduce a NEGF-based quantum fluctuations approach (NEGF-QF)[2] that builds on earlier works [3] to efficiently factorize the two-particle Green function. This method drastically reduces computational costs for advanced self-energy approximations, including GW and T-matrix, while enabling straightforward parallelization. As a result, NEGF-QF allows simulations of systems with up to ten thousand basis states. We demonstrate the approach for large Hubbard clusters and graphene nanoribbons, illustrating its effectiveness for large, strongly correlated systems.

This work was funded by the Deutsche Forschungsgemeinschaft (DFG), Project No. 464370560.

[1] Schlünzen et al., Phys. Rev. Lett. 124, 076601 (2020)
[2] Schroedter et al., to be published (2026)
[3] Schroedter et al., Cond. Matt. Phys. 25, 23401 (2022)

DY 42.4 Wed 15:00 P5

Quantum Chaos in a Classical Counterpart to the Fermi-Hubbard model through an exact Path-Integral Formalism — •Louis Renck[1], Wolfgang Hogger[2], Juan Diego Urbina[2], and Peter Schlagheck[1] — [1]IPNAS, CESAM research unit, Université de Liège, Belgium — [2]Institut für Theoretische Physik, Universität Regensburg, Germany

Understanding quantum chaos in interacting many-fermion systems remains challenging : unlike many-bosons systems - where quantum-classical correspondence can be established using semiclassical tools such as the van Vleck-Gutzwiller propagator [1] -, most interacting fermions models still lack a sensible classical limit where Hamiltonian chaos can be defined.

We propose a candidate to the first classical Hamiltonian for the Fermi-Hubbard model with integrability broken by a random onsite potential. Starting from the fermionic Hamiltonian, we apply a Jordan-Wigner transformation and switch to the Schwinger-boson representation to obtain a bosonic form. A recently developed exact bosonic path-integral formalism [2] then provides a classical Hamiltonian symbol defined over a symplectic phase space. We investigate the resulting quantum-classical correspondence by comparing the effective dynamics with the quantum evolution, and we present quantitative checks of chaos based on spectral properties and out-of-time ordered correlators.

[1]. T. Engl, J. Dujardin, A. Argüelles, P. Schlagheck, K. Richter, and J. D. Urbina, Phys. Rev. Lett. 112, 140403 (2014).
[2]. F. Bruckmann and J. D. Urbina (2018)

DY 42.5 Wed 15:00 P5

Adaptive Fermion Circuits with chiral transport — •Markus Siegl and Michael Buchhold — Department of Theoretical Physics, Universität Innsbruck, Austria

Nonequilibrium quantum transport, where coherent many-body dynamics coexist with directional motion remains a central challenge in modern quantum physics. This project investigates transport phenomena in two coupled fermionic chains designed to break chiral symmetry. Using fermionic adaptive circuits and measure-ment-feedback protocols, we aim to control nonequilibrium dynamics and induce directional motion in an other-wise symmetric quantum system. By linking classical universality, quantum many-body effects, and information transport, the research seeks to uncover new mechanisms for controlled, symmetry-broken quantum transport, establishing a model system for genuinely nonequilibrium quantum matter.

DY 42.6 Wed 15:00 P5

Absorbing-State Dynamics and Feedback Control in Quantum Many-Body Scar Systems — •Lara Schorr — University of Innsbruck

We look at quantum many-body scar states, which are special excited states in non-integrable systems that do not thermalize. To better understand their non-equilibrium dynamics, we translate the problem to a measurement-based quantum circuit equipped with feedback control. Focusing on a spin-1/2 chain with SU(2) symmetry, we show that local unitary feedback enables controlled manipulation of non-local charges, allowing the system to relax into highly entangled dark states. By analyzing the convergence towards the target state, we find that the dynamics resembles an emergent absorbing-state process, in which non-local charges diffuse and annihilate over time. Studying the scaling of convergence times allows us to identify conditions under which the dynamics may exhibit an absorbing-state phase transition.

DY 42.7 Wed 15:00 P5

Floquet-Magnus expansion for driven quantum systems and spin dynamic mean-field theory in NMR — •Antonia Joëlle Bock — TU Dortmund University, Germany

An accurate and reliable theoretical description of periodically driven quantum systems is highly relevant to many applications, such as for magic-angle spinning (MAS) in nuclear magnetic resonance (NMR) and ultracold atoms in driven optical lattices. Typically, the first step in capturing the dynamics is to determine an effective time-independent Hamiltonian, for which one can choose from a broad range of slightly different, hence often confusing, theories. Thus, I specifically investigated two widely used theories: Average Hamiltonian theory (AHT) and the Floquet-van Vleck approach (secular averaging). I was able to quantify the importance of the kick operator for the equivalence between perturbative and numerically exact approaches. This was achieved through analytical calculations and numerical evaluations of exemplary spin systems. These crucial insights then build the foundation for the second step of my project: a dynamic mean-field theory for dense spin ensembles applicable to complex couplings between three or more spins (MAS-DMFT). The recently developed spinDMFT (cp., e.g., Gräßer et al., 2024) has proven to be efficient, accurate and applicable to large spin systems yielding 2-particle interactions.

DY 42.8 Wed 15:00 P5

Phonon mediated indirect spin interaction — •Pablo Reiser and Habib Rostami — University of Bath, Bath, United Kingdom

Due to the lack of inversion symmetry in the hBN monolayer, circular polarized vibration in solids, or chiral phonons, with nonzero angular momentum are allow. These chiral phonons can couple to spins of different nature through their angular momentum. Within this context, we explored the coupling of chiral phonons with non-zero angular momentum to two impurities spins in hBN. Using field theory methods, we obtained the spin susceptibility and studied it*s properties like the mass dependence of the coupling, frequency of oscillation and rate of decay. The momentum transfer due to this coupling may opens the door for non-trivial thermal or spin transport effects.

DY 42.9 Wed 15:00 P5

Dynamical Phases and Instabilities in Periodically Driven Bogoliubov-de Gennes Superconductors — •Subhadip Chakraborty, Animesh Panda, and Ferdinand Evers — Institute of Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

We investigate the nonequilibrium dynamics of a superconductor subjected to a periodic modulation of the interaction strength starting with Bogoliubov-de Gennes (BdG) mean field Hamiltonian. Using numerical solutions of the time-dependent Bogoliubov-de Gennes equations, we first explore several dynamical superconducting regimes. Our analysis reveals a rich variety of phases, including Rabi-Higgs oscillations, synchronized Higgs dynamics, and time-crystalline responses, and shows how their stability varies across driving parameters. In some regions of parameter space, infinitesimal initial seeds of finite momentum pairing grow exponentially during our driving protocol. By computing the momentum-resolved pairing response, we identify the instability bands associated with these finite-momentum modes, quantify their growth rates, and determine their dependence on driving frequency and drive amplitude. These results provide a comprehensive numerical characterization of the dynamical phases and instabilities that arise in periodically driven superconductors before the final steady state is reached.

DY 42.10 Wed 15:00 P5

Higher order Magnus expansion for two-level quantum dynamics — •Chen Wei and Frank Grossmann — Institut für Theoretische Physik, 01062 Dresden, Germany

This study investigates the Magnus expansion[1] for a generic time-dependent two-level system. By using its convergence condition[2], we find that elementary unitary transformations significantly extend the validity of the Magnus expansion. Furthermore, higher order terms admit particular physical interpretations. By virtue of su(2) Lie algebra, the expansion is decomposed into a commutator-free form. To illustrate its usefulness, we study the Landau-Zener[3] model, which displays a special case of non-adiabatic transitions. Using agian the Magnus expansion, Hermitian and non-Hermitian versions of the semiclassical Rabi model are systematically treated by determining the Floquet quasienergy[4] and Bloch-Siegert shift[5]. As a noteworthy by-product, the Magnus expansion provides a quantitative characterization of the adiabatic theorem[6].

[1] W. Magnus, Commun. Pure Appl. Math. 7, 649-673 (1954). [2] M. M. Maricq, J. Chem. Phys. 86, 5647-5651 (1987). [3] C. Zener and R. H. Fowler, Proc. R. Soc. Lond. A 137, 696-702 (1932). [4] J. H. Shirley, Phys. Rev. 138, B979 B987 (1965). [5] F. Bloch and A. Siegert, Phys. Rev. 57, 522-527 (1940). [6] M. Born and V. Fock, Z. Phys. 51, 165-180 (1928).

DY 42.11 Wed 15:00 P5

Distribution of complex amplitudes of chaotic resonance states — •Jan Möseritz-Schmidt and Roland Ketzmerick — TU Dresden, Institut für Theoretische Physik, Dresden, Germany

Resonance states of chaotic scattering systems have complex amplitudes in the position representation. Naively, one would expect that the phase of the complex amplitude is uniformly distributed, however, we observe significant deviations. We find that part of this is a finite-size effect which is already present in the random wave model. It is enhanced by the multifractal structure of chaotic resonance states, which follows from the factorization conjecture. We quantify these deviations using the phase rigidity and analyze its scaling behavior in the semiclassical limit. Numerically, this is demonstrated for the paradigmatic three-disk scattering system.

DY 42.12 Wed 15:00 P5

Complex dynamics and particle-wave correspondence in anisotropic mesoscopic cavities — •Silvan Stopp, Samuel Schlötzer, Lukas Seemann, and Martina Hentschel — Technische Universität Chemnitz, 09107 Chemnitz, Germany

Mesoscopic billiard systems with different geometries are well-known model systems for investigating complex dynamics and quantum chaos. While the breaking of spatial cavity symmetries is typically considered to be the origin of chaotic dynamics, we show that anisotropies, i.e., broken symmetries in momentum space, can also cause chaotic particle dynamics. To this end, we investigate bilayer graphene systems (BLG) [1] and birefringent optical microcavities [2], both of which have preferred propagation directions. Anisotropy prevent angular momentum to be a conserved quantity, and consequently, the angles of incidence and of reflection of a particle trajectory deviate. Therefore, we implementing an advanced ray tracing algorithm that we apply to BLG and birefringent cavities. We show that the presence of anisotropies induces chaotic dynamics even in circular cavities. We investigate the interplay of the cavity shape and the Fermi line geometry and illustrate how it affects the cavity dynamics. In particular, we find that certain trajectories can be stabilized by matching the symmetry in real and momentum space. In addition, we use Kwant and transformation optics to demonstrate ray/particle-wave correspondence in real space as well as in phase space using the Husimi function.

[1] L. Seemann, A. Knothe, M. Hentschel, PRB 107, 205404 (2023)
[2] M. Hentschel, S. Schlötzer, L. Seemann, Entropy 27(2):132 (2025)

DY 42.13 Wed 15:00 P5

Periodic orbit theory approach for a non-Hermitian Riemann operator — •Sebastian Hörhold, Andreas Hötzinger, Juan Diego Urbina, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, Germany

The Riemann Hypothesis (RH) is one of the most important open problems in mathematics. Among the various approaches toward its proof is the Hilbert-Pólya (HP) conjecture, stating that there should exist a Hermitian operator whose eigenvalues t_n are given by the zeros of the Riemann zeta function $\zeta(1/2 + it_n)$. The RH would then follow from the reality of these eigenvalues.

In a recent contribution toward a proof of the RH, a non-Hermitian Hamiltonian has been introduced, referred to as a Riemann operator, whose spectrum contains the t_n, and from which one can construct an HP operator [1]. Our work focuses on a similar Hamiltonian, and we intend to make use of semiclassical tools to support earlier work by Berry and Keating, who obtained a formal asymptotic expression for the counting function of the nontrivial Riemann zeros [2]. Their results suggest a strong connection between the spectral statistics of these zeros and classically chaotic systems.

In this poster contribution, we show the emergence of the Riemann zeros within the spectrum of our non-Hermitian Hamiltonian and discuss how periodic orbit theory can be applied.

[1] E. Yakaboylu, arXiv:2408.15135
[2] M. V. Berry and J. P. Keating, SIAM Review 41.2 pp. 236-266

DY 42.14 Wed 15:00 P5

Echo state network prediction of billiard dynamics — •Anna Skopnik, Lukas Seemann, and Martina Hentschel — Institut für Physik, TU Chemnitz, Germany

Machine Learning has attracted a lot of interest recently. Here, we apply an Echo State Network (ESN) algorithm to two mesoscopic billiard systems in order to explore its usability in the prediction of the internal dynamics of ballistic cavities. First, we study the well-known Limaçon system with chaotic dynamics. Second, we study the more complex dynamics in an anisotropis system inspired by bilayer graphene (BLG) representing a mixed space dynamics with regular and chaotic trajectories. Here, we present preliminary results on the training and hyperparameter optimization for both systems, Limaçon and BLG.

DY 42.15 Wed 15:00 P5

Anomalous Dynamics in Complex Quantum Systems — •Irina Petreska[1], Pece Trajanovski[1,2], Ervin Kaminski Lenzi[3], and Trifce Sandev[1,2,4] — [1]Ss. Cyril and Methodius University in Skopje, Macedonia — [2]Macedonian Academy of Sciences and Arts, Skopje, Macedonia — [3]Universidade Estadual de Maringá, Maringá, Brazil — [4]Korea University, Seoul, Korea

We will give an overview of our recent works related to some generalizations of the Schrödinger equation. Special attention will be paid to the fractional Schrödinger equation, pointing out physical examples where the time-fractional Schrödinger equation naturally emerges under certain geometric constraints. Additionally, we include a long-range interaction term, modeled by an integral operator, which captures spatial nonlocalities. Using the Green's function approach, we derive analytical solutions and explore their implications in the time-space domain. Our findings reveal anomalous behavior arising from the interplay of fractional dynamics, nonlocal potentials and memory effects.

DY 43: Poster: Statistical Physics

Time: Wednesday 15:00–18:00 Location: P5

DY 43.1 Wed 15:00 P5

Extended classical nucleation theory for active phase separation in the reversed Ostwald regime — •Wanja Becker[1], Cesare Nardini[2,3], and Michael te Vrugt[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, 55128 Mainz, Germany — [2]Service de Physique de l'Etat Condensé, CEA, CNRS Université Paris-Saclay, CEA-Saclay, 91191 Gif-sur-Yvette, France — [3]Sorbonne Université, CNRS, Laboratoire de Physique Théorique de la Matière Condensée, 75005 Paris, France

Classical nucleation theory (CNT) is a model to describe how rare fluctuations lead to nucleation and thus describes the kinetics of phase transitions. In Ref. [1], CNT was extended to describe phase separation in Active Model B+ - a scalar field theory for active matter - for the case of positive active surface tension. Here, we further extend the theory to be applicable for negative active surface tensions. In this regime a stable fixed-point radius is expected to be found. Droplets smaller than this radius grow and droplets larger than this radius shrink, i.e. reverse Ostwald ripening. In Ref. [1], the theory was formulated by expanding the

order parameter in powers of 1/R, up to order 1/R. Here, terms of order 1/R^2 are included to describe nucleation for negative surface tension. In doing this the effective potential acquires an additional linear contribution. We calculate the prefactor of the linear contribution numerically to determine whether it suffices to capture the nucleation of droplets at negative surface tension that afterwards grow by reversed Ostwald processes.

[1] M. E. Cates and C. Nardini, Phys. Rev. Lett. 130, 098203 (2023)

DY 43.2 Wed 15:00 P5

Classical fractionally charged quasiparticles in kagome lattices and at interfaces — •Jannis Waldmann, Malte Grunert, and Erich Runge — Theoretical Physics I, Institute of Physics, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Interacting systems of charged particles can show fractionally charged excitations, as is well known from the Fractional Quantum Hall Effect of electrons in a magnetic field. Fractionally charged excitations have also been predicted in the absence of magnetic fields for certain lattices with geometric frustrations, e.g., for quantum mechanical models of spinless fermions on the criss-crossed checkerboard lattice [1,2]. Here, we present results on the transport properties of classical particles with nearest-neighbor repulsion on a kagome lattice including Andreev-like reflection at interfaces between frustrated and 'normal', i.e., non-frustrated matter. This involves a coupling between kagome lattice and an infinite particle reservoir via transport channels. Through kinetic Monte Carlo simulations, we study the transition from classical hopping at high temperatures and electric fields to transport dominated by half-charged quasiparticles at low temperatures and special filling factors.

[1] P. Fulde et al., Ann. Phys. 514, 892-900 (2002)
[2] F. Pollmann et al., J. Magn. Magn. Mat. 310, 966-968 (2007)

DY 43.3 Wed 15:00 P5

Non-markovian master equation for Thioacetylacetone Coupled to bosonic bath — •Zahra Sartipi[2], Richard Gundermann[1], Janet Anders[2,3], and Peter Saalfrank[1] — [1]University of Potsdam, Institute of Chemistry, Theoretical Chemistry, Karl-Liebknecht-Str. 24-25, D-14476 Potsdam, Germany — [2]University of Potsdam, Institute of Physics and Astronomy, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany — [3]Physics and Astronomy, University of Exeter, Exeter EX4 4QL, United Kingdom

The Canonically Consistent Quantum Master Equation (CCQME) is used to address intramolec-ular proton transfer in thioacetylacetone , with an N -level quantum system coupled to an organic solvent. In this setup, the solvent is modeled as a harmonic bath (a continuum of oscillators) characterized by a Drude-cutoff Ohmic spectral density.

The results highlight that while the Redfield and CCQME (canonical consistent quantum master equation) approaches agree in the weak-coupling regime, they diverge at stronger couplings. Redfield incorrectly drives the system toward the canonical Gibbs state of the bare system Hamiltonian, neglecting the influence of correlations, and may thus yield thermodynamically inconsistent predictions. By contrast, CCQME incorporates the bath's effect on the system's energy landscape, ensuring relaxation toward the correct mean-force Gibbs state. This guarantees both positivity and consistency with statistical mechanics, even at stronger coupling.

DY 43.4 Wed 15:00 P5

An O(logN) Kinetic Monte Carlo Algorithm for Transport Simulation with Long-Range Interactions — •Bat-Amgalan Bat-Erdene, Roya Ebrahimi Viand, Karsten Reuter, and Sebastian Matera — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

When transport is controlled by activated events, kinetic Monte Carlo (kMC) simulation is the method of choice. However, a characteristic of charge transport is the presence of long-range Coulomb interactions, leading to a complexity of $O(N)$ in the system size N for the updates of the transition rates. In contrast, kMC with only short-range interactions can be made to scale as $O(\log N)$ per step, and thus Coulomb interactions cause a significant computational overhead. We address this issue by a novel time discretization approach. Starting with exact values for the rates, the approach conducts fast incremental updates ($O(\log N)$) in every step based on a truncated short-range potential. Inevitably, this leads to a deviation of the rates from their true values as simulation proceeds. Therefore, a full $O(N \log N)$ recalculation is conducted once every $O(N)$ steps, resulting in an average cost of $O(\log N)$ per step. We demonstrate the scheme for charge transport on a cubic lattice using our in-house kMC framework. Special emphasis is placed on the balance between discretization error and efficiency, as well as the influence of the truncation radius on both.

DY 43.5 Wed 15:00 P5

Quantifying stochastic resonance in bistable systems: a new measure based on passive observation — •Christian Muñoz[1], Bart Vos[1], Till Münker[1], Dorian Marx[1], Matthias Krüger[2], and Timo Betz[1] — [1]Third Institute of Physics - Biophysics, Georg August University Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Institut für Theoretische Physik, Georg August University Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Stochastic resonance (SR) is a noise-assisted phenomenon of broad relevance whose complexity motivates its study in simple and controllable systems. In this work, SR is investigated using a single Brownian particle confined in a bistable potential created with optical tweezers. In such a system, SR emerges from the interplay between thermal fluctuations and the periodic modulation of the potential landscape. First, several well-established approaches from literature are revised to determine under which conditions SR is enhanced. In particular, the strength of the first peak of the residence time distribution displays a clear maximum. Additionally, we propose a new protocol to quantify SR based on the novel quantity of the mean back relaxation (MBR). The new quantifier, which measures the amplitude of the oscillations that MBR displays, shows quantitative agreement with the average work done by the system. Our findings may provide a new approach for analyzing the stochastic energetics of a system by mere passive observation.

DY 43.6 Wed 15:00 P5

Random Organization in a Many-Body Reaction System — •Mishael Derla and Michael Schmiedeberg — Soft Matter Theory Group, Theoretical Physics: Lab for Emergent Phenomena, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen

Random organization refers to certain simplified simulation protocols of the reversibility-irreversibility transition in sheared colloid suspensions. It displays an absorbing state transition believed to be in the conserved directed percolation universality class. We present a related analytical time-continuous many-body reaction-diffusion model. It features two species of spherical grains (of diameter σ): diffusing active grains A (with diffusion constant D), and motionless inactive grains I. A spontaneously decay $A \to I$ with rate μ and overlapping grains react with $A + I \to 2A$ and $I + I \to 2A$, respectively at rate λ. When $\lambda \gg \mu \gg D\sigma^{-2}$ overlapping grains are almost certainly active and non-overlapping ones almost certainly inactive and hence a time-continuous (or small step-size) version of random-organization is recovered.

DY 43.7 Wed 15:00 P5

Stochastic Simulation Algorithm for Spatiotemporal Chemical Master Equations — •Fatemeh Tavakkoli, Roya Ebrahimi Viand, Bat-Amalgam Bat-Erdene, Karsten Reuter, and Sebastian Matera — Fritz-Haber-Institut der MPG, Berlin

Spatiotemporal chemical master equations (SCME) have a number of applications ranging from biochemistry to sociodynamics, and have gained interest in mathematical physics. Describing high-dimensional Markov jump processes, SCMEs are typically not solvable, neither analytically nor numerically, but need to be addressed by stochastic simulation using kinetic Monte Carlo methods. We present a software framework for this purpose based on the Berlin Extended Stochastic Simulation Software (BeESSS). A simple to use Python frontend allows to define an SCME model and the software generates efficient backend C++ code (controllable by the Python frontend). The sparse nature of BeESSS allows to exploit the local nature of SCMEs where space is decomposed into compartments and only neighboring compartments interact. We demonstrate the tool on Lottka-Volterra-type predator-prey models and use it to evaluate the time complexity and memory limitations of our simulation approach.

DY 43.8 Wed 15:00 P5

Bottom-Up DPD Thermostat Parameterization for Coarse-Grained Molecular Liquids — •Karan Venkatesh and Nico F. A. van der Vegt — Technische Universität Darmstadt

Coarse-grained (CG) models substantially accelerate molecular dynamics simulations but often yield dynamical properties that diverge from those of fine-grained (FG) systems. We introduce a dynamic coarse-graining framework that bottom-up parameterizes a Markovian Dissipative Particle Dynamics (DPD) thermostat in conjunction with a CG model of liquid cyclohexane, enabling more consistent reproduction of FG dynamical behavior. We determine the Markovian friction for the DPD thermostat by extracting its distance dependence from the fluctuations of pair forces measured in the FG simulations. The resulting distance-dependent friction is subsequently scaled by an amplitude optimized through an iterative procedure to match the long-time diffusion coefficient[1]. Compared to standard DPD[2], our bottom-up parameterized model significantly improves the reproduction of velocity autocorrelation functions (VACFs) on all time scales. It also yields a closer match to the frequency-dependent viscosity. Overall, this method offers a physically grounded, systematic route to parameterizing DPD thermostats for molecular liquids, preserving the efficiency of single-site coarse-graining while delivering improved dynamics across all time scales.

[1] V. Klippenstein; N F A van der Vegt; J. Chem. Theory Comput. 2023, 19(4), 1099-1110. [2] C. Junghans; M. Praprotnik; K. Kremer; Soft Matter 2008, 4(1), 156-161.

DY 43.9 Wed 15:00 P5

Reduction of interaction order in hard combinatorial optimization through conditionally independent degrees of freedom — •Alexandru Ciobanu[1], David Dahmen[1], John Paul Strachan[2], and Moritz Helias[1] — [1]Forschungszentrum Jülich, Jülich, Germany — [2]Peter Grünberg Institut (PGI-14), Aachen, Germany

Combinatorial optimization problems have a broad range of applications and map to physical systems with complex dynamics. Among them, the 3-SAT problem is prominent due to its NP-complete nature. In physics terms, its solution corresponds to finding the ground state of a disordered Ising spin Hamiltonian with third-order, or tensor, interactions. The large growth of the number of third-order interactions with number of variables poses technical difficulties for the physical implementation of minimizers. In this work, we employ the renormalization group to create a pairwise interacting system from the original third-order system while preserving the free energy. Our procedure utilizes additional degrees of freedom that now exhibit conditional independence. A step-wise trace of the extra variables while running the minimization is therefore computable, yielding a state-dependent effective interaction. We use the effective interaction to reconstruct the original third-order energy spectrum.

DY 43.10 Wed 15:00 P5

From Gradients to Flux: Towards A General Strategy for Non-Equilibrium Molecular Dynamics Simulations — •Daniel Padilla-González, Diego Veloza-Diaz, Mauricio Sevilla, Kurt Kremer, and Robinson Cortes-Huerto — Max Planck Institute for Polymer Research, Mainz, Germany

The numerical simulation of molecular systems under external gradients is crucial for understanding processes in which local solvation and diffusion play a central role, common to applications in nanofluidics and biological transport. Few computational methods can handle the stationary non-equilibrium, open-boundary conditions present in reality while consistently sampling the grand canonical (GC) ensemble in equilibrium. The Hamiltonian Adaptive resolution simulation (AdResS) provides a framework for this purpose by coupling a fully atomistic region to a coarse-grained reservoir that acts as a thermodynamic bath. AdResS can be combined with particle insertion (PI) steps [1] to reproduce GC conditions and to impose controlled gradients by connecting the atomistic region to multiple reservoirs at different state points [2]. This strategy enables the study of non-equilibrium situations in which particle fluxes appear across the system. In this project, by considering simple liquids and mixtures, we aim to evaluate the applicability of the AdResS+PI methodology to the study of stationary flows generated by temperature, density, and concentration gradients.

[1] J. Chem. Phys. 162, 080901 (2025)
[2] J. Chem. Phys. 152, 194104 (2020)

DY 43.11 Wed 15:00 P5

Coexistence in chemically driven mixtures — •Ellen Meyberg[1], Joshua Robinson[2,3], and Thomas Speck[1] — [1]Institute for Theoretical Physics IV, University of Stuttgart, Stuttgart, Germany — [2]STFC Hartree Centre, Sci-Tech Daresbury, Warrington, United Kingdom — [3]H. H. Wills Physics Laboratory, University of Bristol, United Kingdom

Underlying virtually any biological function is the organization of proteins and other molecules in time and space. A current challenge in statistical physics is to uncover universal principles governing the self-organization of macromolecules in crowded environments and driven away from equilibrium. Usually, Ostwald ripening leads to the macroscopic phase separation. In contrast, aggregates of proteins in living cells typically show "size control" and are stable over an extended time without coarsening, which can be rationalized in terms of reverse Ostwald ripening. We study a thermodynamically consistent, chemically driven two component reaction-diffusion system in which particles of one species attract each other. Combining insights from stochastic thermodynamics and active field theories, we aim to understand how phase coexistence is modified by the chemical activity.

DY 43.12 Wed 15:00 P5

Coarsening in the $1D$ XY model with long-range interactions — •Dustin Warkotsch, Fabio Müller, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, 04103 Leipzig, Germany

We investigate the phase-ordering kinetics of the $1D$ XY model with long-range interactions using a simplified version of the recently established fast, hierarchical Metropolis algorithm. Owing to the sparse predictions concerning the nonequilibrium dynamics of this model in one dimension, we seek to close this gap via Monte Carlo simulations with our highly efficient method. Regarding the scaling behavior of correlation function $C(r,t)$, the structure factor $S(k,t)$ and the characteristic length scale $\ell(t)$, we find consistent behavior for all studied growth exponents $\sigma \leq 1$.

DY 43.13 Wed 15:00 P5

Strong coupling phases of conserved growth models are crumpled — •Debayan Jana and Abhik Basu — Saha Institute of Nuclear Physics (SINP), Kolkata, India

We show that stochastically driven nonequilibrium conserved growth models admit generic strong coupling phases for sufficiently strong nonlocal chemical potentials underlying the dynamics. The models exhibit generic roughening transitions between perturbatively accessible weak coupling phases satisfying an exact relation between the scaling exponents in all dimensions d, and strong coupling phases. In dimensions below the critical dimension d_c, the latter phases are unstable and argued to be crumpled, and thus distinct from the well-known strong coupling rough phase of the Kardar-Parisi-Zhang equation in dimensions $d \geq 2$. At d_c, conventional spatio-temporal scaling in the weak coupling phase is logarithmically modulated and are exactly obtained.

DY 43.14 Wed 15:00 P5

Universality of shocks in conserved driven single-file motion with bottlenecks — •Sourav Pal and Abhik Basu — Theory Division, Saha Institute of Nuclear Physics, a CI of Homi Bhabha National Institute, Kolkata, India

Driven single-file motion, in which particles move unidirectionally along one-dimensional channels, sets the paradigm for wide variety of one-dimensional directed movements, ranging from intracellular transport and urban traffic to ant trails and controlled robot swarms. Motivated by the phenomenology of these systems in closed geometries, regulated by number conservation and bottlenecks, we explore the domain walls (DWs) or shocks in a conceptual one-dimensional cellular automaton with a fixed particle number and a bottleneck. For high entry and exit rates of the cellular automaton, and with sufficiently large particle numbers, the DWs formed are independent of the associated rate parameters, revealing *universality* in their *shapes*, which are however enclosed by nonuniversal boundary layers. In contrast, the DWs do depend upon these parameters, if they are small, and hence have nonuniversal shapes, but without boundary layers. Nonuniversal delocalized DWs can be formed by additional tuning of the control parameters. Experimental verification of our theoretical predictions can be performed via high-resolution ribosome profiling on mRNA loops with slow codons, or video imaging of vehicular flow, ant trails, and robotic swarms on confined tracks.

DY 43.15 Wed 15:00 P5

Dynamics of dense phase separation — •Bibhut Sahoo[1] and Peter Sollich[1,2] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, 37077 Göttingen — [2]Department of Mathematics, King's College London, London

Phase separation in mixtures is a ubiquitous phenomenon in nature. In dense systems, it involves an intriguing interplay of phase separation dynamics with slowing down due to crowding effects. We investigate such systems by encoding the approach to dynamic arrest in the kinetic coefficient at the level of a continuum description. We predict the phase behaviour of such kinetically constrained multicomponent mixtures, including density and composition of both mobile and arrested phases, using a suitable constrained free energy minimization. We probe the coarsening dynamics numerically and find, for the baseline one-component case, a crossover between two distinct domain growth power laws. For binary mixtures with three equilibrium phases (one gas and two demixed liquids), we see a Warren-like scenario where collective diffusion first leads to gas-liquid phase separation without fractionation, before the mixture components eventually start to demix. Surprisingly, this demixing dynamics is interface-induced, i.e. it begins at the interfaces of the initial gas-liquid domains. We rationalize this by controlled numerical experiments starting from constrained (without demixing) gas-liquid equilibria and by theoretical analysis of the local spinodal growth rates.

DY 43.16 Wed 15:00 P5

Linear coupling reduces entropy production in nonequilibrium multicomponent systems — •Vansh Kharbanda[1,2], Anton Burnet[1,2], and Benedikt Sabass[1,2] — [1]Faculty of Physics and Center for NanoScience, Ludwig-Maximilians-Universität München, 80752 Munich, Germany — [2]Fakultät Physik, Technische Universität Dortmund, 44227 Dortmund, Germany

Many biological and synthetic systems operate far from equilibrium and pay an energetic cost quantified by the steady-state entropy production rate (EPR). We investigate how linear coupling between subsystems modifies this dissipation in a class of Hurwitz-stable Langevin dynamics. For networks of diffusively coupled Ornstein-Uhlenbeck processes, we derive closed-form expressions for the EPR of n-coupled two-dimensional units and show that any attractive symmetric coupling reduces the EPR, which monotonically approaches the single-unit value in the strong-coupling limit. This behaviour is traced to a suppression of probability currents, driving the collective closer to detailed balance. We then generalize to higher dimensions and arbitrary symmetric coupling topologies and conjecture a structural criterion: commuting coupling and diffusion matrices together with negative semidefinite coupling are sufficient for a monotonic EPR decrease. Violating this criterion generates mismatch-induced irreversible currents, which can increase EPR. Finally, we illustrate this mechanism in nonlinear biological models of bacterial chemotaxis and inner-ear hair bundles, where coupling substantially lowers dissipation without hindering performance metrics.

DY 43.17 Wed 15:00 P5

Energetics of coupled stochastic circular limit-cycle oscillators — •Anton Francis Burnet[1,2], Vansh Kharbanda[1,2], David Tobias[1], and Benedikt Sabass[3,1,2] — [1]Faculty of Physics and Center for NanoScience, Ludwig-Maximilians-Universität München, 80752 Munich, Germany — [2]Department of Veterinary Sciences, Ludwig-Maximilians-Universität München, 80752 Munich, Germany — [3]Fakultät Physik, Technische Universität Dortmund, 44227 Dortmund, Germany

Stochastic oscillations serve important functions in many biological systems, including hair-cell bundles of the inner ear and neuronal activity. Sustaining coherent cycles in noisy environments requires continuous energy dissipation, quantified by the steady-state entropy production rate (EPR). We study an idealized, analytically tractable model of a stochastic circular limit cycle and examine how mutual diffusive coupling in pairs and populations alters dissipation. Three factors contribute to the EPR: intrinsic frequency asynchrony, tangential velocity fluctuations, and mean tangential velocity. The dynamics are characterized by an effective temperature, which depends on diffusion and intrinsic relaxation timescales. For radial (amplitude), phase (Kuramoto-like), and Cartesian couplings, we derive analytical expressions for the EPR and confirm them numerically. Varying the effective temperature and system size strongly influences how the EPR depends on coupling strength and, in some cases, results in qualitatively distinct behaviors. Moreover, the coupling types affect the tangential velocity distributions differently.

DY 43.18 Wed 15:00 P5

Localized Driving of the Jamming Transition in a Quasi-2D Colloidal Platform — •Jordan D. Groh, Timo Betz, and Bart Vos — Drittes Physikalisches Institut, Göttingen, Deutschland

The jamming transition marks the abrupt emergence of rigidity when a dense assembly of particles is compressed beyond a critical packing fraction. Decades of experiments and simulations have identified its static signatures, a sharp rise of the shear modulus and contact-network percolation, for globally driven systems. What remains largely unexplored is how a jammed material reacts to localized perturbations and whether they can steer the system into new metastable states.

We therefore construct a reproducible quasi-2D colloidal chamber that confines a binary mixture of polyacrylamide hydrogel beads (elastic stress sensors) and polystyrene beads (optically addressable active centres). A small fraction of temperature-responsive pNIPAm beads allows us to tune the effective packing fraction; cooling below the LCST swells them, thereby raising the global packing fraction with high precision. High-speed confocal microscopy provides particle trajectories, from which we locate the jamming point and perform contact-network analysis.

The platform enables calibrated optical forces on single beads and local heating-induced volume changes, yielding full spatiotemporal maps of displacement and stress fields. This testbed will allow us to map a local-driving jamming phase diagram, study force-propagation lengths, and ultimately design amorphous metamaterials with programmable mechanical heterogeneity.

DY 43.19 Wed 15:00 P5

Critical behaviour of ferroelectrics with divergence-free polarization — •Svitlana Kondovych[1], Asle Sudbø[2], and Flavio S. Nogueira[1] — [1]Institute for Theoretical Solid State Physics, Leibniz Institute for Solid State and Materials Research Dresden, Helmholzstr. 20, D-01069 Dresden, Germany — [2]Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

Unconventional phase transitions often display unusually large anomalous dimensions, often attributed to fractionalization and emergent gauge fields [1]. Here we show that similar behaviour can arise without fractionalization when the order parameter is constrained to be divergence-free, as occurs in ferroelectrics where the polarization $\vec{P}$ remains locally charge-neutral, div$\vec{P}$=0 [2]. This constraint forces polarization into loop-like textures and reshapes the critical behaviour.

Our analysis reveals a new universality class in which internal symmetry becomes intrinsically linked to spatial dimensionality [3]. The resulting critical point exhibits strongly enhanced fluctuations and a remarkably large anomalous dimension. These findings show that conventional ferroic materials can exhibit non-Landau criticality driven by local conservation laws. This reveals a new conceptual pathway for unconventional critical phenomena and suggests nanoscale ferroelectrics as experimentally accessible platform for exploring these ideas.

[1] T. Senthil, et al., Science 303:1490 (2004). [2] I. A. Lukyanchuk, et al., Phys. Rep. 1110:1 (2025). [3] S. Kondovych, A. Sudbø, F. S. Nogueira, arXiv:2510.13960 (2025).

DY 43.20 Wed 15:00 P5

Nonequilibrium phase transition in single-file transport at high crowding — •Annika Vonhusen[1], Sören Schweers[1], Artem Ryabov[2], and Philipp Maass[1] — [1]Universität Osnabrück, Institut für Physik, Germany — [2]Charles University, Faculty of Mathematics and Physics, Czech Republic

In driven single-file Brownian motion across periodic energy landscapes, fast particle transport can occur for potential barriers orders of magnitude larger than the thermal energy. The fast transport is mediated by solitary cluster waves forming at high crowding of interacting particles [1]. Cluster waves were first predicted theoretically for hard spheres [2] and shortly after confirmed in experiments [3]. Here we show that persistent cluster wave propagation sets in at a critical density and gives rise to a nonequilibrium phase transition that manifests itself in a singular point of the current-density relation [4]. The critical density varies in a complex manner with the particle size and temperature, which can be understood from a simple geometric principle.

[1] A. P. Antonov, A. Vonhusen, A. Ryabov, P. Maass, Nonlinear Dyn. 113, 31529 (2025).
[2] A. P. Antonov, A. Ryabov, P. Maass, Phys. Rev. Lett. 129, 080601 (2022).
[3] E. Cereceda-López, A. P. Antonov, A. Ryabov, P. Maass, and P. Tierno, Nat. Commun. 14, 6448 (2023).
[4] A. Vonhusen, S. Schweers, A. Ryabov, P. Maass, arXiv:2511.16234 (2025), to appear in Chaos.

DY 43.21 Wed 15:00 P5

Sampling of ground states for the bimodal random-field Ising model — •Jana Lukin, Tony Albers, and Martin Weigel — Institut für Physik, TU Chemnitz, 09107 Chemnitz, Germany

The Gaussian random-field Ising model (RFIM) is well understood, largely because its ground state is non-degenerate and can therefore be computed efficiently using polynomial-time optimization methods. In contrast, the bimodal RFIM exhibits degenerate ground states, which has hindered precise numerical investigations of its critical behavior. Here, we introduce a perturbation to lift this degeneracy. This approach enables the application of a max-flow algorithm to obtain exact ground states and thereby allows a more accurate characterization of the phase transition in the bimodal RFIM.

DY 43.22 Wed 15:00 P5

Critical behaviour of non-reciprocal Ising models — •Max Haessler and Martin Weigel — TU Chemnitz Institut für Physik, Chemnitz, Germany

Equilibrium statistical physics is based on symmetric, Hamiltonian interactions fulfilling Newton*s Third Law. On the other hand, active matter like bacteria or bird flocks, predator-prey relations in nature and social systems violate time-reversal symmetry due to non-reciprocal interactions, hence they are non-equilibrium systems.

We try to investigate the fundamental mechanisms that govern such systems by investigating non-reciprocal modifications of the Ising model.

We especially focus on investigating the impact of the non-reciprocal interactions on the critical behaviour of those models.

DY 43.23 Wed 15:00 P5

Analysis of phase transitions in the random-field Blume-Capel model via exact ground state calculations — •Tony Albers, David Müller-Bender, and Martin Weigel — Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany

The random-field Blume-Capel model is a generalization of the well-known Ising model, where spin variables can take three values (-1,0,1) corresponding to three orientations of the spins with respect to an external field. We perform exact ground-state calculations of this 3-label problem using a suitable transformation to a 2-label problem [1] and an advanced graph-cut method called generic cuts [2]. The obtained ground states can be used to study phase transitions in dependence on the zero-field splitting parameter and the strength of the random field resulting in a phase diagram which is compared to the one obtained by a mean-field approximation [3]. Preliminary results suggest the presence of first- and second-order phase transitions. With the help of a finite-size scaling analysis, we obtain a set of critical exponents for the latter and compare them with the exponents of related universality classes.

[1] C. Arora and S. N. Maheshwari, 2014 IEEE Conf. Comput. Vis. Pattern Recognit., 1346 (2014)
[2] C. Arora, S. Banerjee, P. K. Kalra, and S. N. Maheshwari, IEEE Trans. Pattern Anal. Mach. Intell. 37, 1323 (2015)
[3] S. Mukherjee and Sumedha, J. Stat. Phys. 188, 22 (2022)

DY 43.24 Wed 15:00 P5

Shear-driven diffusion process and its generalizations — •Trifce Sandev — Macedonian Academy of Sciences and Arts, Skopje, Macedonia — Ss. Cyril and Methodius University in Skopje, Macedonia — Korea University, Seoul, Korea

We consider different generalizations of the shear-driven diffusion process, which represents a two-dimensional Brownian motion in presence of a linear shear flow. One possible generalization is the shear-driven anomalous diffusion motion which occurs due to the long-tailed waiting time of the particle, effect described by a two-dimensional Fokker-Planck equation with memory kernel. Another possible generalization is the shear-driven finite-velocity diffusion, that is a shear-driven motion, but now, at random times, the walker changes its direc-

tion to the opposite one. The corresponding process can be described by a two-dimensional telegrapher's-like equation. We also explore the corresponding processes under stochastic resetting and find that the systems reach non-equilibrium stationary states in the long time limit that also result in saturation of the evolution of the corresponding mean squared displacement, variance, skewness and kurtosis.

DY 44: Poster: Active Matter, Soft Matter, and Fluids

Time: Wednesday 15:00–18:00 Location: P5

DY 44.1 Wed 15:00 P5

Directed autonomous motion of active Janus particles induced by wall-particle alignment interactions — •Poulami Bag — Presidency University Kolkata

We propose a highly efficient mechanism to rectify the motion of active particles by exploiting particle-wall alignment interactions. Through numerical simulations of active particles' dynamics in a narrow channel, we demonstrate that a slight difference in alignment strength between the top and bottom walls or a small gravitational drag suffices to break upside-down symmetry, leading to rectifying the motion of chiral active particles with over 60% efficiency. In contrast, for achiral swimmers to achieve rectified motion using this protocol, an unbiased fluid flow is necessary that can induce orbiting motion in the particle's dynamics. Thus, an achiral particle subject to Couette flow exhibits spontaneous directed motion due to an upside-down asymmetry in particle-wall alignment interaction. The rectification effects caused by alignment we report are robust against variations in self-propulsion properties, particle's chirality, and the most stable orientation of self-propulsion velocities relative to the walls. Our findings offer insights into controlled active matter transport and could be useful to sort artificial as well as natural microswimmers (such as bacteria and sperm cells) based on their chirality and self-propulsion velocities.

DY 44.2 Wed 15:00 P5

Emergent Interaction in Attractively Coupled Active Particles — •Ritwick Sarkar and Urna Basu — S. N. Bose National Centre for Basic Sciences, India.

We investigate the dynamics of N pair-wise harmonically coupled active Brownian particles (ABPs) in the presence of thermal fluctuations. The harmonic coupling and the bounded nature of the active noise ensure that the relative distance between each pair of particles eventually reaches a stationary state. Depending on the interplay between the active time-scale and the relaxation time-scale associated with the harmonic coupling, three regimes emerge: strong, moderate, and weak coupling. We analytically show that in the strong coupling regime, an effective short-range repulsion emerges between ABP pairs with speed heterogeneity, both in the presence and absence of thermal fluctuations. The short-range repulsion also persists when the ABP pairs are coupled by a generic long-range attractive potential.

[1] Ritwick Sarkar, Urna Basu, Soft Matter 21, 3595-3603 (2025).

[2] Ritwick Sarkar, Sreya Chatterjee, and Urna Basu, J. Phys. A: Math. Theor. 58 415001 (2025).

DY 44.3 Wed 15:00 P5

AMEP: Analyzing Active and Soft Matter Simulations — •Kay-Robert Dormann[1], Lukas Hecht[1], Kai Luca Spanheimer[2], Aritra K. Mukhopadhyay[1], Mahdieh Ebrahimi[1], Suvendu Mandal[1], and Benno Liebchen[1] — [1]Institut für Physik kondensierter Materie, Technische Universität Darmstadt, Darmstadt, Germany — [2]Institut für Theoretische Physik II, Heinrich-Heine-Universität, Düsseldorf, Germany

AMEP [1] is a Python library that focuses on the fast and user-friendly analysis of active and soft matter simulations. It can natively analyze data from molecular dynamics, Brownian dynamics, and continuum simulations from software such as LAMMPS, HOOMD-blue, and GROMACS. With a plethora of methods for calculating observables and visualizing results, AMEP is suitable for calculating complex observables equally for advanced studies of active and soft matter, as well as for beginners in the field. Computationally expensive methods are parallelized to run on any system from laptops and workstations to high-performance computing clusters.

The methods range from correlation functions and order parameters to cluster detection and coarse-graining methods. Due to the Python-based implementation, the methods can be easily extended and individualized. Information and examples are available at https://amepproject.de. AMEP can be installed via pip and conda.

[1] L. Hecht et al., Comput. Phys. Commun. 309, 109483 (2025).

DY 44.4 Wed 15:00 P5

Environmental Control of Self-Aligning Chiral Bristlebots — •Timo Wagner, Thomas Ihle, and Horst-Holger Boltz — University Greifswald, Institute for Physics, Greifswald

The subject of our work is the interplay of two very topical aspects of active matter systems, self-alignment and chirality, with complex environments. Chirality refers to a handedness of the dynamics manifesting itself in circular trajectories and self-alignment is a specific realization of physical memory in which the direction of the actual velocity and that of the self-propulsion are not identical, but are coupled. We present experimental results of an implementation of self-aligning chiral dynamics by custom augmentation of commercial toy bristlebots (Hexbugs) and extend the accessible parameter range by inferring a numerical model capable of reproducing the observable data. In particular, we study the control of edge currents (cf. Caprini et al, arXiv:2509.05053) by chiral environments. Additionally, we show that this simple system is sufficient to observe mode-switching between collectively moving and arrested states in active solids (cf. Hernandez-Lopez et al, PRL 132, 238303 (2024)).

DY 44.5 Wed 15:00 P5

Stochastic Path Integral for the Active Brownian Particle in a Harmonic Potential — •Mike Brandt[1], Carsten Littek[2], and Falko Ziebert[1] — [1]Institut für Theoretische Physik Philosophenweg 19, D-69120 Heidelberg, Germany — [2]Institut für Theoretische Physik Philosophenweg 12, D-69120 Heidelberg, Germany

We present a path-integral approach for the motion of active particles in harmonic traps, developed in our recent preprint [arXiv:2509.26296]. We apply the Martin-Siggia-Rose formalism to the overdamped Langevin equations of an active Brownian particle (ABP). The associated action can be separated into an exactly solvable passive reference motion and an "activity operator" to be treated perturbatively. This method allows for the calculation of the exact, time-dependent correlation functions for the ABP in a harmonic potential. Furthermore, the probability density can be perturbatively expanded in a series, which already captures important qualitative features of the system at low orders. This is exemplified by discussing the transition between a ring-shaped distribution for a weak potential and a peaked distribution for a strong potential in the long-time limit. Finally, we present full time-dependent expressions for the mean-square displacement of the Brownian circle swimmer (BCS), along with comparisons to simulations.

DY 44.6 Wed 15:00 P5

Continuum models for active matter: Derivation and overview — •Juliette Wegner and Sebastian Heidenreich — Physikalisch-Technische Bundesanstalt Braunschweig und Berlin, Abbestr. 2-12, 10587 Berlin, Germany

Turbulence and collective motion in active matter provide an interesting insight into non-equilibrium systems. Many different models have been suggested to describe the prevalent dynamics, mainly including polar and nematic systems. Each of these systems is developed under different assumptions considering different systems, but their similarities and differences are often not obvious.

In our poster we start from a simple micro-swimmer model to derive a general continuum model incorporating both nematic and polar order parameter equations, following the procedure from [1]. To this general continuum model, we then systematically introduced further restrictions and assumptions to derive more specific models which are in line with popular continuum models from literature. Specifically, we obtain models with nematic and polar symmetries similar to those studied by Saintillan and Shelley, as well as active Nematics, and active Polar suspension. Finally, we also consider theories that only incorporate the overall bacterial motion, such as the Toner Tu equation or the hydrodynamic approach of Slomka and Dunkel.

[1] Henning Reinken, Sabine HL Klapp, Markus Bär, and Sebastian Heidenreich. Derivation of a hydrodynamic theory for mesoscale dynamics in microswimmer suspensions. Physical Review E, 97(2):022613, 2018.

DY 44.7 Wed 15:00 P5

Active Brownian ellipsoids in three spatial dimensions — •Sebenzile Tsabedze and Michael te Vrugt — Institut für Physik, Johannes Gutenberg-Universität Mainz, 55128 Mainz, Germany

We investigate ellipsoidal active Brownian particles with alignment interactions in three spatial dimensions that are propelled orthogonal to their symmetry axis. Their propulsion direction makes the particles biaxial, implying that their dynamics is considerably more complex than in the usually considered case of particles being propelled along their symmetry axis. We use Brownian dynamics simulations and assume the particles to interact via a Gay-Berne potential (for the ellipsoidal repulsion) and a Heisenberg potential (for the interaction).

DY 44.8 Wed 15:00 P5

Dynamics of Aligning Active Matter: Mapping to a Schrödinger Equation and Exact Diagonalization — •Tara Steinhöfel, Horst-Holger Boltz, and Thomas Ihle — University Greifswald, Institute for Physics, Greifswald

We investigate models of Viscek-like particles with long-ranged interactions subject to noise and alignment interactions of polar and nematic symmetries. It is shown how the relevant N-particle Fokker–Planck equation can be mapped onto a Schrödinger equation in imaginary time for arbitrary particle numbers. Focusing on the minimal case of $N = 2$, we construct a complete eigenbasis by exact diagonalization of the corresponding self-adjoint Hamiltonian. In a treatment formally equivalent to standard quantum mechanics, this yields the fully time-resolved relaxation of the N-particle-probability density from arbitrarily correlated initial conditions into the stationary state. By marginalization, the one-particle angular modes which include the usual hydrodynamic modes are obtained; we discuss their relaxation backed by agent-based simulations and give comparisons for the resulting exact relaxation rates to mean-field and to predictions from approximate field theories (G. Spera, C. Duclut, M. Durand, J. Tailleur, PRL 132, 078301 (2024)). Furthermore, we discuss possible extensions of the method to $N \geq 3$ particles, as well as modifications due to non-reciprocal interactions.

DY 44.9 Wed 15:00 P5

Absence of chiral long-range order in the 2d non-reciprocal Vicsek model — •Chul-Ung Woo[1], Heiko Rieger[1], and Jae Dong Noh[2] — [1]Department of Theoretical Physics and Center for Biophysics, Saarland University, Saarbrücken, Germany — [2]Department of Physics, University of Seoul, Seoul, Korea

Nonreciprocal interactions in active matter have been predicted to generate homogeneous chiral phases, in which the polarization order parameter rotates at a constant frequency as a result of a nonreciprocal phase transition. Here we revisit the non-reciprocal Vicsek model in two space dimensions with short-range interactons and ask whether the putative chiral phase survives in the thermodynamic limit. Using large-scale simulations, we show that a spatially homogeneous chiral state, while long-lived in small systems, is generically unstable to the spontaneous nucleation of spiral defects that invade the system and drive it into spatio-temporal chaos. The global chiral order parameter, τ exhibits a robust finite-size scaling $\tau(J_-; L) = J_-\tau_r(LJ_-)$, where $J_{=}J_{AB} - J_{BA}$ is the anti-symmetric part of the interaction matrix, with the asymptotic behavior $\tau_r(x) \sim x^{-1}$ at large x, implying that global chirality vanishes in the thermodynamic limit. Controlled droplet-seeding experiments and a Boltzmann kinetic description support the droplet nucleation and growth scenario for the breakdown of chiral order. Our results demonstrate that paradigmatic non-reciprocal flocking models display chiral long-range order only in mean-field, whereas it is only metastable in two space dimensions and replaced there by spatio-temporal chaos.

DY 44.10 Wed 15:00 P5

Phase properties of constant density interacting flocks — •Astik Haldar and Heiko Rieger — Center for Biophysics & Department of Theoretical Physics, Universität des Saarlandes, Saarbruecken 66123, Germany

We present a field-theoretic study of a mixture of two polar Malthusian species in two dimensions with distinct aligning and propulsion strengths. The system exhibits rich phase behavior, including oriented flocking states (both parallel and anti-parallel) and a coherently rotating chiral phase. We map the parameter regions for these phases and characterize their universal properties.

DY 44.11 Wed 15:00 P5

Influence of shape on dynamic properties of magnetic active particles — •Ekaterina Novak[1], Elena Pyanzina[1], Tatyana Belyaeva[1], and Sofia Kantorovich[2] — [1]Ekaterinburg, Russia — [2]University of Vienna, Vienna, Austria

This study investigates the influence of shape on the dynamic properties of active magnetic particles. The focus is on ellipsoidal particles of two variations and spherical particles, aiming to understand the relationship between particle shape and motion characteristics. The research is motivated by the need to improve the control and efficiency of active particles, which have significant potential in medical and technological applications, such as precise drug delivery.

Active particles, inspired by natural systems like bacteria, can convert chemical energy into directed motion. However, challenges arise in maintaining precise control over their orientation and direction over time. By introducing a rigidly fixed permanent dipole moment and utilizing a strong external magnetic field, it is possible to minimize thermal fluctuations and achieve precise control.

The study also explores the anisotropic properties of ellipsoidal particles, which can have two possible orientations of the magnetic moment depending on the material. This behavior is analogous to magnetic cubes with integrated nanomotors. The findings from this research contribute to the development of optimal particle shapes for effective transportations, opening new possibilities in various fields.

The work was financially supported by the RSF grant No. 25-22-00327.

DY 44.12 Wed 15:00 P5

Order and shape dependence of mechanical relaxation in proliferating active matter — Jonas Isensee[1,2], •Finn Albrecht[1,2], Lukas Hupe[1,2], and Philip Bittihn[1,2] — [1]MPI for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for the Dynamics of Complex Systems, University of Göttingen, Germany

The collective behavior of dense, proliferating anisotropic active matter, such as elongated cells or bacteria, arises from an interplay between growth, division, and mechanical interactions, often mediated by particle shape. In classical models of prolate, rod-like growth, flow-induced alignment and division geometry reinforce one another, leading to robust nematic order under confinement. Here we introduce a complementary regime by considering smooth convex particles whose geometry can be oblate for part or all of their growth cycle, creating a tunable competition between these two alignment mechanisms. Using agent-based simulations of particles with tunable curvature profiles in both channel and open-domain geometries, we systematically vary particle shapes to span regimes of cooperation and competition between ordering cues. We find that oblate growth can reverse classical flow-alignment, destabilize microdomain formation in intermediate regimes, and, in combination with variations in curvature, lead to entirely new global order patterns. These findings are then reconciled using an order- and shape-dependent mechanical relaxation interpretation that is supported by explicit measurements.

DY 44.13 Wed 15:00 P5

The impact of particle shape for self-diffusiophoresis — •Leif Peters[1], Benjamin J. Walker[2], and Christina Kurzthaler[1,3,4] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany — [2]Department of Mathematics, University College London, WC1H 0AY London, UK — [3]Center for Systems Biology Dresden, Pfotenhauerstraße 108, 01307 Dresden, Germany — [4]Cluster of Excellence, Physics of Life, TU Dresden, Arnoldstraße 18, 01062 Dresden, Germany

Self-diffusiophoretic micron-sized particles are paradigmatic examples of synthetic microswimmers where the swimming behavior depends not only on the patterning of the chemically active surface, i.e., the activity and phoretic mobility, but also on the particle shape itself. Accounting for the governing chemical and hydrodynamic equations we investigate how the particle shape influences the self-propulsion velocity and the agent's chemotactic behavior. To derive analytical expressions for anisotropic and curved particles we employ slender body theory and the Lorentz reciprocal theorem. Furthermore, we corroborate our results with a boundary element method. Our numerical framework allows going beyond the slender-particle limit and lays the foundation for addressing the physics of hydro-chemically interacting active agents and the emergent collective phenomena.

DY 44.14 Wed 15:00 P5

Dynamics of thermophoretic Janus particles in homogeneous light fields — •Samad Mahmoudi, Franziska Michaela Braun, and Regine von Klitzing — Institute of Condensed Matter Physics,TU Darmstadt, Hochschulstraße 8 64289 Darmstadt

We study the thermophoretic motion and orientational dynamics of individual Au-polystyrene Janus particles under uniform laser illumination. Light-driven Janus colloids serve as a model system for active Brownian motion and non-equilibrium transport in soft matter. The particles are illuminated by a defocused, approximately homogeneous laser spot and observed with dark-field microscopy. Image-processing routines in Python yield long-time trajectories, center-of-mass positions and in-plane orientations of the gold cap. From the mean-squared displacement we extract effective self-propulsion velocities and compare them with active Brownian particle models and simple expectations for thermophoretic motion. Our first measurements show that the tracking procedure resolves both translational and rotational motion of single Janus particles and yields thermophoretic velocities in the expected range for micrometer-sized swimmers. In future work, we will use this analysis to study how light gradients and cap design can create transient barriers for Janus particles and control their thermophoretic motion.

DY 44.15 Wed 15:00 P5

Static and dynamic states of compound drops on heated substrates — •Dominik Thy, Jan Diekmann, and Uwe Thiele — Institute of Theoretical Physics, University of Münster, Wilhelm-Klemm-Str. 9, 48149 Münster, Germany

We present a mesoscopic thin-film model for interface dominated compound drops including a vertical temperature gradient [1]. Starting with established findings for the passive case, i.e., (isothermal) gradient dynamics that show relaxation to equilibrated compound drops of different configurations [2], we then drive the system out of equilibrium. To this end, we introduce a vertical temperature gradient that renders the system active by introducing thermal Marangoni flows. We discuss different static and dynamic states.

[1] Pototsky, Bestehorn, Merkt, Thiele. The Journal of Chemical Physics, 2005. doi: 10.1063/1.1927512.

[2] Diekmann, Thiele. Physical Review Fluids, 2025. doi: 10.1103/physrevfluids.10.024002.

DY 44.16 Wed 15:00 P5

Evaporation Induced Salt Precipitation in Porous Media: A Lattice Boltzmann Approach — •Alexander Reinauer[1], Louis Oberer[1], Alexander Schlaich[2], and Christian Holm[1] — [1]Institute for Computational Physics, Stuttgart, Germany — [2]Institute for Physics of Functional Materials, Hamburg University of Technology, Hamburg, Germany

We present a lattice Boltzmann model for simulating coupled evaporation and salt precipitation in porous media. The approach integrates Shan-Chen multiphase flow with a volume-based discretization of salt transport and incorporates a precipitation rule, which converts fluid cells into solid crystals once the local concentration exceeds a crystallization threshold.

The model is validated by reproducing analytical predictions for crystal growth. Besides, it features a tunable evaporation rate, enabling pore-scale studies of evaporation-induced salt precipitation. Investigations of the wettabilities of both the salt and the porous matrix reveal a pronounced impact on precipitation patterns. The simulations show distinct shifts in pore-clogging behavior depending on the relative wetting properties, with highly wetting crystals causing the strongest clogging and the slowest evaporation, arising from how wetting influences the spatial distribution of precipitation.

DY 44.17 Wed 15:00 P5

Power-Law to Maxwell Transition in Soft Glassy Materials under Large Amplitude Oscillations — •Raffaele Mendozza[1], Shanay Zafari[1], Sarah Köster[1], and Peter Sollich[1,2] — [1]Institute for Theoretical Physics, University of Göttingen, Göttingen, Germany — [2]Department of Mathematics, King's College London, London, United Kingdom

Soft glassy materials, such as colloidal suspensions and biological networks, exhibit complex rheological behaviour. We present a modified version of the Soft Glassy Rheology (SGR) model, introducing an upper cutoff on the yield rate that prevents unphysical yield rate increases at large strains. In the nonlinear response to step strains, the modified model exhibits a crossover from short-time exponential (Maxwell-like) relaxation to the power law relaxation obtained in the original model. This qualitatively reproduces results from strain-ramp experiments on actin networks. Under large amplitude oscillatory strain (LAOS) we similarly find Maxwell-like viscoelastic spectra at higher frequencies, crossing over to the original SGR power-law spectrum at low frequencies. We demonstrate that this can be rationalized qualitatively by Fourier transforming the nonlinear step strain results. The nonlinear spectra break the usual phase angle relations for power law (linear) response, however, which we explain using a quasistatic approximation. The stress response to LAOS at fixed frequency becomes more anharmonic for increasing strain amplitudes up to a critical value; beyond this point, harmonicity is eventually restored due to the crossover to Maxwell behavior.

DY 44.18 Wed 15:00 P5

Gelation versus bundling in parallel-aligned directed polymers — •Panayotis Benetatos and Minsu Yi — Department of Physics, Kyungpook National University, Daegu, South Korea

In many soft-matter and biological systems, bundles of similarly charged parallel-aligned filaments form when a short-range attraction overcomes the longer-range electrostatic repulsion. It is also known that permanent cross-links in parallel-aligned directed polymers can yield a directed gel with a finite in-plane shear modulus. Because permanent cross-links effectively act as a short-range attraction, we are motivated to investigate the interplay of gelation versus bundling in such a system. Using the theoretical tools of replica field theory, where the cross-links are treated as quenched disorder following the Deam-Edwards distribution, we show that the effective attraction due to spring-like permanent cross-links is too weak to induce bundling before the gelation transition.

DY 44.19 Wed 15:00 P5

Thermoresponsive liquid-liquid phase behaviour of biomolecular condensates in programmable thermal landscapes — •Ilona Kundi[1], Falko Schmidt[1], Rasmus Krogh Norrild[2], Alexander Kai Büll[2], and Frank Cichos[1] — [1]Peter Debye Institute for Soft Matter Physics, Leipzig University, 04103 Leipzig, Germany — [2]Department of Biotechnology and Biomedicine, DTU, 2800 Kgs. Lyngby, Denmark

Liquid-liquid phase separation (LLPS) of biomolecules drives the formation of membraneless organelles in cells. The LLPS behavior of the intrinsically disordered N-terminal region of the DEAD-box helicase DDX4 (DDX4N) is examined under precisely controlled and reconfigurable local temperature fields.

Locally tunable thermal landscapes are generated by scanning a focused laser beam over an absorbing metal thin film, creating microscale temperature profiles around DDX4N condensates. Here, the spatiotemporal evolution of condensate nucleation, growth, coarsening, and dissolution is tracked, linking local thermal forces to mesoscale LLPS dynamics.

By repeatedly cycling the temperature across the LLPS boundary, kinetic and thermodynamic parameters of the DDX4N phase transition are measured, revealing switching thresholds, hysteresis, and condensate material properties. Controlled microthermal perturbations thus provide a powerful means to probe and program protein LLPS, establishing a versatile platform for testing models of thermoresponsive intrinsically disordered proteins.

DY 44.20 Wed 15:00 P5

Rheology of Semi-Flexible Polymer Networks — •Sanjay Bhandarkar[1] and Peter Sollich[1,2] — [1]Institute for Theoretical Physics, University of Göttingen, Germany — [2]Department of Mathematics, King's College London, London

Semiflexible polymers, both in solution and organized into networks, continue to be a major focus in biological physics owing to their critical relevance to the structural and mechanical functions of living systems. The mechanics of the cytoskeleton emerges from the collective properties of semiflexible biopolymers such as actin filaments, microtubules, and intermediate filaments [1,2]. We investigate the rheology of semiflexible polymer networks using molecular dynamics simulations, performing Small-Amplitude Oscillatory Shear (SAOS) tests on permanently cross-linked systems to demonstrate how filament stiffness and monomer density control the frequency dependence of the complex shear modulus G*. In addition, we examine the connection between power-law rheology and the self-similar structural features observed in biopolymer networks and gels [3,4]. We further analyze how crosslinking dynamics and activity-induced stresses modify the network mechanics. Together, this rheological framework lays the groundwork for future models that incorporate more detailed structural and biochemical complexity.

[1] P. Kollmannsberger and B. Fabry, 2011
[2] Broedersz, C. P. and MacKintosh, F. C., 2014
[3] J. Martin, D. Adolf, and J. P. Wilcoxon, 1989
[4] M. Bantawa et al., 2023

DY 44.21 Wed 15:00 P5

Dynamic magnetic susceptibility of magnetic elastomers taking into account the internal magnetic anisotropy of particles — •Alla Dobroserdova[1] and Sofia Kantorovich[2] — [1]Ekaterinburg, Russia — [2]University of Vienna, Vienna, Austria

Magnetic elastomers are non-magnetic elastic matrices with embedded magnetic particles. These systems can be controlled using an external magnetic field, which provides the basis for their practical applications in both industry and medicine.

The aim of this study is to investigate the dynamic magnetic response of magnetic elastomers. Two previously developed elastomer models suitable for molecular dynamics simulations are used. This study reveals the dependence of the response on the intensity of interparticle interactions, the rigidity of the elastic non-magnetic matrix, and the internal magnetic anisotropy of the particles.

Support by RSF (project 25-22-00270) is acknowledged.

DY 44.22 Wed 15:00 P5

Computer simulation of the dynamic susceptibility of ellipsoidal multicore particles: the effect of inter-core interaction — •Vladimir Zverev[1], Ekaterina Novak[1], Andrey Kuznetzov[2], and Sofia Kantorovich[2] — [1]Ekaterinburg, Russia — [2]University of Vienna, Vienna, Austria

This report presents a study of the magnetic dynamic susceptibility of MNPs under the influence of a low-amplitude alternating plane-polarized magnetic field. We consider ellipsoidal MNPs modeled as a collection of spherical subparticles with fixed spatial positions relative to each other. This corresponds to a scenario where nanoparticles are embedded in a polymer or other rigid non-magnetic matrix. The modeling employs the molecular dynamics simulations using the ESPResSo software package, which accounts for magnetic anisotropy. The model is based on the concept proposed in [1]. The core idea is that the orientation of the magnetic moment in a subparticle is determined by solving the stochastic Landau-Lifshitz-Gilbert equation in a reference frame fixed to the particle body, neglecting precession and the Barnett effect. To form a single-domain-like particle assembly, their common convex hull approximates an elongated ellipsoid of revolution with a preset aspect ratio, enabling comparison with spherical particles.

The work was financially supported by the Russian Science Foundation grant No. 25-22-00338.

[1] Pyanzina E. S. et al. Dynamic Magnetic Response of Multicore Particles: The Role of Grain Magnetic Anisotropy and Intergrain Interactions //Journal of Molecular Liquids. - 2025. - P.126842.

DY 45: Focus Session: Physics of AI – Part I (joint session SOE/DY)

The focus session is organized by Claudius Gros (Goethe-Universität Franfurt), Moritz Helias (Forschungszentrum Jülich), Peter Sollich (Georg-August-Universität Göttingen)

This focus session brings together experts in the field of physics-inspired theory of machine learning and artificial intelligence, who aim to supplement the engineering-driven success of AI by a principled theory of neural information processing. Contributions will address how statistical and dynamical perspectives explain learning in modern AI systems and how these insights support interpretability as well as prediction of performance, generalization, and the required resources.

Time: Thursday 9:30–11:15 Location: GÖR/0226

Invited Talk DY 45.1 Thu 9:30 GÖR/0226

Generative AI and diffusion models: a statistical physics approach — •Giulio Biroli — Ecole Normale Superieure, Paris, France

Generative AI represents a groundbreaking development within the broader *Machine Learning Revolution,* significantly influencing technology, science, and society. In this colloquium, I will focus on the state-of-the-art *diffusion models*, which are currently used to generate images, videos, and sounds. They are very fascinating algorithms for physicists, as they are very much connected to concepts from stochastic thermodynamics, particularly time-reversed Langevin dynamics. These diffusion models start from a simple white noise input and make it evolve through a Langevin process to generate complex outputs such as images, videos, and sounds. I will show that statistical physics provides principles and methods to characterise this generation process. Specifically, I will discuss how phenomena such as the transition from memorization to generalization and the emergence of features can be understood through the lens of symmetry breaking, phase transitions, slow dynamics, and methods used to study disordered systems.

DY 45.2 Thu 10:00 GÖR/0226

Statistical Physics of Classifier-free Diffusion Guidance — •Enrico Ventura[1], Beatrice Achilli[1], Carlo Lucibello[1], and Luca Ambrogioni[2] — [1]Bocconi University, Milan, Italy — [2]Radboud University, Nijmegen, The Netherlands

Classifier-free Guidance (CFG) is a simple yet effective technique that helps diffusion models better follow a user's prompt. By combining standard unconditional diffusion with diffusion conditioned on a specific class of the data, it steers generation toward samples (e.g. images, videos or text) that more clearly reflect the intended content. We propose a description of the sampling dynamics of a diffusion model under CFG based on the statistical mechanics of disordered systems. Specifically, we study the time-dependent transformation of the diffusion potential providing a quantitative prediction of the way a complex target distribution is deformed to improve data generation. Moreover, we leverage our results to propose alternative theory-based guidance schedules that enhance such beneficial effects.

DY 45.3 Thu 10:15 GÖR/0226

Fundamental operating regimes, hyper-parameter fine-tuning and glassiness: towards an interpretable replica-theory for trained restricted Boltzmann machines — •Alberto Fachechi[1], Elena Agliari[1], Miriam Aquaro[1], Anthony Coolen[2], and Menno Mulder[2] — [1]Department of Mathematics, Sapienza University of Roma, P. le A. Moro 5, 00185 Roma, Italy — [2]Theoretical Biophysics, DCN Donders Institute, Faculty of Science, Radboud University, 6525 AJ Nijmegen, The Netherlands

Since the seminal work by Amit, Gutfreund and Sompolinsky, statistical mechanics of spin-glasses with structural disorder has acquired a crucial role in theoretical investigations of artificial neural networks, as it enables the representation of their generalization and information processing capabilities as phases within the space of parameters. We study the relaxation towards equilibrium of the training procedure of restricted Boltzmann machines with a binary visible layer and a Gaussian hidden layer with an unlabelled dataset consisting of noisy realizations of a single ground pattern. We develop a statistical mechanics framework to describe the network generative capabilities by exploiting replica theory. We outline the effective control parameters (e.g., the relative number of weights to be trained, the regularization parameter), whose tuning can yield qualitatively different operative regimes. We also provide analytical and numerical evidence for the existence of a sub-region in the space of the hyperparameters where replica-symmetry breaking occurs.

DY 45.4 Thu 10:30 GÖR/0226

Mirror, Mirror of the Flow: How Does Regularization Shape Implicit Bias? — •Tom Jacobs, Chao Zhou, and Rebekka Burkholz — CISPA Helmholtz Center, Saarbrucken, Germany

Implicit bias plays an important role in explaining how overparameterized models generalize well. Explicit regularization like weight decay is often employed in addition to prevent overfitting. While both concepts have been studied separately, in practice, they often act in tandem. Understanding their interplay is key to controlling the shape and strength of implicit bias, as it can be modified by explicit regularization. To this end, we incorporate explicit regularization into the mirror flow framework and analyze its lasting effects on the geometry of the training dynamics, covering three distinct effects: positional bias, type of bias, and range shrinking. The mirror flow framework relies on Noether style parameter symmetry preservation, the regularization controls them. Our analytical approach encompasses a broad class of problems, including sparse coding, matrix sensing, single-layer attention, and LoRA, for which we demonstrate the utility of our insights. To exploit the lasting effect of regularization and highlight the potential benefit of dynamic weight decay schedules, we propose to switch off weight decay during training, which can improve generalization, as we demonstrate in experiments.

DY 45.5 Thu 10:45 GÖR/0226

Generalization performance of narrow one-hidden layer networks in the teacher-student setting — Rodrigo Pérez Ortiz[1], •Gibbs Nwemadji[2], Jean Barbier[3], Federica Gerace[1], Alessandro Ingrosso[4], Clarissa Lauditi[5], and Enrico Malatesta[6] — [1]Alma Mater Studiorum * Università di Bologna (Unibo), Bologna, Italy — [2]International School of Advanced Studies (SISSA), Trieste, Italy — [3]The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy — [4]Radboud University, Nijmegen, The Netherlands — [5]Harvard University, Cambridge, US — [6]Bocconi University, Milano, Italy

Generalization on simple input-output distributions is best studied in the teacher-student setting, but fully connected one-hidden-layer networks with generic activations still lack a complete theory. We develop such a framework for networks with a large but finite number of hidden neurons, using statistical-physics tools to obtain closed-form predictions for both Bayesian and ERM estimators through a few summary statistics. We also identify a specialization transition when the sample size matches the number of parameters. The resulting theory accurately predicts generalization errors for networks trained with Langevin dynamics or standard full-batch gradient descent.

DY 45.6 Thu 11:00 GÖR/0226

Testing generalization through tiny task switching frameworks — •Daniel Henrik Nevermann and Claudius Gros — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Deutschland

With an ever-growing interest in advancing the performance and efficiency of large language models (LLMs), and therein particularly the transformer architecture, the need for tiny testing frameworks is pressing, as many researchers cannot afford to train models on large GPU clusters. We here propose a tiny testing framework, extending the recently published IARC task switching framework, that despite being trivial to implement offers suitable complexity to be non-trivial to learn for small scale transformer models with a few million parameters or less. Beyond model benchmarking, the framework is also suitable for probing phenomena relevant to problems arising in physics of AI, where controlled, interpretable testbeds are essential. The proposed training and evaluation scheme relies on integer sequences to be predicted by the model. These integer sequences are generated by simple deterministic tasks designed to abstract typical challenges arising in natural language processing, such as short and long range correlations, or context awareness. Within the sequences, tasks are randomly switched, where a switch is indicated by a control token. An important quality of LLMs is the ability to generalize at inference time. We here extend the existing task switching framework with new tasks able to probe models generalization capacities in a tiny, yet meaningful manner.

DY 46: Many-body Quantum Dynamics I (joint session DY/TT)

Time: Thursday 9:30–12:45 Location: HÜL/S186

DY 46.1 Thu 9:30 HÜL/S186

Nonequilibrium transport in adaptive fermionic circuits — •Paul Weiss[1], Karim Chahine[2], and Michael Buchhold[1] — [1]Department of Theoretical Physics, Universität Innsbruck, Austria — [2]Institute for Theoretical Physics, University of Cologne, Germany

We investigate nonequilibrium dynamics in one-dimensional adaptive fermionic circuits, where monitored fermions undergo local unitary evolution conditioned on measurement outcomes. By tuning the measurement strength and the duration of the unitary gates, the dynamics can be continuously interpolated between incoherent, classical transport and coherence-dominated quantum transport. In the classical limit, we recover the asymmetric simple exclusion process (ASEP), while in the quantum regime we uncover a coherent analogue of the Burgers equation along with coherence-enhanced Kardar-Parisi-Zhang (KPZ) transport. Our analytical approach, based on transport equations and Keldysh field theory, is supported by numerical simulations.

DY 46.2 Thu 9:45 HÜL/S186

Frustration-Free Control and Absorbing-State Transport in Entangled State Preparation — •Tobias Dörstel[1,2], Thomas Iadecola[3,4,5], Justin H. Wilson[6,7], and Michael Buchhold[1,2] — [1]Department of Theoretical Physics, University of Innsbruck, Austria — [2]Institute for Theoretical Physics, University of Cologne, Germany — [3]Department of Physics, The Pennsylvania State University, USA — [4]Institute for Computational and Data Sciences, The Pennsylvania State University, USA — [5]Materials Research Institute, The Pennsylvania State University, USA — [6]Department of Physics and Astronomy, Louisiana State University, USA — [7]Center for Computation and Technology, Louisiana State University, USA

We study frustration-free control, a measurement-feedback protocol for quantum state preparation that extends the concept of frustration-free Hamiltonians to stochastic dynamics. The protocol drives many-body systems into highly entangled target states, common dark states of all measurement projectors, through minimal local unitary corrections that realize an absorbing-state dynamics without post-selection. We show that relaxation to the target state is governed by emergent transport of nonlocal charges, such as singlet excitations in SU(2)-symmetric dynamics. While measurement-feedback annihilates compatible charge configurations, both measurement and scrambling unitaries induce charge transport and thus determine the convergence time. Mapping a baseline model of SU(N) SWAP measurements with local corrections to a solvable absorbing random walk yields a runtime scaling $t \sim L^z$ with transport exponent $z = 2$.

DY 46.3 Thu 10:00 HÜL/S186

Quantum typicality approach to energy flow between two spin-chain domains at different temperatures — Laurenz Beckemeyer[1], •Markus Kraft[1], Mariel Kempa[1], Dirk Schuricht[2], and Robin Steinigeweg[1] — [1]University of Osnabrück, Department of Mathematics/Computer Science/Physics,D-49076 Osnabrück, Germany — [2]Institute for Theoretical Physics, Utrecht University, 3584CC Utrecht, The Netherlands

We discuss a quantum typicality approach to examine systems composed of two subsystems at different temperatures. While dynamical quantum typicality is usually used to simulate high-temperature dynamics, we also investigate low-temperature dynamics using the method. To test our method, we investigate the energy current between subsystems at different temperatures in various paradigmatic spin-1/2 chains, specifically the XX chain, the critical transverse-field Ising chain, and the XXZ chain. We compare our numerics to existing analytical results and find a convincing agreement for the energy current in the steady state for all considered models and temperatures.

[1] Beckemeyer et al. arXiv:2507.23439

DY 46.4 Thu 10:15 HÜL/S186

Revisiting boundary-driven method for transport: Finite-size effects and the role of system-bath coupling — •Mariel Kempa[1], Markus Kraft[1], Sourav Nandy[2], Jacek Herbrych[3], Jiaozi Wang[1], Jochen Gemmer[1], and Robin Steinigeweg[1] — [1]University of Osnabrueck, Osnabrueck, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]Wroclaw University of Science and Technology, Wroclaw, Poland

Understanding transport in interacting quantum many-body systems is a central challenge in condensed matter and statistical physics. Numerical studies typically rely on two main approaches: Dynamics of linear-response functions in closed systems and Markovian dynamics governed by master equations for boundary-driven open systems. While the equivalence of their dynamical behavior has been explored in recent studies, a systematic comparison of the transport coefficients obtained from these two classes of methods remains an open question. Here, we address this gap by comparing and contrasting the dc diffusion constant $\mathscr{D}_{\mathrm{dc}}$ computed from the aforementioned two approaches. We find a clear mismatch between the two, with $\mathscr{D}_{\mathrm{dc}}$ exhibiting a strong dependence on the system-bath coupling for the boundary-driven technique, highlighting fundamental limitations of such a method in calculating the transport coefficients related to asymptotic dynamical behavior of the system. We trace the origin of this mismatch to the incorrect order of limits of time $t \to \infty$ and system size $L \to \infty$, which we argue to be intrinsic to boundary-driven setups.

DY 46.5 Thu 10:30 HÜL/S186

Synchronized Aharonov-Bohm Motifs via Engineered Dissipation — •Christopher Wächtler and Gloria Platero — ICMM-CSIC, Madrdi, Spain

The interplay between external gauge fields and lattice geometry can induce extreme localization dynamics through complete destructive interference. We show that combining this flux-induced localization with engineered dissipation leads to robust spin synchronization in rotationally symmetric spin geometries, referred to as Aharonov-Bohm motifs, with cyclic symmetries of any order. The synchronized dynamics is independent of initial conditions and features entanglement among spins within each motif. We further demonstrate that multiple motifs can fully synchronize when coupled, which is achieved by applying additional collective dissipation acting on all intra-motif spins. These results reveal a direct connection between flux-induced localization, dissipative engineering, and collective quantum synchronization.

DY 46.6 Thu 10:45 HÜL/S186

Krylov space dynamics of ergodic and dynamically frozen Floquet systems — •Luke Staszewski[1], Asmi Haldar[2], Pieter Claeys[1], and Alexander Wietek[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Laboratoire de Physique Theorique - IRSAMC, Toulouse

In isolated quantum many-body systems periodically driven in time, the asymptotic dynamics at late times can exhibit distinct behavior such as thermalization or dynamical freezing. Understanding the properties of and the convergence towards infinite-time (nonequilibrium) steady states however remains a challenging endeavor. We propose a physically motivated Krylov space perspective on Floquet thermalization which offers a natural framework to study rates of convergence towards steady states and, simultaneously, an efficient numerical algorithm to evaluate infinite-time averages of observables within the diagonal ensemble. The effectiveness of our algorithm is demonstrated by applying it to the periodically driven mixed-field Ising model, reaching system sizes of up to 30 spins. Our method successfully resolves the transition between the ergodic and dynamically frozen phases and provides insight into the nature of the Floquet eigenstates across the phase diagram. Furthermore, we show that the long-time behavior is encoded within the localization properties of the Ritz vectors under the Floquet evolution, providing an accurate diagnostic of ergodicity.

15 min. break

DY 46.7 Thu 11:15 HÜL/S186

Chaotic many-body quantum dynamics, spectral correlations, and energy diffusion — •Dominik Hahn and John Chalker — Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

We present results on the quantum dynamics of a minimal model with spatial structure and local interactions. The model features a time-independent Hamiltonian, in contrast to the widely studied quantum circuits, and is analytically tractable in the limit of large local Hilbert space dimension and weak intersite coupling. In this regime, we show that the energy dynamics are governed by a classical master equation exhibiting diffusive behavior. Furthermore, we demonstrate that the spectral form factor can be expressed exactly in terms of the solution to this master equation, demonstrating how the linear ramp emerges at long times, while locality gives rise to an additional enhancement at short times.

DY 46.8 Thu 11:30 HÜL/S186

Dissipative diffusion in quantum state preparation — •Tim Pokart[1], Lukas König[1], Sebastian Diehl[2], and Jan Carl Budich[1,3,4] — [1]Institute of Theoretical Physics, Technische Universität Dresden — [2]Institut für Theoretische Physik, Universität zu Köln, 50937 Cologne, Germany — [3]Würzburg-Dresden Cluster of Excellence ct.qmat, 01062 Dresden, Germany — [4]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

Dissipative quantum protocols that engineer a desired state as their dark state provide a powerful route to preparing quantum many-body states. We investigate a number conserving variant of such a dissipative protocol which is able to stabilize a topologically nontrivial phase. We show that the protocol admits a unique and stable dark state. Furthermore, we find that the cooling is diffusive in nature, supported by both analytical arguments and numerical simulations.

DY 46.9 Thu 11:45 HÜL/S186

First principles simulation of spin diffusion using dynamic mean-fields — •Timo Grässer[1], Matthias Ernst[1], and Götz S. Uhrig[2] — [1]Institute of Molecular Physical Science, ETH Zurich, 8093 Zurich, Switzerland — [2]Condensed Matter Physics, TU Dortmund University, 44227 Dortmund, Germany

The transfer of a globally conserved polarization among a homogeneous spin ensemble is called spin diffusion and one of the most important phenomena in the broad field of magnetic resonance. Describing spin diffusion theoretically is a notoriously difficult task due to the large number of spins involved. We use a description through dynamic mean-fields (dubbed spinDMFT [1]) to derive an effective model for spectral spin diffusion. The approach is benchmarked for two crystalline test samples, malonic acid and dipotassium α-D-glucopyranose-1-phosphate dihydrate, yielding a remarkable agreement with experimental data and requiring only little computational effort. This strongly supports the use of spinDMFT, which may be extended in future works to understand spin diffusion in dynamic nuclear polarization (DNP) experiments [2].

[1] T. Gräßer et al., Phys. Rev. Research 3, 043168 (2021), DOI 10.1103/PhysRevResearch.3.043168

[2] J. Eills et al., Chem. Rev. 123, 1417 (2023), DOI 10.1021/acs.chemrev.2c00534

DY 46.10 Thu 12:00 HÜL/S186

Simulating universal long-time dynamics in integrable quantum spin chains — •Angelo Valli[1], Catalin Pascu Moca[2], Miklos Antal Werner[3], Marton Kormos[1], Doru Sticlet[6], Balazs Dora[1], Ziga Krajnik[4], Tomaz Prosen[5], and Gergely Zarand[1] — [1]Budapest University of Technology and Economics, Budapest (Hungary) — [2]University of Oradea, Oradea (Romania) — [3]Wigner Research Centre for Physics, Budapest (Hungary) — [4]New York University, New York (USA) — [5]University of Ljubljana, Ljubljana (Slovenia) — [6]National Institute for R&D of Isotopic and Molecular Technologies, Cluj-Napoca (Romania)

We introduce a novel tensor-network approach to calculate cumulants of the full counting statistics to unprecedentedly long times. We investigate spin-transfer in quantum spin chains, where the superdiffusive transport with dynamical exponent z=3/2 has been conjectured to fall within the Kardar-Parisi-Zhang (KPZ) universality class of classical interface growth. Recent experimental evidence on quantum simulators challenged this hypothesis. Our results extend far beyond the experimental timescales and provide unambiguous evidence that spin transfer in integrable quantum spin chains is indeed incompatible with KPZ universality. However, spatio-temporal fluctuations of the spin analogue of surface roughness exhibit a self-similar Family-Vicsek (FV) scaling, relating roughness, growth, and dynamical exponents in all transport regimes and across models with SU(N) symmetry. Our results shed light on how classical universal scaling laws extend to the quantum many-body realm.

DY 46.11 Thu 12:15 HÜL/S186

Few-body structures of Quantum impurity problems in the Heisenberg picture — •Maxime Debertolis — University of Bonn

Quantum impurity problems are known to exhibit a simplified representation of their ground state or for quench protocols when an optimized single-particle basis is chosen. This work extends the study of single-particle rotations taylored to operators in the Heisenberg picture. We present the concept of natural super-orbitals for many-body operators, defined as the eigenvectors of the one-body super-density matrix associated with a vectorized operator. These objects are related to measures of non- Gaussianity of operators associated to the occupations of the natural super-orbitals. We perform a numerical investigation of the natural super-orbitals corresponding to both the time-evolution operator and a time-evolved local operator in the t-V model and in a quantum impurity model using tensor network simulations. In the quantum impurity model, occupations of the natural orbitals for both operators decay exponentially at all times. More surprisingly, the non-Gaussianity of the local operator saturates in time. This indicates that only a small number of orbitals contribute significantly to quantum correlations, enabling a compact matrix-product-operator representation. This framework opens the door to future research that leverages the compressed structure of operators in their natural super-orbital basis, enabling for instance the computation of out-of-time-order correlators in large interacting systems over extended time scales.

DY 46.12 Thu 12:30 HÜL/S186

Propagating the Hierarchical Equations of Motion (HEOM) using the Multi-Configurational Time-Dependent Hartree method (MCTDH) — •Luisa R. Grether[1], Uwe Manthe[2], Samuel L. Rudge[1], and Michael Thoss[1] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg im Breisgau, Deutschland — [2]Theoretische Chemie, Fakultät für Chemie, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Deutschland

The Hierarchical Equations of Motion (HEOM) are a powerful, numerically exact approach for simulating the time evolution of an open quantum system. Over the past decade, several tensor-train- and tensor-network-based approaches have been suggested and realized to make the HEOM applicable to ever larger model systems [1,2].

In this contribution, we build upon the existing twin-space formulation of the HEOM [2] and introduce a novel approach employing the Multi-Configurational Time-Dependent Hartree method (MCTDH) [3] for the time propagation of the HEOM. We demonstrate the applicability of the resulting HEOM+MCTDH method by presenting electron transport calculations for a nanojunction model, for which fully quantum results have not been available previously.

[1] Q. Shi *et al.*, J. Chem. Phys. **148**, 174102 (2018).

[2] Y. Ke *et al.*, J. Chem. Phys. **156**, 194102 (2022).

[3] H.-D. Meyer *et al.*, Chem. Phys. Lett. **165**, 73 (1990).

DY 47: Statistical Physics: General I

Time: Thursday 9:30–12:30 Location: ZEU/0114

DY 47.1 Thu 9:30 ZEU/0114

Microcanonical ensemble out of equilibrium — •Roman Belousov[1], Jenna Elliott[1,2], Florian Berger[3], Lamberto Rondoni[4,5], and Anna Erzberger[1,2] — [1]European Molecular Biology Laboratory (EMBL), Heidelberg, Germany — [2]Heidelberg University, Heidelberg, Germany — [3]Utrecht University, Utrecht, The Netherlands — [4]Politecnico di Torino, Turin, Italy — [5]Istituto Nazionale di Fisica Nucleare (INFN), Turin, Italy

The microcanonical ensemble serves as the fundamental representation of equilibrium thermodynamics in statistical mechanics by counting all possible realizations of a system's states. Ensemble theory connects this idea with probability and information theory, leading to the notion of Shannon-Gibbs entropy and, ultimately, to the principle of maximum caliber describing *trajectories* of systems—in and out of equilibrium. While the latter phenomenological generalization reproduces many results of nonequilibrium thermodynamics, its physical justification remains an open area of research. What is the microscopic origin and physical interpretation of this variational approach? What guides the choice of relevant observables? We address these questions by extending Boltzmann's method to a microcanonical caliber principle. Thereby we systematically develop generalized local detailed-balance relations, clarify the statistical origins of inhomogeneous transport, and provide an independent derivation of key equations from stochastic thermodynamics. This approach introduces a *dynamical* ensemble theory, which we verify in numerical simulations of spatially extended, driven, and active systems.

DY 47.2 Thu 9:45 ZEU/0114

Ensemble dependence of the critical behavior of a system with long range interaction and quenched randomness — •Nir Schreiber, Reuven Cohen, and Simi Haber — Department of Mathematics, Bar Ilan University, Ramat Gan, Israel 5290002

A system with long range interaction (LRI) is usually non-additive. In other words, such a system with volume V and energy E, cannot be divided into two subsystems with energies E_1, E_2 , where $E = E_1 + E_2 + o(V)$.

The canonical and the microcanonical ensembles are expected to be equivalent when describing additive systems. Conversely, non-additivity may result in peculiar microcanonical phenomena that are not observed in the canonical ensemble, such as negative specific heat or the presence of microstates that are inaccessible to the system, leading to breaking of ergodicity.

The Blume-Emery-Griffiths (BEG) model with mean-field-like interaction is a simple example of a model with LRI. We employ that model to demonstrate inequivalence of the two ensembles, without interfering with the interaction content. Specifically, we consider a hybrid system governed by the BEG Hamiltonian, where the spins are randomly quenched such that some of them are "pure" Ising and the others admit the BEG states. It is found, by varying the concentration of the Ising spins while keeping the parameters of the Hamiltonian fixed, that the model displays different canonical and microcanonical phase portraits in concentration-temperature plain. Indications that these portraits are rich and rather unusual are provided.

DY 47.3 Thu 10:00 ZEU/0114

Quasicrystals with large rotational symmetries: Amorphous-like on small but ordered at large lengths scale — Alan Rodrigo Mendoza Sosa[1,2], Atahualpa S. Kraemer[1], Erdal C. Oğuz[2], and •Michael Schmiedeberg[3] — [1]Departamento de Física, Facultad de Ciencias, Universidad Nacional Autónoma de México, Ciudad Universitaria, 04510, Mexico City, Mexico — [2]Key Laboratory of Soft Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing, 100190, China — [3]Soft Matter Theory group, Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

We study hyperuniformity in quasicrystals with large rotational symmetry. Hyperuniform systems are characterized by anomalously suppressed long-wavelength (i.e., large-length-scale) density fluctuations compared to those found in ordinary gases and fluids as well as in amorphous solids. We show that the degree to which the large-scale fluctuations are suppressed reveals a new characteristic length-scale. Below this length the patterns behave like amorphous systems while only above this length the long-ranged order becomes important leading to hyperuniformity in all cases.

DY 47.4 Thu 10:15 ZEU/0114

Emergence of mixed orientational ordering in quasi-one-dimensional superdisk and superball fluids — •Sakineh Mizani[1], Martin Oettel[1], Péter Gurin[2], and Szabolcs Varga[2] — [1]Institute for Applied Physics, University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — [2]Physics Department, Centre for Natural Sciences, University of Pannonia, PO Box 158, Veszprém, H-8201 Hungary

We investigate the collective behavior of hard anisotropic particles confined in quasi-one-dimensional channels where particle centers are constrained to a line but particles can rotate freely. For superdisks and superballs with tunable curvature, equilibrium properties are calculated using an exact transfer-operator method. We reveal the emergence of a novel state of mixed orientational order which is characterized by a close-packing state with particles having two distinct orientations, distributed randomly over the line [1]. This ordering is highly sensitive to particle shape: small deviations from ideal spherical symmetry can stabilize or destabilize the mixed phase, demonstrating the the subtle interplay between particle geometry and confinement. Our results provide new insights into entropically driven ordering in confined systems, offering potential guidelines for designing colloidal assemblies and understanding phase behavior in narrow channels. [1] S. Mizani et al, arXiv:2510.06918, J. Mol. Liq. (accepted).

DY 47.5 Thu 10:30 ZEU/0114

Scaling of the Mpemba effect in the Ising model — •Janett Prehl and Martin Weigel — Institute of Physics, Technisch Universität Chemnitz, Chemnitz, Germany

The Mpemba effect – originally observed by Mpemba and Osborne for water [1] – describes the counterintuitive situation in which a hotter system relaxes faster than an initially colder one when both are instantaneously brought into contact with the same (cold) reservoir. Lately this phenomenon has been identified in various systems undergoing phase transitions [2 – 4]. Here, we investigate the Mpemba effect in the 2D Ising model with a critical temperature T_c. Using Monte Carlo simulations with different update dynamics, we study how initial temperatures and different initial magnetization influence the coarsening dynamics of different structural properties while quenching below T_c. In detail we investigate observables such as the energy per spin $\langle e \rangle$ and the average domain length $\langle \ell \rangle$. While Mpemba-like curve crossings appear for several conditions, they occur in the finite-size limited regime and weaken with increasing system size L. In contrast, non-zero initial magnetization enhances the effect, producing robust inversions in relaxation behavior.

[1] E. B. Mpemba and D. G. Osborn, *Phys. Educ.* **4** (1969) 172.
[2] M. Baity-Jesi et al., *PNAS* **116** (2019) 15350.
[3] N. Vadakkayil and S. K. Das, *Phys. Chem. Chem. Phys.* **23** (2021) 11186.
[4] A. K. Chatterjee, S. Takada, and H. Hayakawa, *Phys. Rev. Lett.* **131** (2023) 080402.

DY 47.6 Thu 10:45 ZEU/0114

Work extraction from a single negative-temperature bath considered as a temperature gradient-driven heat flow — •Wolfgang Bauer — Dept. of Internal Medicine I, Comprehensive Heart Failure Centre, UKW, Würzburg, Germany — EPV, Institute of Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany}

Work can dissipate as heat within a bath. The reverse, i.e. extracting work from a thermal bath without changing the state of the working system contradicts the 2nd law of thermodynamics. However, this does not hold for a bath at negative absolute temperature. Our approach reconciles the 2nd law with sole work extraction from a bath at negative temperature. We consider not only a single, but rather a large assembly of working systems. Within the assembly the working systems may exchange mutually energy by weak thermal coupling. This assembly is now assigned from Shannon entropy a canonical temperature. While this framework may seem unconventional for macroscopic working machines, it naturally becomes clear for very small, molecular-scale machines. We show for paradigmatic examples of working machines, that their initial canonical temperature is positive. Consequently, sole extraction of work from a bath at negative temperature represents simply heat flow from a hot system (bath at negative temperature) to a cool system (assembly of working machines), consistent with the 2nd law of thermodynamics.

15 min. break

DY 47.7 Thu 11:15 ZEU/0114

Advancing Stochastic 3-SAT Solvers by Dissipating Oversatisfied Constraints — •Joachim Schwardt[1,2] and Jan Budich[2,1] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Institute of Theoretical Physics at TU Dresden

We introduce and benchmark a stochastic local search heuristic for the NP-complete satisfiability problem 3-SAT that drastically outperforms existing solvers in the notoriously difficult realm of critically hard instances. Our construction is based on the crucial observation that well established previous approaches such as WalkSAT are prone to get stuck in local minima that are distinguished from true solutions by a larger number of oversatisfied combinatorial constraints. To address this issue, the proposed algorithm, coined DOCSAT, dissipates oversatisfied constraints (DOC), i.e. reduces their unfavorable abundance so as to render them critical. We analyze and benchmark our algorithm on a randomly generated sample of hard but satisfiable 3-SAT instances with varying problem sizes up to N = 15000. Quite remarkably, we find that DOCSAT outperforms both WalkSAT and other well known algorithms including the complete solver Kissat. The essence of DOCSAT may be seen as a way of harnessing statistical structure beyond the primary cost function of a combinatorial problem to avoid or escape local minima traps in stochastic local search.

DY 47.8 Thu 11:30 ZEU/0114

Quest for optimal quantum resetting: Protocols for a particle on a chain — •Pallabi Chatterjee, S. Aravinda, and Ranjan Modak — Department of Physics, Indian Institute of Technology Tirupati, Tirupati 517619, India

In the classical context, it is well known that, sometimes, if a search does not find its target, it is better to start the process anew. This is known as resetting. The quantum counterpart of resetting also indicates speeding up the detection process by eliminating the dark states, i.e., situations in which the particle avoids detection. In this work, we introduce the most probable position resetting(MPR) protocol, in which, at a given resetting step, resets are done with certain probabilities to the set of possible peak positions that could occur because of the previous resets, followed by uninterrupted unitary evolution, irrespective of which path was taken by the particle in previous steps. In a tight-binding lattice model, there exists a twofold degeneracy (left and right) of the positions of maximum probability(peak). The survival probability with optimal restart rate approaches zero when the particle is reset with equal probability on both sides path independently. This protocol significantly reduces the optimal mean first-detected-passage time, and it performs better even if the detector is far apart compared to the usual resetting protocols in which the particle is brought back to the initial position. We propose a modified protocol, an adaptive two-stage MPR, by making the associated probabilities of going to the right and left a function of steps. We see a further reduction of the optimal mean FDT and improvement in the search process.

DY 47.9 Thu 11:45 ZEU/0114

Quantification of correlations by Fisher matrix — •Jakub Grabarczyk and Krzysztof Byczuk — Faculty of Physics, University of Warsaw, Poland

Quantum Fisher Information (QFI) is a concept based on relative entropy used to measure the distinctiveness of the given statistical ensemble. When applied to a lattice model, it quantifies the measurable difference between two instances of the model characterized by different parameter values. In my work, I demonstrate the significance of QFI in understanding microscopic properties of correlated quantum particles. The results are verified numerically. I compare the QFI across several important lattice models including the bosonic and fermionic Hubbard models as well as the Heisenberg model. Furthermore, I discuss how QFI relates to physically measurable quantities.

DY 47.10 Thu 12:00 ZEU/0114

Universal irreversibility—an information loss paradigm — •Jürgen Stockburger — Institut for Complex Quantum Systems, Ulm University

I develop a general prescription to incorporate irreversibility into any physical dynamics governed by a reversible microscopic dynamics with interactions. A description of irreversibility is introduced from the perspective that reversibility is *infeasible* due to insufficient means, not as a fundamental alteration of any microscopic theory.

With an arbitrary partitioning into subsystems, a coupled dynamics between a projected (decorrelated) and a residual (complementary) state is formulated, still fully equivalent to the reversible dynamics. All partitions are treated equally, without designation of "system" and "bath". With a (variable) truncation of the memory of the residual state, I recognize the fact that correlations in the distant

past are undetectable in the present. The notion of irrecoverable correlation information is also implicit in current open-system approaches such as repeated interaction models [1]; the need to consider heat baths equally as a "system of interest" arises, e.g., in the context of quantum bolometry [2]. The framework of *entropy augmentation through subadditive excess* (EASE) introduces not only a universal view on irreversibility, it also provides a roadmap for actual computation [3].

[1] F. Ciccarello *et al.*, Phys. Rep. **954**, 1 (2022)
[2] B. Karimi *et al.*, Nat. Comm. **11**, 367 (2020)
[3] Stockburger, J.T., Eur. Phys. J. Spec. Top. (2025).
https://doi.org/10.1140/epjs/s11734-025-01923-2

DY 47.11 Thu 12:15 ZEU/0114

Temperature as joules per bit — Charles Alexandre Bédard[1], •Sophie Berthelette[2], Xavier Coiteux-Roy[3], and Stefan Wolf[2,4] — [1]École de technologie supérieure, Montreal, Canada — [2]Università della Svizzera italiana, Lugano, Switzerland — [3]University of Calgary, Calgary, Canada — [4]Facoltà indipendente di Gandria, Gandria, Switzerland

In statistical mechanics, entropy is defined as a fundamental quantity. However, its unit, J/K, involves that of temperature, which is only subsequently defined — and defined in terms of entropy. This circularity arises with the introduction of Boltzmann's constant into the very expression of entropy. The J/K carried by the constant prevents entropy from finding a unit of its own while simultaneously obfuscating its informational nature. Following the precepts of information theory, we argue that entropy is well measured in bits and coincides with information capacity at thermodynamic equilibrium. Consequently, not only is the temperature of a system in equilibrium expressed in J/bit, but it acquires a clear meaning: It is the cost in energy to increase its information capacity by 1 bit. Viewing temperature as joules per bit uncovers the strong duality exhibited by Gibbs long ago between available capacity and free energy. It also simplifies Landauer's cost and clarifies that it is a cost of displacement, not of erasure. Replacing the kelvin with the bit as an SI unit would remove Boltzmann's constant from the seven defining constants.

DY 48: Nonlinear Dynamics and Time-Delay Systems

Time: Thursday 9:30–11:00 Location: ZEU/0118

DY 48.1 Thu 9:30 ZEU/0118

From Case Counts to Contact Networks: Inferring Epidemic Coupling in Space and Time — •Adrian Pelcaru and Dirk Brockmann — Center Synergy of Systems (SynoSys), TUD Dresden University of Technology, Dresden, Germany

Inferring spatio-temporal transmission structure from incidence data alone is a central problem in epidemic modelling, with implications for real-time surveillance and for how we interpret mobility and contact information. We analyse discrete-time renewal SIRS models on a network of metapopulations that incorporate infection-age structure, seasonality, mobility between regions, and time-varying local contact rates. In the analysis, these ingredients are combined into an effective spatio-temporal contact kernel that quantifies how cases in region m at a given infection age contribute to new infections in region n one day ahead. Stacking multi-region incidence histories across lags into a delay-embedded state, the renewal dynamics define a map on this reconstructed space whose local Jacobian is the convolution operator determined by the contact kernel and the susceptibles. Aggregating the kernel over infection age with suitable weights yields a time-dependent effective contact matrix and associated effective distances that summarise how infections propagate between regions. This construction provides a transparent link between mechanistic assumptions about mobility and varying infection rates and the resulting effective couplings in space and time, and identifies a natural operator that can, in principle, be compared to reconstructions from incidence data to detect systematic deviations from mobility-based expectations.

DY 48.2 Thu 9:45 ZEU/0118

Beyond the Balance: A Minimal Model Unifying Regime Shifts, Long Transients, and Critical Transitions — •Misha Chai and Holger Kantz — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, D 01187, Germany

By the late 20th century, ecologists recognized that classical equilibrium views — nature is deterministic and always converges to a single, stable state — often fail to capture real-world dynamics. A nonequilibrium perspective emerged: ecological systems are frequently dominated by long transients that can persist over a super-long periods of time, with recurrent cyclic and chaotic behavior, until a sudden regime shifts changes the dynamics and transitions the system to an unpredictable new state.

However, models that integrate these key features — alternative stable states, stochastic drivers, long transients, and critical transitions — while also quantifying stability via resilience, remain rare.

We propose a minimal model that encapsulates these key properties of nonequilibrium ecology, while remaining amenable to theoretical analysis.

DY 48.3 Thu 10:00 ZEU/0118

Anticipated synchronization in systems with distributed delay — •David Ortiz, Tobias Galla, and Raúl Toral — Instituto de Física Interdisciplinar y Sistemas Complejos IFISC (CSIC-UIB), Campus UIB, 07122 Palma de Mallorca, Spain

Anticipated Synchronization (AS) describes counterintuitive situations in which a system synchronizes with the future state of another, even though the coupling between the systems is perfectly causal. Thus, the driven system 'forecasts' the driver. Common setups include two identical copies of a system, coupled with a fixed delayed interaction. AS has been reported in chaotic, excitable and spatially extended systems.

We extend AS to linear and nonlinear systems coupled with distributed delay. This models situations with uncertainty on the delay, or systems in which there are multiple distinct delay channels. The damped harmonic oscillator can be studied analytically, and shows stable AS provided the coupling strength and mean delay are not too large. We compute the anticipation time, and show that the driven system amplifies the oscillations in the driver. Our theoretical predictions are confirmed by numerical simulations. Numerically, we also investigate nonlinear chaotic and excitable systems. We confirm that AS can occur in the presence of distributed delay. Similar to the case of linear systems, we again find instances of signal enhancement.

DY 48.4 Thu 10:15 ZEU/0118

Dynamics of Temporal Localized States in an Injected Resonant Saturable Absorber Mirror — •Martin P. Szymiczek[1], Elias R. Koch[1], Julien Javaloyes[2], and Svetlana V. Gurevich[1,2,3] — [1]Institut für Theoretische Physik, Universität Münster — [2]Universitat de les Illes Balears, Palma — [3]Center for Data Science and Complexity, Universität Münster

We are interested in the dynamical behaviour of temporal localized states (TLS) and corresponding frequency combs in an injected microcavities subjected to a strong time-delayed feedback. A nonlinear optical system consist of a short injected microcavity with a thin slice of a saturable absorber, coupled to a long external cavity introducing a time delay and closed by a feedback mirror. We disclose sets of multistable bright TLSs coexisting on their respective bistable homogeneous backgrounds and show that they are mainly generated through the locking of domain walls leading to a collapsed snaking structure. The results provide insights into the control and design of emission in delay-coupled micro-resonator systems.

DY 48.5 Thu 10:30 ZEU/0118

FPGA-integrated analog simulations of time-delayed differential equations — •Matthias Hering[1], Julien Javaloyes[2], and Svetlana V. Gurevich[1,2,3] — [1]Institute of Theoretical Physics, Münster, Germany — [2]Departament de Física and IAC[3], Universitat de les Illes Balears, Spain — [3]Center for Data Science and Complexity, Münster, Germany

Real-world complex systems can be strongly influenced by time-delays due to unavoidable finite signal propagation speeds and time-delayed dynamical systems (TDSs) have proven to be a fertile framework for the modeling of nonlinear phenomena. However, they are difficult to study experimentally due to the need for precise delay elements. We present a hybrid implementation by integrating a digital feedback loop powered by an FPGA into an analog circuit to realize a damped harmonic oscillator with a piecewise nonlinear, delayed restoring force. Operating at 125 MS/s enables the FPGA to enable a clean reconstruction of the system*s dynamics up into the MHz regime without digital artifacts. The experiment not only reproduces the expected Turing bifurcation in the long delay limit, but also reveals the formation of robust localized states and square-waves patterns.

DY 48.6 Thu 10:45 ZEU/0118

Experimental realisation of thermalisation in a nonlinear non-Hermitian optical lattice — •Julia Görsch[1], Joshua Feis[1], Andrea Steinfurth[1], Sebastian Weidemann[1], Georgios G. Pyrialakos[2], Matthias Heinrich[1], Mercedeh Khajavikhan[2], Alexander Szameit[1], and Demetrios N. Christodoulides[2] — [1]Institute of Physics, University of Rostock, Rostock, Germany — [2]Ming Hsieh Department of Electrical and Computer Engineering, University of Southern California, Los Angeles, California, USA

Optical thermodynamics has emerged as an efficient framework for describing and predicting the dynamics of strongly multimode, nonlinear systems. Yet, in non-Hermitian settings, many of the theoretically predicted effects have remained experimentally unexplored. Here, we report the first experimental observation of thermalisation in a nonlinear, non-Hermitian optical lattice using a platform based on coupled optical fiber loops. This arrangement emulates light propagation in a one-dimensional lattice by coupling two fiber loops of unequal length via a beam splitter, thereby mapping pulse evolution onto a doubly discrete (1+1)D lattice. Within this system, we engineer a pseudo-Hermitian lattice whose non-Hermiticity arises from anisotropic nearest-neighbor coupling, implemented via a tunable beam-splitting ratio combined with amplitude modulation. Following excitation with a superposition of eigenmodes, the system undergoes a clear thermalisation process - despite its intrinsic non-Hermiticity - revealing a previously inaccessible regime of non-Hermitian optical thermodynamics and opening the door to further experimental investigations.

DY 49: Active Matter V (joint session DY/BP)

Time: Thursday 9:30–12:45 Location: ZEU/0160

Invited Talk DY 49.1 Thu 9:30 ZEU/0160

Active memory and non-reciprocity as pathways to pattern formation in conserved scalar fields — •Supropriya Saha and Vaishnavi Gajendragad — Max Planck Institute for Dynamics and Self-organisation

Active phase separation has emerged as a field within active matter that investigates pattern formation in number-conserving scalar fields. The field has also gained momentum from developments in biological systems, where phase separation has been implicated in the formation of biological condensates. In this talk, I will explore two different paths to non-Hermiticity in number-conserving scalar fields. Non-Hermiticity, or the emergence of complex eigenvalues in the linear dynamics of scalar densities, is associated with traveling patterns that break time-reversal symmetry and parity.

The first pathway I will discuss is a feedback mechanism in which particles store and use information about their past trajectories to influence their time evolution. I will present a model in which the particle velocity acquires an active contribution that depends on its past trajectory, weighted by a memory kernel. This memory kernel is independent of the thermal noise acting on the particle, implying a microscopic violation of detailed balance. The number density of these particles is described by a modified Cahn*Hilliard equation that incorporates this non-equilibrium effect. The second pathway involves non-reciprocal interactions between two or more species. I will describe the phenomenology observed in both cases, focusing on the role of fluctuations, nonlinearities, and the stability of the resulting patterns.

DY 49.2 Thu 10:00 ZEU/0160

Self-propulsion via non-transitive phase coexistence in chemically active mixtures — •Yicheng Qiang, Chengjie Luo, and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany

Chemical activity is common in many active matter systems. For example, active reactions can lead to the self-propulsion of particles, which can finally give rise to rich collective dynamics, including phase separation, even in the absence of attractive interactions. With interactions that already favor phase separation, chemical activity and multiple coexisting phases will further intertwine. To unveil the basic effect of active reactions on coexistence, we study mixtures where solvent species interconvert while solutes segregate. We demonstrate that active reactions alter the chemical potential balance between the coexisting phases and defy the construction of pseudo-pressure balance. As a result, the transitivity of phase coexistence is broken, and the bulk compositions depend on the contact topology among all the coexisting phases. With cyclic topologies, the pressure imbalance leads to self-propelled phases and other complex dynamics such as budding and engulfment.

DY 49.3 Thu 10:15 ZEU/0160

Contraction waves in pulsating active liquids: from pacemaker to aster dynamics — Tirthankar Banerjee[1], Thibault Desaleux[1], Jonas Ranft[2], and •Etienne Fodor[1] — [1]Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg City, Luxembourg — [2]Institut de Biologie de l'ENS, Ecole Normale Supérieure, CNRS, Inserm, Université PSL, 46 rue d*Ulm, 75005 Paris, France

We propose a hydrodynamic theory to examine the emergence of contraction waves in dense active liquids composed of pulsating deformable particles. Our theory couples the liquid density with a chemical phase that determines the periodic deformation of the particles. This mechanochemical coupling regulates the interplay between the flow induced by local deformation, and the resistance to pulsation stemming from steric interaction. We show that this interplay leads the emergent contraction waves to spontaneously organize into a packing of pacemakers. We reveal that the dynamics of these pacemakers is governed by a complex feedback between slow and fast topological defects that form asters in velocity flows. In fact, our defect analysis is a versatile platform for investigating the self-organization of waves in a wide range of contractile systems. Our results shed light on the key mechanisms that control the rich phenomenology of pulsating liquids, with relevance for biological systems such as tissues made of confluent pulsating cells. Refs: arXiv:2509.19024, arXiv:2407.19955

DY 49.4 Thu 10:30 ZEU/0160

Topology of pulsating active matter: Defect asymmetry controls emergent motility — •Luca Casagrande[1], Alessandro Manacorda[2], and Étienne Fodor[1] — [1]Department of Physics and Materials Science, University of Luxembourg, Luxembourg City, Luxembourg — [2]CNR Institute of Complex Systems, Uos Sapienza, Rome, Italy

When heartbeats become irregular, spiral waves and motile defects emerge at the surface of cardiac tissues [1]. Capturing the emergence of defect motility despite the absence of any cellular flows is a theoretical challenge which has recently been tackled by models of actively deforming particles [2-4]. The interplay between individual pulsation of particles sizes, synchronization, and repulsion yields deformation waves resembling those of cardiac tissues. Combining particle-based and hydrodynamic approaches, we examine the statistics of defects in the collective deformation of particles. We rationalize defect motility as stemming from the breakdown of time-reversal and spatial symmetries, and provide predictions for the deformation profile near the defect core to quantify motility. [1] A. Karma, Annu. Rev. Condens. Matter Phys., 4, 313-337 (2013) [2] Y. Zhang, É. Fodor, Phys. Rev. Lett., 131, 238302 (2023) [3] A. Manacorda, É. Fodor, Phys. Rev. E, 111, L053401 (2025) [4] W. Piñeros, É. Fodor, Phys. Rev. Lett., 134, 038301 (2025)

DY 49.5 Thu 10:45 ZEU/0160

Avalanche statistics in dense active matter — •Vinay Vaibhav[1] and Peter Sollich[1,2] — [1]Institut für Theoretische Physik, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Department of Mathematics, King's College London, The Strand, London, UK

Reorganization processes in dense active matter remain a central open question in non-equilibrium physics. In particular, how persistent self-propulsion drives local rearrangements and triggers collective failure events is not well understood. Here, we investigate such activity-induced rearrangements, that sometimes rapidly cascade to avalanches, in a dense assembly of self-propelled particles with extremely persistent activity. These systems evolve through abrupt transitions between mechanically stable configurations, giving rise to rich intermittent behavior. Using large-scale simulations, we systematically characterize avalanche statistics across a range of system sizes and activity protocols. We quantify the scaling properties of avalanche-size distributions for two widely studied active matter models: active Brownian particles and active Ornstein-Uhlenbeck particles. By comparing these classes of dynamics, we identify how the nature of the propulsion mechanism influences the exponents associated with the avalanche size distribution. In addition, we report the frequency and temporal organization of avalanches. Our results provide a unified picture of how persistent activity drives rearrangements in dense active systems and highlight the connections between active intermittency, mechanical stability, and avalanche dynamics.

15 min. break

DY 49.6 Thu 11:15 ZEU/0160

Coupling intracellular processes and extracellular environment in a Cellular Potts model — •Cornelis Mense[1,2], Falko Ziebert[1,2], and Ulrich Schwarz[1,2] — [1]ITP, Heidelberg — [2]BioQuant, Heidelberg

The Cellular Potts Model (CPM) is a computationally very efficient framework to study cell dynamics, wherein cells are simulated through Hamiltonian based update rules on a discretised lattice. The model has traditionally been used to predict cell migration and shape in scenarios such as immune response, morphogenesis, cancer, and wound healing. In contrast to e.g. active gel models, however, the CPM usually does not represent subcellular processes. Here, we propose an extension to the CPM by which cells can contract their bulk to both actively transport material and strain their substrate. This model allows us to represent feedback loops between intracellular processes, cell shape and the mechanical and geometrical properties of the extracellular environment. Migration can emerge both as internal symmetry break or as response to an external gradient. We apply it to some standard situations of experimental interest, in particular 3D-printed scaffolds for cell adhesion and migration.

DY 49.7 Thu 11:30 ZEU/0160

Exact Stationary State of a d-dimensional Run-and-Tumble Particle in a Harmonic Potential — •Mathis Guéneau[1], Grégory Schehr[2], and Satya N. Majumdar[3] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany — [2]Sorbonne Université, Laboratoire de Physique Théorique et Hautes Energies, CNRS UMR 7589, 4 Place Jussieu, 75252 Paris Cedex 05, France — [3]LPTMS, CNRS, Univ. Paris-Sud, Université Paris-Saclay, 91405 Orsay, France

We study the stationary state of a run-and-tumble particle (RTP) confined in a harmonic potential in arbitrary dimension d. Owing to isotropy, all statistical properties of the steady state are fully encoded in the distribution of a single coordinate. This coordinate follows an effective one-dimensional dynamics with a piecewise-constant self-propulsion velocity drawn from a prescribed distribution. We obtain the exact stationary distribution by identifying a stick-breaking process and a Dirichlet process in the dynamics, and by using known results for these processes. This framework allows us to compute exactly the full radial distribution, the joint law of the coordinates, and their moments, and to extend these results to include thermal noise. We further characterize the shape transition of the stationary state, from active-like to passive-like behavior, and show that it can be analyzed for arbitrary external potentials.

DY 49.8 Thu 11:45 ZEU/0160

Jerky active particles — •Hartmut Löwen and Stephy Jose — Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf

We introduce jerky active particles, a generalization of inertial active Brownian particles subjected to jerk, the time derivative of acceleration. These particles can be realized by feedback in active macroscopic granules or in mesoscopic colloids moving in a viscoelastic background with memory. We analytically derive their mean squared displacement (MSD) and show that there is a gigantic dynamical spreading with extremely high scaling exponent of the MSD as a function of time [1]. We also generalize jerky dynamics to a chiral active particle and demonstrate that the mean displacement shows damped and exploding Lissajous-like patterns alongside the well-known classical spira mirabilis [2]. Our work on jerky chiral active particles opens a new route to explore rich dynamical effects in active matter.

[1] H. Löwen, Physical Review E 112, 045412 (2025)

[2] S. Jose, H. Löwen, Chiral jerky active particles, New Journal of Physics (in press), see also arXiv:2508.18180

DY 49.9 Thu 12:00 ZEU/0160

Diffusion of active particles on curved manifolds — •Maxim Root[1], Lorenzo Caprini[2], and Hartmut Löwen[1] — [1]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf, Germany — [2]Physics Department, Sapienza University of Rome, 00185 Rome, Italy

Active Matter rarely exists in isolated idealized systems. In nature, it is rather typical that active particles are surrounded by complex environments and experience external forces. So far, passive Brownian motion constrained to curved surfaces [1,2] was studied extensively and similar work was done on clusters of active particles [3]. In this talk we explore the emergent effects of active particles constrained to two-dimensional curved surfaces and in presence of an external homogeneous force field, e.g., gravity. This is done for an overdamped active particle that exhibits persistent motion on a short time scale and diffusion in the long-time limit. The lateral long-time diffusion coefficient is computed for different scenarios and criteria for localization are derived.

[1] T. Ohta and S. Komura, *Lateral diffusion on a frozen random surface*, EPL **132**, 50007 (2020)

[2] A. Naji and F. L. H. Brown, *Diffusion on ruffled membrane surfaces*, J. Chem. Phys. **126**, 235103 (2007)

[3] E. D. Mackay et al., *Emergent Dynamics of Active Systems on Curved Environments*, arXiv:2505.24730 (2025)

DY 49.10 Thu 12:15 ZEU/0160

Modeling dissipation in quantum active matter — Alexander P. Antonov[1], Sangyun Lee[2], Benno Liebchen[3], Hartmut Löwen[1], Jannis Melles[1], Giovanna Morigi[4], Yehor Tuchkov[2], and •Michael te Vrugt[2] — [1]Institut für Theoretische Physik II, Weiche Materie, Heinrich-Heine-Universität Düsseldorf — [2]Institut für Physik, Johannes Gutenberg-Universität Mainz — [3]Institut für Physik der kondensierten Materie, Technische Universität Darmstadt — [4]Theoretische Physik, Universität des Saarlandes

In classical active matter systems, dissipation plays a major role. Currently, there is an increased focus in exploring quantum mechanical active matter systems, for which the question of how to model dissipation is far from obvious. In fact, for open quantum systems, a variety of quantum heat bath models have been proposed that are valid in different physical situations. Here, we compare the effects of different quantum heat baths based on a recently proposed quantum active matter model [Phys. Rev. Res. **7**, 033008 (2025)]. We find that the choice of the quantum heat bath strongly influences the dynamics at short timescales, which is the regime in which quantum effects are most relevant.

DY 49.11 Thu 12:30 ZEU/0160

Active Magnetic Particles in Magnetic Gradient Fields — •Laris Berekovic, Margaret Rosenberg, and Hartmut Löwen — Heinrich-Heine University Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf

Active particles are common in nature, underlying many complex phenomena. Since the motion of active particles has no intrinsic directionality, steering the particles' motion requires an additional control parameter, such as a magnetic interaction. In this contribution, we present an analysis of the effect of magnetic vortex fields created by a current carrying wire on the ground states and motion of active Brownian particles (ABP) carrying a fixed magnetic dipole moment. We present an analytical solution for the single-particle case, compute the ground state for multiple particles via simulated annealing in the passive case and explore the activity-induced phase transition created by increasing the self-propulsion. We find new forms in the ground state, as well as a rich variety of activity-induced structures. These results can be applied to ferrofluid systems, biophysical systems of magnetotactic bacteria or form the basis of more complex industrial applications.

DY 50: Focus Session: Controlling Microparticles and Biological Cells by Ultrasound (joint session BP/CPP/DY)

Recently ultrasound has emerged as a very promising physical modality to control the behavior of microparticles and even of biological cells, which can be moved and stimulated by sound waves. For biological cells, one can further control the effect of sound through gene expression (sonogenetics), similar to the control by light (optogenetics). However, because the wavelength of sound is much larger than the one of light, one of the challenges is to localize the effect of sound waves, e.g. by using gas bubbles. Here, we bring together experimental and theoretical researchers who currently explore the potential of ultrasound to control active and passive microsystems and to develop new applications ranging from biomedicine to soft robotics.

Organized by Peer Fischer and Ulrich S. Schwarz (Heidelberg)

Time: Thursday 10:15–12:45 Location: BAR/0106

See BP 30 for details of this session.

DY 51: Networks: From Topology to Dynamics – Part III (joint session DY/SOE)

Time: Thursday 11:15–12:45 Location: ZEU/0118

DY 51.1 Thu 11:15 ZEU/0118

Remote Tipping in Networks — •Philip Marszal[1], Malte Schröder[1], and Marc Timme[1,2] — [1]Chair of Network Dynamics, Center for Advancing Electronics Dresden (cfaed) and Institute of Theoretical Physics, TUD Dresden University of Technology, 01062 Dresden, Germany — [2]Lakeside Labs, Lakeside B04b , 9020 Klagenfurt, Austria

Tipping of a single unit in a complex networked system can trigger large-scale cascades that shift the system's macroscopic state. Typically, such cascades propagate diffusively, with each tipping event destabilizing adjacent units.

Here we report a novel form of tipping cascade in systems of coupled bistable oscillators, that results in the tipping of non-adjacent nodes. One node can trigger transitions in distant nodes while intermediate neighbors remain unaffected. Which nodes tip and which ones remain unaffected depends intricately on the local oscillator dynamics and the underlying network structure. We study the transition between locally spreading and non-local cascades and characterize the conditions necessary for the emergence of non-local cascades.

DY 51.2 Thu 11:30 ZEU/0118

Ponderomotive Route to Tipping in Open Networks — Seungjae Lee[1], •Marisa Fischer[1], and Marc Timme[1,2,3] — [1]Chair for Network Dynamics, Institute of Theoretical Physics and Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, 01062 Dresden, Germany — [2]Center Synergy of Systems, Technische Universität Dresden, 01062 Dresden, Germany — [3]Lakeside Labs, Lakeside B04b, 9020 Klagenfurt, Austria

External fluctuations impact the dynamics of complex networked systems, from cells and ecosystems to engineered infrastructures. Strong external forcing may cause tipping that compromises such systems' functionality. Here, we identify a generic ponderomotive route to tipping in open, periodically driven systems. Upon increasing the driving amplitude, the time-average of the oscillatory responses persistently shifts away from the original system's operating point – a system-level ponderomotive effect. We characterize the shift as the fixed-point solution of a slow dynamics resulting from a two-time-scale analysis. A bifurcation point of the shift defines the tipping point beyond which the system settles into another collective state, diverges gradually, or exhibits finite-time blow-up. The ponderomotive shift together with its bifurcation yields the novel type of *ponderomotive tipping*. It generically emerges across disparate systems from science and engineering and is independent of their diverse post-tipping dynamics.

DY 51.3 Thu 11:45 ZEU/0118

Linear dynamics on infinite networks — •Bernd Michael Fernengel — HIFMB, Oldenburg, Germany

Linear evolutionary equations are often used to describe the time evolution of a physical system. Their solution operator can be written in an exponential form of exp(t A), with some generator A. When the generator is a finite dimensional matrix, we can interpret its time evolution as a hopping dynamics on a finite network, where the dynamics of the network can be transferred to the dynamics of the solution operator.

In order to study special types of solution operators for non-interacting systems of countable dimensions, we construct countable, infinitely large networks using the iterated Cartesian product of finite graphs, where the dynamics is known. We discuss the possibilities to infer properties like the time evolution and the stationary solution of the infinite network from finite approximations via the thermodynamic limit. This is closely related to the question, under which conditions it is possible to approximate a countable, infinite system by finite subsystems.

DY 51.4 Thu 12:00 ZEU/0118

Localizing sparse perturbation sources in driven nonlinear networks — •Julian Luca Fleck, Jose Casadiego, and Marc Timme — Chair of Network Dynamics, Center for Advancing Electronics Dresden (cfaed) and Institute of Theoretical Physics, TUD Dresden University of Technology, 01062 Dresden, Germany

Network dynamical systems under the influence of external perturbations abound in nature and engineered systems, ranging from neural circuits to electrical power grids. The external driving can drastically change the system's operating mode and be fatal for system stability. Localizing sources of perturbations in a network is crucial to mitigate systems failure. We present a linear response approach to infer the location from a multivariate time series of a recorded subset of nodes. We employ a compressed-sensing algorithm to locate one or multiple perturbation sources utilizing the sparsity of such locations. The approach additionally yields the time series of the unmeasured nodes and the external driving. We test for random linear systems, and illustrate the applicability to electrical power grids.

DY 51.5 Thu 12:15 ZEU/0118

Elucidating structure-function relationships in physical networks via ensnarlment — •Yu Tian[1,2,3,4], Chinmayi Subramanya[1,3,4], and Carl Modes[1,3,4] — [1]Center for Systems Biology Dresden, Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems — [3]Max Planck Institute of Molecular Cell Biology and Genetics — [4]Dresden University of Technology, Dresden, Germany

Understanding physical networks – whose structure is constrained by the physical properties of their nodes and links – is a growing interdisciplinary challenge, especially in biological systems. Physical constraints such as volume exclusion and non-crossing conditions, along with biological functionality, can drive these networks into non-optimal spatial configurations. One prominent feature is that cycles may go through each other's interior space, which may not be unraveled without removing edges, leading to an ensnarled state. Characterizing the ensnarlment in the space, and its interplay with the functional behaviours of the network, is essential for revealing structure-function relationships in such systems. In this work, we introduce a graph-theoretic framework based on the linking operator, obtained by the Gauss linking integral applied to the cycles in the network. This approach enables a multiscale analysis of entanglement, spanning local, intermediate, and global structures. Our goal is to reveal how topological complexity shapes, and is shaped by, biological functions, providing new insights into the organizational principles of physical and biological networks.

DY 51.6 Thu 12:30 ZEU/0118

Transient stability properties for transitions between stationary power flows — •Leo Heidweiler[1,2] and Frank Hellmann[2] — [1]TU Dresden — [2]Potsdam Institute for Climate Impact Research

The increasing incorporation of renewable energy sources into electrical power grids fundamentally changes their dynamical behaviour and introduces new challenges for system stability. While network expansion and operation are traditionally based on stationary power flow analysis, dynamical effects following line faults, such as loss of synchronization of a single generator or whole part of the network, may occur even when a stable post-fault power flow exists and operational constraints are fulfilled. Direct assessment of transient stability, however, requires time-resolved simulations that are computationally expensive and unsuitable for large-scale planning and real-time applications. This motivates the question of whether transient stability properties can be inferred from static characteristics of the network, such as power flow solutions and topology.

In this work, we develop stability indicators for the IEEE39 Bus power system and investigate their predictability using PowerDynamics.jl, a Julia Library for numerical Power Grid simulations. In particular, we make use of the complex oscillator formulation of Power Systems and machine learning. This helps us assess whether stability margins can be predicted from stationary quantities alone or whether intrinsically dynamical information is indispensable. If so, we can deduce what minimal dynamical information is sufficient for reliable prediction.

DY 52: Statistical Physics of Biological Systems III (joint session BP/DY)

Time: Thursday 15:00–18:15 Location: BAR/SCHÖ

DY 52.1 Thu 15:00 BAR/SCHÖ

Efficiency of Droplet Formation and Dissolution by Chemical Reactions — •Gerrit Wellecke[1,2], Riccardo Rossetto[1,2], Jan Kirschbaum[1], and David Zwicker[1] — [1]Theory of Biological Fluids, Max Planck Institute for Dynamics and Self-Organization, Am Faßberg 17, 37077 Göttingen, Germany — [2]University of Göttingen, Institute for the Dynamics of Complex Systems, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Droplets formed by phase separation are vital for intracellular organization, and cells often control the formation and dissolution of these droplets through chemical reactions. To understand how cells can influence droplets in space and time, we consider a ternary system that exhibits a bistability between homogeneous and phase-separated states. We use a thermodynamically consistent approach to describe the diffusive and reactive dynamics, which allows us to quantify the energy dissipation and entropy production during transitions between these states. We find that reaction-controlled droplet formation and dissolution in the

bistable regime are fundamentally different processes. While droplet formation is generally aided by relaxation to equilibrium, we find that a droplet's size determines whether it is best dissolved internally or externally. Further, our model identifies plausible mechanisms by which cells may regulate their intracellular droplets, providing insights that could guide the development of synthetic soft matter systems with tunable droplet behaviour.

DY 52.2 Thu 15:15 BAR/SCHÖ

Size control and fluctuations of chemically active droplets — •Guido Kusters and David Zwicker — Max Planck Institute for Dynamics and Self-Organization, Göttingen, Germany

Biological cells use liquid-liquid phase separation to dynamically compartmentalize their environment for various applications, many of which require size control. This process is challenging because (i) large droplets tend to grow at the expense of smaller ones, and (ii) thermal fluctuations can disturb droplets since cells are typically small and soft. Chemical reactions can, in principle, control droplet sizes, but there are no clear guidelines on how to robustly achieve size control. To provide guidelines, we consider a binary fluid model driven out of equilibrium by chemical reactions. We reveal two different classes of size-controlled droplets, depending on the ratio of droplet radius to the reaction-diffusion length. Moreover, we determine parameter regimes in which droplets become small. To study fluctuations in this case, we use fluctuation-dissipation arguments to predict the size fluctuations of size-controlled droplets, consistent with our numerical simulations. Taken together, our theory allows us to predict the chemical reactions necessary for maintaining small droplets, e.g., in biological cells or synthetic applications.

DY 52.3 Thu 15:30 BAR/SCHÖ

Anomalous diffusion and directed coalescence of condensates out of equilibrium — •Andriy Goychuk — Helmholtz Centre for Infection Research, Braunschweig, Germany — Lower Saxony Center for Artificial Intelligence and Causal Methods in Medicine, Hannover, Germany

Phase separation is ubiquitous in engineered and in biological systems. For example, biomolecular condensates contribute to the organization of the cytoplasm and nucleoplasm in cells. Here, I will first extend our understanding of textbook phase separation models by showing how condensates consisting of nonpolar molecules can effectively polarize and undergo coarsening by directed coalescence when subjected to a global drift, for example due to electrostatic potential gradients, chemical concentration gradients, or gravitation. Next, to better model the intracellular solution, I will incorporate viscoelastic stress propagation and nonequilibrium fluctuations. In this context, the Brownian motion of condensates has been barely explored despite being a cornerstone of statistical and colloidal Physics. If the active stresses, for example generated by molecular motors, have a different correlation time than the viscoelastic relaxation time of the solution, then the fluctuation-dissipation theorem is broken and the mixture is driven out of equilibrium. In this case, the size-dependence of the center-of-mass diffusion coefficient of the condensates can be either suppressed or enhanced, and the droplet can show superdiffusive motion. Together, these findings improve our understanding of the dynamics of domains in viscoelastic media and conserved order parameters in general.

DY 52.4 Thu 15:45 BAR/SCHÖ

A Minimal Theoretical Framework Linking Translation Activity to Stress-Induced Condensates — •Pascal S. Rogalla[1], Alessandro Barducci[1], and Luca Ciandrini[1,2] — [1]Centre de Biologie Structurale, Université de Montpellier, CNRS, INSERM, Montpellier, France. — [2]Institut Universitaire de France

The formation of intracellular membraneless organelles, such as stress-granule-like condensates formed via liquid-liquid phase separation (LLPS), is a common response to cellular stress. RNA, including mRNA, promotes the assembly of many of these condensates, while the resulting aggregation of mRNAs reduces their availability for translation and thereby modulates ribosome loading. This establishes a feedback loop between condensate formation and translational activity. Here we develop a minimal physical model that makes this coupling explicit by combining Flory-Huggins theory for LLPS with the Totally Asymmetric Simple Exclusion Process (TASEP) for ribosomal traffic on mRNAs. This hybrid framework provides a proof-of-principle description of how LLPS and translation dynamically influence one another. Our analysis reveals that the phase behaviour of both subsystems becomes mutually dependent: a low-occupancy ribosomal phase promotes mRNA aggregation, whereas a high-occupancy phase suppresses condensate formation. These results suggest that cells may regulate condensate formation through translation modulation and, conversely, that LLPS can reshape the translatome. This provides a first proof-of-principle framework for quantifying stress-induced reorganisation of the translational landscape.

DY 52.5 Thu 16:00 BAR/SCHÖ

Optimal sensing through phase separation — •Henry Alston[1], Mason Rouches[2], Arvind Murugan[2], Aleksandra Walczak[1], and Thierry Mora[1] — [1]Laboratoire de Physique, Ecole Normale Superieure — [2]The James Franck Institute & Department of Physics, The University of Chicago

Cells are constantly tasked with making accurate measurements of their surroundings. A paradigmatic example is the sensing of signalling molecule concentrations: the work of Berg and Purcell derived limits for the precision and speed of this sensing through ligand-receptor binding. However, recent experimental work has identified the formation of condensates (liquid droplets coexisting with the cell cytoplasm through phase separation) as a potential mechanism for selectively initiating downstream processes by effectively amplifying small concentration differences between competing signalling molecules. Using a minimal model for droplet nucleation and growth in a fluid mixture, we observe that phase separation can distinguish concentration differences of 1% in minutes, a significant improvement upon well-established pathways for precise concentration sensing.

DY 52.6 Thu 16:15 BAR/SCHÖ

Thermodynamics of DNA sequence recognition by a transcription factor — •Jonas Neipel[1,2,3], Anne Schwager[1], Yahor Savich[1,2,3], Douglas Diehl[1], Anthony A. Hyman[1], Frank Jülicher[2,3], and Stephan W. Grill[1,3] — [1]Max Planck Institute for Molecular Cell Biology and Genetics, Dresden Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden Germany — [3]Center for Systems Biology Dresden, Dresden, Germany

Transcription factors (TFs) are proteins that regulate the transcription of genes by binding to specific genomic positions defined by the DNA sequence. The sequence of preference of a TF is typically characterized by a single sequence motif that maximizes binding affinity. However, eukaryotic TFs bind to a spectrum of low affinity binding sites that vastly outnumber canonical motif sequences in the genome. Here, we develop an Ising model of DNA sequence recognition that yields quantitative prediction of TF binding energies across sequence space for the human TF KLF-4. The model is parametrized by in vitro experiments, where we quantify relative binding energies for various sequences in a competitive assay using fluorescence anisotropy. Strikingly, we find that the thus fully parametrized thermodynamic model quantitatively predicts KLF-4 occupancy across the human genome. Finally, we discuss how this genomic energy landscape guides the formation of TF condensates.

15 min. break

DY 52.7 Thu 16:45 BAR/SCHÖ

Kinetic inference of entropy production — •Ivan Di Trelizzi — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Nonequilibrium steady states, from planetary dynamics to biological processes, constantly dissipate energy to their environment, producing entropy at a constant rate. Quantifying this dissipation is key to understanding how far systems operate from equilibrium but remains experimentally challenging. I will present a new approach to infer entropy production directly from trajectory data, using measurable kinetic quantities known as traffic and inflow rate, without requiring knowledge of microscopic forces or fluxes. The method remains effective even under partial observation, providing a practical framework to quantify nonequilibrium behaviour in complex physical and biological systems.

DY 52.8 Thu 17:00 BAR/SCHÖ

Frequency-space trajectory Fisher Information to quantify sensitivity in complex living systems — •Zhiheng Wu[1] and Isabella Graf[1,2] — [1]European Molecular Biology Laboratory, Heidelberg, Germany — [2]Department of Physics and Astronomy, Heidelberg University, Heidelberg, Germany

Living systems sense their environment by stochastically mapping external signals onto internal states. For example, several animals including fruit flies and pit vipers encode small changes in the ambient temperature in terms of changes in the interspike time of neurons. The sensitivity of these measurements can be evaluated by the so-called Fisher information (rate). While living systems constantly adapt to changing environments, calculations of Fisher information have so far mostly focused on static signals and internal states. To evaluate measurement sensitivity in the non-static case, we evaluate the trajectory Fisher information and show that, under common assumptions, it can be expressed as an integral over frequency space involving the power spectral density. This expression provides a tractable way to quantify information in adaptive and complex biological systems and we discuss some interesting applications.

DY 52.9 Thu 17:15 BAR/SCHÖ

Ergodicity shapes inference in biological reactions driven by a latent trajectory — •Ricardo Martinez-Garcia[1], Benjamin Garcia de Figueiredo[2], Justin Calabrese[1], and William Fagan[3] — [1]CASUS-HZDR, Görlitz, Germany. — [2]Princeton University, Princeton NJ, USA. — [3]University of Maryland, College Park MD, USA.

Many natural phenomena, from intracellular reactions to predator-prey encounters, can be described as counts of events triggered at random intervals when an underlying dynamical system enters reactive regions of its phase space. These reactions control biological functions across scales, from cellular processes to ecosystem services and stability. We compute the exact distribution of inter-count times under the only assumption that the latent dynamical system is

Markovian and ergodic, recovering widely used Poisson statistics as a limiting case. These results limit what information about the latent process can be inferred from a local detector, which we explore in two biophysical scenarios. First, in estimating an animal's activity from detector crossings, we show that mean counts may fail to capture movement parameters, encoded in higher-order moments. Second, we show that the variance of inter-reaction times imposes a fundamental limit on how precisely detector measurements can infer the size of an ensemble of trajectories, generalizing the Berg-Purcell limit for chemosensation. Overall, we develop a flexible framework for quantifying inter-event time distributions in reaction-diffusion systems that shows which properties of latent processes are inferable from observed reactions.

DY 52.10 Thu 17:30 BAR/SCHÖ

Information Bottleneck in Gene Regulation — •Marianne Bauer — TU Delft

Biological systems need to process information in order to perform specific functions. In the context of gene regulation, regulatory regions process transcription factor signals in order for cells to differentiate towards correct fates. Previously, we have shown that the information bottleneck (IB) framework provides a useful framework for understanding regulatory binding site regions. Here, I will discuss two recent collaborative advances to provide an improved biological understanding from IB based predictions. First, using two complementary models for clustering transcription factors at binding site sensors, we can study information transfer during early fly embryo development with local transcription factor clustering. We find that weak cooperativity or clustering can allow for maximal information transfer, especially about the relevant variable, and that weak clustering also allows the binding site sensors to achieve optimality consistent with the IB bound. Second, we investigate how optimal activation changes when multiple binding site elements can process information, and find that activation profiles consistent with IB optimality resemble gene expression profiles in the early fly embryo.

DY 52.11 Thu 17:45 BAR/SCHÖ

Binary karyotypes are universally selected for across cancers — •Lucija Tomašić[1], Shane A. Fiorenza[1], Hajime Okada[2], Thomas W. van Ravesteyn[3], Uri Ben-David[2], Geert J.P.L. Kops[3], and Nenad Pavin[1] — [1]Univ. of Zagreb, Zagreb, Croatia — [2]Tel Aviv University, Tel Aviv, Israel — [3]Hubrecht Institute, Utrecht, the Netherlands

Aneuploidy, an abnormal chromosome number, is a defining feature of most cancers, yet its vast diversity has made it difficult to identify universal evolutionary rules. By analyzing over 90,000 patient-derived cancer karyotypes using a new visualization approach and mathematical modeling, we uncover a simple organizing principle. Across cancer types, and even in yeast, aneuploid genomes overwhelmingly assemble into "binary karyotypes" composed of only two chromosome copy numbers. Despite the enormous space of theoretically possible chromosome configurations, these states dominate patient data, comprising more than three-quarters of observed karyotypes. Our model shows that this pattern arises from a modest but consistent fitness advantage of binary karyotypes over more complex configurations. This principle also provides insight into how aneuploid cells withstand stress responses, as binary karyotypes exhibit lower rates of tumor suppressor gene inactivation. Together, our results identify binary karyotypes as a conserved evolutionary class of aneuploidy, governed by global organizational rules that may reveal shared vulnerabilities across cancers.

DY 52.12 Thu 18:00 BAR/SCHÖ

Inertial instability of blood in cross microchannels — •Joséphine Van Hulle and Christian Wagner — Experimental Physics, Saarland University, Germany

A localized reduction of vessel diameter (stenosis) increases the local blood flow speed and can trigger downstream recirculation which promotes conditions for the vessel blockage (thrombosis). The role of fluid elasticity in these flows remains underexplored. We isolate the extensional effects using cross-slot microfluidics, which creates an elongation plane with a well-defined inertial instability. By varying the hematocrit and plasma composition, we show that red blood cell deformability and plasma viscoelasticity lower the critical Reynolds number for the onset of vortex formation. These results highlight that even weak elastic stresses of blood can favor recirculation, a characteristic rarely modeled but necessary for physiologically realistic arterial simulations.

DY 53: Many-body Quantum Dynamics II (joint session DY/TT)

Time: Thursday 15:00–16:30 Location: HÜL/S186

DY 53.1 Thu 15:00 HÜL/S186

general framework for understanding and modeling irreversibility: relaxator Liouville dynamics — •Martin Janssen and Janos Hajdu — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

Irreversibility is explained as an emergent phenomenon brought about by a separation between two characteristic time scales: the time t_s up to which relevant degrees of freedom of a system are tracked is extremely much shorter than the spectral resolution time t_e necessary to resolve the spectrum of all degrees of freedom involved. A relaxator that breaks reversibility condenses in the Liouville operator of the relevant degrees of freedom. The irrelevant degrees of freedom act as an environment. The relaxator Liouville equation is a most general equation of motion in a many body quantum system and contains memory effects and initial correlations of all degrees of freedom, generalizing the well known semi-group dynamics. Stationary states turn out to be generically unique and independent of the initial conditions and exceptions are due to degeneracies. Equilibrium states lie in the relaxator's kernel yielding a stationary Pauli master equation and a non negative entropy production rate is identified. Kinetic equations for one-particle densities are constructed as special cases and Kubo's linear response theory is generalized to relaxator Liouville dynamics. In weak coupling between system and environment the relaxator can be factorized in environmental correlations and bilinear system operators.

DY 53.2 Thu 15:15 HÜL/S186

Ground-State Exploration Driven by Thermal and Quantum Fluctuations — •Yoshiaki Horiike[1] and Yuki Kawaguchi[1,2] — [1]Department of Applied Physics, Nagoya University, Nagoya, Japan — [2]Research Center for Crystalline Materials Engineering, Nagoya University, Nagoya, Japan

Simulated annealing provides a heuristic solution to combinatorial optimization problems. The cost function of a problem is mapped onto the energy function of a physical many-body system, and, by using thermal or quantum fluctuations, the system explores the state space to find the ground state, which may correspond to the optimal solution of the problem. Studies have highlighted both the similarities and differences between thermal and quantum fluctuations. Nevertheless, fundamental understanding of thermal and quantum annealing remains incomplete, making it unclear how quantum annealing outperforms thermal annealing. Here, we investigate the many-body dynamics of thermal and quantum annealing by examining all possible interaction networks of $\pm J$ Ising spin systems up to seven spins. Our comprehensive investigation reveals that differences between thermal and quantum annealing become prominent for particular interaction networks, indicating that the structure of the energy landscape distinguishes the two dynamics. We identify the microscopic origin of these differences through probability fluxes in state space, finding that the two dynamics are broadly similar but that quantum tunnelling produces qualitative differences. (arXiv:2511.16457)

DY 53.3 Thu 15:30 HÜL/S186

Symmetry re-breaking in an effective theory of quantum coarsening — •Federico Balducci[1], Anushya Chandran[2], and Roderich Moessner[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Boston University, Boston, MA

We present a simple theory accounting for two central observations in a recent experiment on quantum coarsening and collective dynamics on a programmable quantum simulator [T. Manovitz et al., Nature 638, 86 (2025)]: an apparent speeding up of the coarsening process as the phase transition is approached; and persistent oscillations of the order parameter after quenches within the ordered phase. Our theory, based on the Hamiltonian structure of the equations of motion in the classical limit of the quantum model, finds a speeding up already deep within the ordered phase, with subsequent slowing down as the domain wall tension vanishes upon approaching the critical line. Further, the oscillations are captured within a mean-field treatment of the order parameter field. For quenches within the ordered phase, small spatially-varying fluctuations in the initial mean-field lead to a remarkable long-time effect, wherein the system dynamically destroys its long-range order and has to coarsen to re-establish it. We term this phenomenon symmetry re-breaking, as the resulting late-time magnetization can have a sign opposite to the initial magnetization.

DY 53.4 Thu 15:45 HÜL/S186

Pairing-induced phase transition in the non-reciprocal Kitaev chain — •Pietro Brighi and Andreas Nunnenkamp — Faculty of physics, University of Vienna, Boltzmanngasse 5, 1090, Vienna, Austria

Investigating the robustness of non-reciprocity in the presence of competing interactions is central to understanding non-reciprocal quantum matter. In this

work, we use reservoir engineering to induce non-reciprocal hopping and pairing in the fermionic Kitaev chain, and reveal the emergence of a pairing-induced phase transition. The two phases appear in the spectrum of the non-Hermitian Kitaev Hamiltonian describing the dynamics of correlations, separated by an exceptional point. In the non-reciprocal phase, dynamics are characterized by directionality and slow relaxation, and the steady state supports non-reciprocal density and spatial correlations. At strong pairing, we uncover an unexpected density wave phase, featuring short relaxation times, a modulation in particle occupation and strikingly different correlation spreading depending on pairing non-reciprocity. Our work highlights the non-trivial breakdown of non-reciprocity due to superconducting pairing and invites experimental investigation of non-reciprocal fermionic systems.

DY 53.5 Thu 16:00 HÜL/S186

Harnessing spin qubit decoherence to probe strongly interacting quantum systems — Marcin Płodzień[1], •Sambunath Das[2], Maciej Lewenstein[1,3], Christina Psaroudaki[4], and Katarzyna Roszak[2] — [1]Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels (Barcelona), Spain — [2]Institute of Physics of the Czech Academy of Sciences, Na Slovance 1999/2, 182 00 Prague, Czech Republic — [3]Passeig Lluis Companys 23, 08010 Barcelona, Spain — [4]Laboratoire de Physique de l' École Normale Supérieure, Université PSL, CNRS, Sorbonne Université, Université de Paris, 75005 Paris, France

Using a mobile qubit as a probe to study the properties of a larger quantum system is a novel technique that leverages the quantum nature of the probe, the system under study, and the interaction between them [1-3]. By analyzing qubit decoherence, one accesses to properties that are difficult to measure classically. We apply this method to the anisotropic Heisenberg XXZ spin-1/2 chain, an archetypal example of strongly correlated system, and show that qubit dynamics encode key system parameters, including quantum phase transitions and perturbation propagation velocity [4]. This demonstrates the effectiveness of small quantum probes for exploring large quantum systems.

References: 1. F. Casola, T. van der Sar et al, Nat. Rev. Mat. 3, 17088 (2018). 2. J. F. Rodriguez-Nieva, K. Agarwal et al. Phys. Rev. B 98, 195433 (2018). 3. S. Chatterjee, J. F. Rodriguez-Nieva et al, Phy. Rev. B 99, 104425 (2019). 4. M Płodzień, S. Das et al, Phy. Rev. B 111, L161115 (2025).

DY 53.6 Thu 16:15 HÜL/S186

Enhancing efficiency of local-information time evolution — •Moksh Bhateja[1], Jonas Rigo[2], and Markus Schmitt[2,3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Universität Regensburg, Regensburg, Germany — [3]PGI-8: Forschungszentrum Jülich, Jülich, Germany

The time evolution of an initially unentangled system under the von Neumann equation generally leads to rapid entanglement growth. This poses challenges for numerical tractability. The Information Lattice framework addresses this by systematically discarding accumulated non-local information (i.e., entanglement) to maintain computational feasibility. Within the local-information time evolution (LITE) approach, we propose Rényi-2 entropy as a measure of information, eliminating the need for matrix decomposition. When combined with additional approximations, this approach significantly enhances the efficiency and scalability of simulations in terms of both system size and duration of time evolution. We demonstrate the accuracy of this method by computing high-quality diffusion coefficients and local observables for a large non-integrable system.

DY 54: Statistical Physics: General II

Time: Thursday 15:00–17:45 Location: ZEU/0114

DY 54.1 Thu 15:00 ZEU/0114

Fluctuating hydrodynamics of non-equilibrium interacting many-body systems — •Felipe Pereira-Alves and Aljaž Godec — Mathematical Physics and Stochastic Dynamics, Institute of Physics, University of Freiburg (GER)

Extending fluctuating hydrodynamics to non-equilibrium systems remains a significant theoretical challenge. In this work we investigate, on the level of distribution-valued fluctuating hydrodynamics, general short-range interacting systems as well as the long-range interacting Dyson process evolving from deterministic non-equilibrium initial conditions. We characterize the probability measure of the distribution-valued fluctuation field during the relaxation to equilibrium and illustrate the results on the example of discretely (in space) observed fluctuation field and compare the results to particle-resolved simulations.

DY 54.2 Thu 15:15 ZEU/0114

Non-ergodicity and breakdown of hydrodynamics in a one-dimensional cold gas — Taras Holovatch[1,2], Yuri Kozitsky[3], Krzysztof Pilorz[3], and •Yurij Holovatch[1,2,4,5] — [1]Yukhnovskii Institute for Condensed Matter Physics of the NAS of Ukraine, Lviv, Ukraine — [2]L4 Collaboration and Doctoral College for the Statistical Physics of Complex Systems, Lviv-Leipzig-Lorraine-Coventry, Europe — [3]Institute of Informatics and Mathematics, Maria Curie-Skłodowska University, Lublin, Poland — [4]Centre for Fluid and Complex Systems, Coventry University, Coventry, UK — [5]Complexity Science Hub, Vienna, Austria

We study dynamics of a 1D chain of elastically interacting particles with masses alternating between two different values, M,m,M,m,.. . Its dynamics is initiated by giving unit velocity in the positive direction to the particle located at the origin. For random particle positions, the resulting long-time behavior was found (S. Chakraborti et al., SciPost Phys. 2022, 13, 074) to posses rather remarkable features: (i) a shock front develops in the bulk of the gas and is governed by Euler hydrodynamics, (ii) the recoiled particles in the splatter move ballistically. In our study we have found (T. Holovatch et al., Phys. Rev. E 2025, 112, L052101) that for equidistant particle positions there exist mass ratios M/m for which (i) the splatter is absent; (ii) the number of simultaneously moving particles is at most three; (iii) the blast front moves in the ballistic way. We support our explicit calculations by MD simulations.

DY 54.3 Thu 15:30 ZEU/0114

Geometry-induced timescales in viscoelastic fluids — •Rupayan Saha[1], Niloyendu Roy[2], Debankur Das[1], Clemens Bechinger[2], and Matthias Krüger[1] — [1]Institute for Theoretical Physics, Georg-August-Universität Göttingen, Göttingen 37073, Germany — [2]Fachbereich Physik, Universität Konstanz, Konstanz 78457, Germany

Recoil experiments provide a powerful window into the non-Markovian properties of complex fluids, revealing memory effects that are usually obscured in conventional rheological measurements. While translational recoil of colloidal probes in viscoelastic media has been successfully modelled with **few distinct timescales**, orientational recoil exhibits an **unbounded** relaxation spectrum, manifested in the divergence of the recoil amplitude with increasing shear-time (t_{sh}) or system size (L). To resolve its physical origin, we design a **first-principles theoretical framework** rooted in the *geometric constraints of torsional flow*. Our model, based on concentric spherical shells, demonstrates that the orthogonality between angular momentum propagation and torsional stress storage generates **a radial scaling law for relaxation modes**. The theory thus establishes **geometry**—not material-complexity—as the primary candidate for engineering complex memory in soft matter. We finally elucidate why such *long relaxation times* have not been previously discovered through conventional rheology.

DY 54.4 Thu 15:45 ZEU/0114

Ion and Water Density Profiles in Nano-Confinement — •Haoyuan Quan, Maximilian Becker, Hanne Antila, and Roland Netz — Freie Universität Berlin, Berlin, Germany

Confined salt solutions are important in biology and in technical applications, such as environmentally friendly energy conversion, yet even basic trends of how ion and water densities change in confinement remain unclear. Using molecular dynamics simulations of graphene slits in equilibrium with bulk aqueous salt solutions, we determine concentration profiles of a variety of alkali-halide ion pairs as a function of slit width and bulk concentration. Using ion and water depletion lengths, which clearly reflect ion-specific effects, we construct a robust and thermodynamically consistent theory to describe water and ion concentrations in confined systems for varying slit widths and bulk salt concentrations.

DY 54.5 Thu 16:00 ZEU/0114

The electron transfer process at the electrode/electrolyte solution interface: A stochastic model and its Monte Carlo implementation — •Diego Veloza-Diaz[1], Friederike Schmid[1], Robinson Cortes-Huerto[2], Pietro Ballone[2], and Nancy C. Forero-Martinez[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany — [2]Max Planck Institute for Polymer Research, Germany

A kinetic model of the electron transfer at the electrode/electrolyte interface is developed, implemented in a Monte Carlo framework, and applied to simulate this process in idealised systems consisting of the primitive model of electrolyte limited by an impenetrable conducting surface. A charged, spherical interface surrounding an equally spherical sample of electrolyte is introduced to model a single-electrode system, providing a computational analogue to the conceptual half-cell picture widely used in electrochemistry. The electron transfer itself is described as a simple surface-hopping process underlying a first-order reaction corresponding to one of the coupled M/M+ and X*/X half-reactions. Then, electron transfer at the interface is combined with the self-diffusion of ions in the electrolyte, which supply reagents and disperse products, allowing the system to settle into a stationary non-equilibrium state. Simulations of the primitive model of an electrolyte in contact with a charged, impenetrable surface show that, after

a brief transient, the system sustains a steady current through the half-cell. Since the simulated interface is very idealised, strategies to overcome the limitations of the present model are outlined and briefly discussed.

DY 54.6 Thu 16:15 ZEU/0114

Fermion as a non-local particle-hole excitation — •Girish Setlur — Department of Physics, Indian Institute of Technology Guwahati

We show that the fermion, in the context of a system that comprises many such entities, which, by virtue of the Pauli exclusion principle, possesses a Fermi surface at zero temperature, may itself be thought of as a collection of non-local particle-hole excitations across this Fermi surface. This result is purely kinematical and completely general, not restricted to any specific dimension, and is applicable to both continuum and lattice systems. There is also no implication that it is applicable only to low-energy phenomena close to the Fermi surface. We are able to derive the full single-particle dynamical Green function of this fermion at finite temperature by viewing it as a collection of these non-local particle-hole excitations. The Green function of the fermion then manifests itself as a solution to a first-order differential equation in a parameter that controls the number of particle-hole pairs across the Fermi surface, and this equation itself reveals variable coefficients that may be identified with a Bose-Einstein distribution, implying that there is a sense in which the non-local particle-hole excitations have bosonic qualities while not being exact bosons at the level of operators. We also recall the definition of the non-local particle-hole operator that may be used to diagonalize the kinetic energy of free fermions of the sort mentioned above. Number-conserving products of creation and annihilation operators of fermions are expressible as a (rather complicated) combination of these non-local particle-hole operators.

15 min. break

DY 54.7 Thu 16:45 ZEU/0114

Emergence of generic first-passage time distributions for large Markovian networks — •Julian B. Voits[1] and Ulrich S. Schwarz[1,2] — [1]Institute for Theoretical Physics, University of Heidelberg, Germany — [2]BioQuant-Center for Quantitative Biology, University of Heidelberg, Germany

In many situations of practical interest, for example for decision-making in biological systems, it is sufficient to characterize a stochastic process by the time at which a final, absorbing state is reached (first-passage time). A prominent example is kinetic proofreading, where cells achieve remarkably accurate decisions through non-equilibrium reaction cycles. Earlier work studying corresponding models observed that as the system size grows, the first-passage time distributions converged to one of two universal forms on the time scale of its mean: either quasi-deterministic (delta-like) or quasi-memoryless (exponential). Building on the graph-theoretical interpretation of first-passage processes, here we provide a unifying explanation for these universal limits based on the distribution of the eigenvalues of the generator matrix. Then, we derive general conditions under which the distribution converges to either the deterministic or exponential limit. We demonstrate the theory by applying it to a generic birth-death process and conclude by discussing illustrative cases where the simple limiting behavior does not hold, which contradicts the naive expectation that a forward bias is sufficient to lead to a deterministic outcome.

DY 54.8 Thu 17:00 ZEU/0114

Derivation of a multi-dimensional non-equilibrium generalized Langevin equation — •Benjamin Hery — Department of Physics, Freie Universität Berlin, 14195 Berlin, Germany

The Mori-Zwanzig formalism is a powerful theoretical framework for deriving generalized Langevin equations (GLEs) for observables of interest using evolution and projection operators. Using a multi-dimensional Mori projection operator, we derive a non-equilibrium Mori GLE for a multi-dimensional observable of interest $\vec{A}$ that consists in a Markovian force, a running integral over time of a non-Markovian friction force, and a orthogonal force that is often interpreted as a random force. We study the structure of the derived GLE in three limiting cases: when the components of $\vec{A}$ are uncorrelated, when the system is at equilibrium, and when both conditions happen at the same time. In particular, we highlight the presence of a contribution to the Markovian force that takes the form of an instantaneous friction force which only vanishes when the components of $\vec{A}$ are uncorrelated.

DY 54.9 Thu 17:15 ZEU/0114

Predicting Friction Modifications under Harmonic Confinement via Perturbative Mori Projections — •Felix Riesterer and Roland Netz — Department of Physics, Freie Universität Berlin, Germany

Previous studies have shown that external potentials can alter friction, yet a comprehensive theoretical explanation for this effect is still lacking. This issue is particularly relevant for enhanced sampling techniques, such as umbrella sampling, where applied biases can distort dynamical observables.

We present a theoretical framework based on perturbative projections within the Mori Generalized Langevin Equation (GLE). The approach provides an explicit first-order prediction of the friction correction due to an external potential using only unbiased simulations. Furthermore, it clarifies the conditions under which such corrections arise.

To validate the theory, we perform molecular dynamics simulations of a Lennard-Jones fluid (argon) confined in a harmonic potential of varying strength. The theoretical predictions capture the friction enhancement to first order in the potential stiffness. These results demonstrate how harmonic umbrella sampling can modify friction, highlighting the potential impact on the interpretation of dynamical quantities obtained from biased simulations.

DY 54.10 Thu 17:30 ZEU/0114

Perturbative projection of many-body systems with applications in enhanced sampling of biomolecules — •Joan Salas-Llabrés — Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany

Using a modification of the well-known Mori-Zwanzig projection operator formalism, a Generalized Langevin Equation (GLE) is derived for a general observable of interest that only depends on the phase space positions, from a many-body Hamiltonian in the presence of a constant linear external potential. In particular, the friction memory kernel is analytically computed, and via an operator perturbative expansion, it is expanded in terms of the external potential up to first order in the potential strength. We name this approach "perturbative projection", and it allows to see the effects that this bias can have on the effective dynamics of a reaction coordinate, in particular on its friction. To test the obtained analytical expression and thus compare to some order of approximation the change in friction with direct results, we choose the conformational dynamics of alanine nonapeptide in water, obtained via molecular dynamics simulations. The results show agreement over a range of bias strengths. This provides new insight into the effects of an external bias on the dynamics of a system of interest, pointing to its fundamental nature in the level of its Hamiltonian, and which in particular has important consequences for the analysis of results coming from enhanced sampling techniques.

DY 55: Focus Session: Emergent Transport in Active Systems (joint session DY/BP)

Collective motion and directed transport are hallmark phenomena of active matter, arising from the interplay of self-propulsion, interactions, and nonequilibrium fluctuations. Even in the absence of global biases, assemblies of active particles can exhibit spontaneous currents, self-organized chemotaxis, and rectified transport due to broken symmetries or nonlinear feedbacks. Directed transport often emerges in inhomogeneous environments, where variations in particle activity or interaction strength can bias motion and organization. Activity gradients represent a particularly relevant example, providing a tunable mechanism to steer collective motion and pattern formation. These processes link microscopic activity to macroscopic material behavior and transport. This focus session aims to bring together theorists and experimentalists working on the fundamental mechanisms and control of emergent transport in active systems.

Organized by Abhinav Sharma (Augsburg) and Jens-Uwe Sommer (Dresden)

Time: Thursday 15:00–18:00 Location: ZEU/0160

Invited Talk DY 55.1 Thu 15:00 ZEU/0160

Out-of-equlibrium synthetic cells: the future of active matter — •Laura Alvarez — Univ. Bordeaux, CNRS, CRPP, UMR 5031

Colloidal active swimmers are broadly used as model systems to design microswimmers, yet their rigid and solid architecture limits their adaptability and functionality. A promising alternative is using bioinspired soft compartments

for the design of cell-mimetic functional architectures while avoiding the complexity of living cells.

Here, I will showcase our latest results on driving giant unilamellar vesicles (GUVs) out of equilibrium via controlled external actuation to mimic and study life-like processes. We fabricate phase-separated Janus lipid vesicles, harnessing membrane fluidity to obtain reconfigurable motion. Under external electric fields, these asymmetric compartments self-propel and display transient run-and-tumble-like dynamics arising from the coupling between mobile membrane domains and the field. By tuning lipid composition and using temperature as an external trigger, we modulate membrane fluidity and phase separation, enabling in situ control over the frequency of tumble events. Beyond motility, we exploit electric fields to induce controlled shape transformations and vesicle division events, showing that the same actuating scheme can access higher-order cell-like functions. In parallel, we use light to drive strong, localized membrane fluctuations, providing a route to study active, non-thermal shape dynamics in soft compartments. These results highlight synthetic cell membranes as versatile platforms in which different functions can be triggered using simple external fields.

DY 55.2 Thu 15:30 ZEU/0160

Biohybrid active matter: active cargo transport by motile cells — Jan Albrecht[1], Lara S. Dautzenberg[1], Manfred Opper[2], Carsten Beta[1], and •Robert Grossmann[1] — [1]University of Potsdam, Potsdam, Germany — [2]Technical University Berlin, Berlin, Germany

We describe the transport of polystyrene beads whose motion is actively driven by cells via direct mechanical contact. We will first discuss the stochastic dynamics of a single cell-cargo pair, focusing on the existence of an optimal cargo size that enhances the diffusion of the load-carrying cells, and estimate the active forces exerted by cells to move colloids. Furthermore, we present the collective transport of these micron-sized particles on a monolayer of motile cells. The colloids' mean-square displacement shows a crossover from superdiffusive to normal-diffusive dynamics. The particle displacement distribution is, however, distinctly non-Gaussian even at macroscopic timescales exceeding the measurement time. We attribute the non-Gaussian statistics to heterogeneity and non-stationarity of the dynamics, and particularly apply a likelihood-based inference framework to estimate the heterogeneity of the bead dynamics from their discretely sampled trajectories. We showcase how this approach can deal with information-scarce situations and provides natural uncertainty bounds for heterogeneity estimates. Similar transport properties are expected for many composite active matter systems. These results thus provide the basis for the future design of cellular microcarriers and for more advanced transport tasks in complex, disordered environments, e.g. tissues.

Invited Talk DY 55.3 Thu 15:45 ZEU/0160

Chemotactic like behavior in by active Brownian particles: from single particles to to polymers — •Hidde Vuijk — University of Augsburg, Universitätsstraße 1, 86159, Augsburg, Germanz

Active Brownian particles can be used as simplified models for microscopic, motile organisms. This research investigates the behavior of such self-propelled objects in spatial gradients of activity, where their self-propulsion speed varies with position. A single active particle tends to accumulate in low-activity regions. When activity is assumed to be proportional to fuel, this corresponds to antichemotactic like behavior. We demonstrate how this behavior can be reversed by structuring particles into simple complexes. For example, by connecting active particles to passive cargo or linking them into chains, we predict a crossover from accumulation in low-activity regions to accumulation in high-activity regions, that is chemotaxic like behavior. These active dimers and polymers can autonomously move up an activity gradient, accumulating where the fuel concentration is highest. This emergent gradient-sensing arises from the physical interactions, offering a novel mechanism for the design of active matter and providing insight into how primitive life forms without complex information processing might have located nutrients.

DY 55.4 Thu 16:15 ZEU/0160

Fluctuation-induced transition in transport of active colloidal cells — •Shashank Ravichandir[1,2], Jens-Uwe Sommer[1,2], and Abhinav Sharma[1,3] — [1]Leibniz Institute of Polymer Research, Dresden, Germany — [2]Technical University Dresden, Dresden, Germany — [3]University of Augsburg, Augsburg, Germany

The transport of active-passive assemblies and their self-localization behavior have been studied in some detail in recent years [1,2]. The "chemotactic" property these exhibit has been attributed to the separation of time scales, i.e between the persistence time of the active particle and the characteristic time scale associated with the interaction between the particles (ex - harmonic springs). We consider a gas of active particles enclosed in a circular vesicle and observe that the transport behavior of the vesicle depends on the density of the enclosed gas or the number of active particles. This is a new mechanism for achieving desired transport of active colloidal cells as no new timescales are introduced by changing the number of active particles. This transition in transport behavior of these vesicles seems to be driven by fluctuations. The proposed model is also experimentally reproducible, contrary to the active-passive assemblies that have been studied so far.

[1] H. D. Vuijk et al., Phys. Rev. Lett., 126(20), 2021. [2] P. L. Muzzeddu et al., Phys. Rev. Lett., 133(11), 2024.

15 min. break

Invited Talk DY 55.5 Thu 16:45 ZEU/0160

From non-reciprocal torques towards shape-flexible and res-ponsive prototypic worms — •Holger Stark and Jeanine Shea — Institute of Physics and Astronomy, Theoretical Physics, Techni-sche Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Non-reciprocal interactions as seen in active matter allow the formation of novel collective states that are only observable in the non-equilibrium. They may serve as prototypes for mimicking what is observed in the real world or for guiding robotic applications.

We start from non-reciprocal orientational interactions, where an active Brownian particle turns away from its neighbors [1]. By varying range and strength of the torque, we discover novel states such as travelling bands or dynamic flocking. Reversing the sign, makes the orientational interaction cohesive. We combine it with aligning torques and again for varying range and torque strength observe multiple, rotary, and persistent worms as well as an aster state [2]. In particular, the persistent worm represents a prototype for a flock of active constituents, either natural or robotic, which shows a remarkable flexibility and integrity when performing shape changes. This becomes obvious when hunting a prey, which leaders inside the worm sense via some chemotactic mechanism. In contrast to the macroscopic world, here without inertia, moving on a straight line seems the best strategy to escape. We also observe that the worm stays intact, even when squeezing through a narrow, long pore.

[1] M. Knezevic, T. Welker & H. Stark, Sci. Rep. 12, 19437 (2022).
[2] Jeanine Shea & Holger Stark, EPJE 48, 22 (2025).

DY 55.6 Thu 17:15 ZEU/0160

Directed motion of active collectives in activity gradients — •Hossein Vahid[1], Jens-Uwe Sommer[1,2], and Abhinav Sharma[1,3] — [1]Leibniz-Institut für Polymerforschung Dresden, 01069 Dresden, Germany — [2]Technische Universität Dresden, 01069 Dresden, Germany — [3]Institute of Physics, University of Augsburg, Universitätsstraße 1, 86159 Augsburg, Germany

Directed motion appears across all scales of active matter, from biomolecular condensates inside cells to large assemblies of migrating filaments. By simulating active particles and polymers, we identified the mechanisms that enable activity gradients to steer these collectives and control their assembly [1,2]. In cohesive mixtures, droplets climb activity gradients, fragment when the activity becomes too intense, and reassemble in low activity regions. This creates a robust cycle of positioning without needing any biochemical feedback. Similarly, in assemblies of active polar polymers, spatial gradients in activity, combined with temporally stochastic propulsion, generate net body forces on dimers, asters, and multiarm structures. This biases their motion toward high-activity regions and stabilizes long-lived entangled clusters even at low concentrations.

[1] H. Vahid, J.-U. Sommer, A. Sharma, Self-Organization and Cyclic Positioning of Active Condensates, arXiv preprint arXiv:2510.15771 (2025). [2] H. Vahid, J.-U. Sommer, A. Sharma, Collective dynamics in active polar polymer assemblies, Phys. Rev. Res. 7, L042031 (2025).

DY 55.7 Thu 17:30 ZEU/0160

Activity hallmarks in kinetic theory: Exceptional Points, Disorder Regularization, Non-Reciprocal Orientation-Displacement Coupling — •Horst-Holger Boltz and Thomas Ihle — University Greifswald, Institute for Physics, Greifswald

The dynamics of active systems are not subject to the same constraints as that of passive classical systems. This is particularly true for self-propelled particles with alignment interactions that have orientation-displacement coupling, i.e. the alignment is dependent on the relative position of the interacting particles to each other. We present recent work within first-principle kinetic theory that highlights key hallmarks of these more generalized dynamics. In particular, we discuss the effect of a cascade of exceptional points in the relevant dynamical operators under finite noise and also how to generally include noise in collision-based kinetic theory beyond mean-field. This allows us to provide analytical insights into the numerically established scaling relations (Kürsten, 2025) underlying the critical exponents in flocking transitions. Also, we are going to explain how to derive a systematic mesoscopic description for aligning self-propelled particles with orientation-displacement coupling and will present results showing a flocking transition in a system of a single species with purely anti-aligning torques and without any forces, simplifying an earlier reported flocking by turning-away mechanism (Das et al, 2024).

Boltz, Ihle, in preparation; Kürsten, arXiv:2402.18711 (2025); Das et al, Phys. Rev. X 14, 031008 (2024); Boltz et al, Entropy, 26(12), 1054 (2024); Ihle et al, arXiv:2303.03357 (2023)

DY 55.8 Thu 17:45 ZEU/0160

Rouse Polymers in Time-dependent Nonequilibrium Baths — •Bhavesh Valecha[1] and Abhinav Sharma[1,2] — [1]Mathematisch-Naturwissenschaftlich-Technische Fakultät, Institut für Physik, Universität Augsbur, Augsburg, Germany — [2]Leibniz-Institut für Polymerforschung Dresden, Institut Theory der Polymere, Dresden, Germany

Directed transport is a characteristic feature of numerous biological systems in response to nutrient and chemical gradients. These signals are often time-dependent owing to the high complexity of interactions in these systems. In this study, we focus on the steady-state behavior of polymeric systems responding to such time varying signals. We model them as ideal Rouse chains submerged in a time-dependent and inhomogeneous nonequilibrium bath, which is described by a spatially and temporally varying self-propulsion wave field experienced by the monomer units. Through a coarse-graining analysis, we show that these chains display rich emergent response to the temporal stimuli as a function of their length and topology. In particular, for slow moving waves, short chains composed of up to 3 monomers drift against self-propulsion wave, whereas, longer chains drift in the direction of the wave. In contrast, for fast moving waves, all chains drift along the wave regardless of their length. Moreover, we find that the star topology displays the highest drift for both slow and fast moving waves. We confirm these analytical predictions with robust numerical simulations, showing that response of polymeric systems to temporal stimuli can be controlled by the topology or the length of the polymer.

DY 56: Members' Assembly

Time: Thursday 18:00–19:00 Location: ZEU/0160

All members of the Dynamics and Statistical Physics Division are invited to participate.

DY 57: Statistical Physics of Biological Systems IV (joint session BP/DY)

Time: Friday 9:30–12:45 Location: BAR/SCHÖ

Invited Talk DY 57.1 Fri 9:30 BAR/SCHÖ

Swimming in complex environments — •Christina Kurzthaler — Max Planck Institute for the Physics of Complex Systems

Microorganisms are omnipresent in the ocean, the human body, and our soils and therefore play an important role for various geological, biological, and medical processes. To optimize their survival and perform biological functions many microorganisms convert chemical energy into directed motion. In this talk, I will illustrate the underlying physical concepts and show concrete examples of our research, focusing on the interactions of microorganisms with their complex habitats. I will first discuss the motion of sperm in complex fluids and address their emergent dynamics in the presence of a hyperactivation agonist, modifying the sperm beating pattern. Second, I will focus on the first-passage-time statistics of active agents moving towards a target boundary. Our results highlight how swim gait impacts spreading and search efficiency in active systems with potential consequences for sperm motion in the reproductive tract and the accumulation of microbial communities.

DY 57.2 Fri 10:00 BAR/SCHÖ

Motor shot noise explains active fluctuations in a single cilium — •Maximilian Kotz[1], Veikko F. Geyer[2], and Benjamin M. Friedrich[1] — [1]Cluster of Excellence Physics of Life, TU Dresden, Dresden, Germany — [2]B CUBE, TU Dresden, Dresden, Germany

Molecular motors drive seemingly regular motion, making living matter move - yet also cause non-equilibrium fluctuations that can serve as a probe of internal motor dynamics. Here, we use motile cilia as a model system to investigate how small-number fluctuations shape collective dynamics. Motile cilia exhibit regular bending waves; this motion is driven by the self-coordinated activity of thousands of molecular motors inside the cilia's cytoskeletal core. By developing, to the best of our knowledge, the first stochastic model of cilia beating, we show that the finite number of motors leads to active fluctuations on the mesoscale, sufficient to explain frequency jitter in beating cilia observed in experimental data. We rigorously compare observables of this model, including the quality factor of the oscillation, to experimental data in which motors have been partially extracted from cilia. This is a strong test of this stochastic model. The model also reproduces other phenomena of experimental data, like correlation lengths of intra-cilium synchronization and noise-induced phase slips. We propose that active fluctuations are important new observables, which can guide theoretical models of motor dynamics in beating cilia and other motor systems.

DY 57.3 Fri 10:15 BAR/SCHÖ

Theory of Forces Between Crosslinked Filaments — •Cedrik Barutel and Sebastian Fürthauer — Institute of Applied Physics TU Wien Austria

The cytoskeleton drives essential cellular processes like cell division and chromosome segregation. It consists of filaments that are crosslinked by proteins, many of which are molecular scale motors that consume ATP to do work. The forces that crosslinking proteins generate between cytoskeletal filaments are the key drivers of active cellular mechanics. We derive a generic theory to describe such crosslinking forces.

We construct a theory to describe and predict the forces generated collectively by crosslinking proteins between biofilaments using symmetries, conservation laws, and out-of equilibrium thermodynamic principles. Our approach identifies the full set of phenomenological coefficients governing entropic, active, and frictional crosslinking forces, which allows a quantitative comparison between the effects of different crosslinker mixtures between two filaments. We demonstrate the power and validity of this framework by quantitatively explaining a set of different experimental setups, which combine the effects of passive and active crosslinks

DY 57.4 Fri 10:30 BAR/SCHÖ

Modeling Cooperative Remodeling and Energy Landscapes in the Bacterial Flagellar Motor — •Nils-Ole Walliser — Laboratoire Charles Coulomb, University of Montpellier, Montpellier, France

Bacteria use the flagellar motor to adapt their motility to changing mechanical conditions. This rotary motor tunes its torque by recruiting and releasing torque-generating stator units. I will present statistical-physics-based models that use single-motor measurements to infer interaction potentials and energy landscapes in the bacterial flagellar motor. First, using single-motor bead assays that resolve stepwise changes in rotation speed and thus stator occupancy, we model stator recruitment as a finite-size lattice gas and infer stator-stator cooperativity from occupancy fluctuations. This reveals moderate attractive interactions and shows that the motor operates in a regime that balances responsiveness to load changes with noise in stator number. Second, I will discuss experiments where the motor load is actively perturbed, uncovering a strong asymmetry in the relaxation to the steady state when starting from higher versus lower stator occupancy. A two-state catch-bond model quantitatively explains this stoichiometry-dependent asymmetry and captures the mechanosensitive nature of stator anchoring to the cell wall. Finally, I will show how high-temporal-resolution rotation traces can be used to reconstruct, in a model-independent way, the tilted periodic energy landscape of the rotor/LP ring within a Smoluchowski framework, yielding barrier heights, torque and internal friction.

DY 57.5 Fri 10:45 BAR/SCHÖ

Anisotropic (sub)diffusion of organelles in living cells — •Aranyak Sarkar, Pooja Yadav, and Matthias Weiss — Experimental Physics I, University of Bayreuth, Universitätsstraße 30, 95447 Bayreuth

Eukaryotic cells are neatly organized into distinct, membrane-enclosed compartments ('organelles') with specific duties. A prominent example are peroxisomes, which feature vesicle-like shapes with radii $0.1 - 1\ \mu$m that are dispersed across the cytoplasm. Using time-lapse fluorescence microscopy, we have tracked the motion of individual peroxisomes over extended periods. Analysis of the experimental data revealed two distinct modes of motion: a prevailing (sub)diffusive motion and a quite rare super-diffusive characteristics that is associated with motor-driven transport along microtubules. Focussing on the seemingly unremarkable subset of (sub)diffusive trajectories, we have found a significant anisotropy in the motion that persisted even when microtubules were disrupted. In particular, diffusive steps along the cells' long axis were seen to be favored over steps in the perpendicular direction, indicating an anisotropic materials characteristic of the cytoplasm. Using a simple model, we were able to capture and explain the observed features of the anisotropic diffusion of organelles.

15 min. break

DY 57.6 Fri 11:15 BAR/SCHÖ

Understanding Influenza A Virus particles detaching from reconstructed cell surfaces — •Thomas Kolbe[1,2], Pierre Gaspard[1], and Bortolo Matteo Mognetti[1,2] — [1]CENOLI, Université Libre de Bruxelles (ULB) — [2]IB2 - Interuniversity Institute of Bioinformatics in Brussels

Influenza infection is a multistage process that involves the trafficking of viral particles across the cell membrane. Before endocytosis, virions target the membrane by binding hemagglutinin ligands to sialic acid residues on cell receptors. After budding, neuraminidase cleaves these residues, enabling virions to detach from the infected cell surface.

We examine detachment dynamics through simulations and theoretical analysis. We explain experimental findings showing that the time required for virions to detach can decrease as the single-trajectory average number of bonds increases - a counterintuitive result specific to neuraminidase activity. Furthermore, we demonstrate that the detachment time is not governed by a Poisson distribution but depends on multiple factors, including ligand-receptor reaction rates, virion size, and receptor diffusion constant. These results clarify how biochemical parameters regulate the residence time of virions at the cell surface.

DY 57.7 Fri 11:30 BAR/SCHÖ

Band pattern formation of erythrocytes in density gradients is due to competing aggregation and net buoyancy — •Felix Maurer[1], Camila Romero[1], Nikolas Lerch[1], Thomas John[1], Lars Kaestner[1,2], Christian Wagner[1,3], and Alexis Darras[1,4] — [1]Experimental Physics, Saarland University, Saarbruecken, Germany — [2]Department of Theoretical Medicine and Biosciences, Saarland University, Homburg, Germany — [3]Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg — [4]School of Physics, University of Bristol, Bristol, United Kingdom

Centrifugation of biological matter in density gradient solutions is a standard method for separating cell types or components. It is also used to separate RBCs by age, as they lose water and become denser over their lifespan. When the density gradient is prepared with Percoll, discrete bands of RBCs are systematically observed, despite the continuous density distribution of RBCs. We developed a continuity equation incorporating cell aggregation to describe the macroscopic evolution of RBC volume fraction in a density gradient, considering a continuous RBC density distribution. Numerical solutions demonstrate that the competition between net buoyancy and aggregation is sufficient to create band patterns. Our model reproduces the temporal evolution observed in experiments, but also predicts several types of bifurcation-like behaviors for the steady-state patterns in constant gradients, depending on RBC volume fraction and aggregation energy.

DY 57.8 Fri 11:45 BAR/SCHÖ

Adaptive self-organization in excitable biological collectives — •Bianca Ariani[1,3], Yunus Sevinchan[2,3], and Pawel Romanczuk[2,3] — [1]Bernstein Center for Computational Neuroscience, Berlin — [2]Science of Intelligence, TU Berlin — [3]Institute for Theoretical Biology, HU Berlin

Biological collectives often display complex, context-dependent behavior, such as coordinated responses to predators, despite individuals following simple local rules. This class of phenomena is broadly understood as self-organization.

We examine a system showing rich spatio-temporal dynamics: Sulphur Mollies, Mexican freshwater fish whose group behavior resembles a stochastic excitable medium. To probe the mechanisms behind their collective activity, we study a bio-inspired agent-based model in which individuals estimate the shoal's mesoscale activity from the cues they perceive as they move. Each agent adjusts its sensitivity to cues through a simple homeostatic plasticity rule, allowing the group to regulate its collective state. This formulation links individual adaptation to population-level patterns.

Our results show that local adaptive regulation reproduces key qualitative features of the biological system. More generally, they illustrate how distributed plasticity mechanisms can support robust self-organization in complex biological collectives.

DY 57.9 Fri 12:00 BAR/SCHÖ

Visual-based Collective Shepherding in Swarm Robotic System — •Yating Zheng[1,2] and Pawel Romanczuk[1,2] — [1]Department of Biology, Humboldt Universität zu Berlin, Berlin, Germany — [2]Research Cluster of Excellence 'Science of Intelligence', Berlin, Germany

Collective shepherding presents a rich example of two interacting multi-agent systems coupled through non-reciprocal interactions. While most existing models assume that shepherd agents have global knowledge of the flock-an unrealistic premise for physical or biological systems-we introduce a vision-based, locally interacting model that captures the essential physics of shepherd-flock coordination. The model produces robust, self-organized behavior among shepherds without explicit communication, and we analyze how key control parameters, such as flock size and the number of shepherds, shape the resulting dynamics.

The framework also performs effectively in more challenging regimes, including the manipulation of non-cohesive agents and passive (non-self-propelled) agents, demonstrating its broad dynamical applicability. We further validate the model on a mixed-reality swarm-robotic platform, where physical robots successfully shepherd a virtual flock.

Overall, these results provide a minimal yet powerful physics-based description of multi-agent herding using only local visual information, offering insight into non-reciprocal collective behavior and enabling scalable real-world implementations in swarm robotics.

DY 57.10 Fri 12:15 BAR/SCHÖ

Polymer theory shows DNA motors extrude loops in the monomeric mode — Kirill Polovnikov[1,2] and •Dmitry Starkov[2] — [1]Institute for Physics and Astronomy, University of Potsdam, Potsdam-Golm, Germany — [2]Moscow, Russia

Cohesin-dependent loop extrusion is a key active mechanism of DNA organization, yet it remains unclear whether chromatin loops in living cells are generated primarily by individual cohesin motors or by higher-order structures. To fill this major gap, we build an analytical polymer-physics model that extracts a missing parameter - *the linear density of loops* - directly from Hi-C data. We focus on short genomic distances, where contact statistics simplify, resulting in a perturbative expression for the contact probability of a looped chain under a finite contact-detection radius. Our theory recapitulates a characteristic dip in the *logarithmic derivative* of the contact-probability that is *broadly observed in experiments*. By fitting this minimal model to a diverse range of mammalian Hi-C datasets, we infer approximately six loops per megabase. Independent imaging and mass spectrometry measurements of cohesin density are consistent with our inferred loop density, supporting the monomeric mode of DNA motors extrusion.

DY 57.11 Fri 12:30 BAR/SCHÖ

Universal loop statistics from active extrusion — •Anastasia Chervinskaya[1] and Kirill Polovnikov[1,2] — [1]Moscow, Russia — [2]Institute for Physics and Astronomy, University of Potsdam, Potsdam-Golm, Germany

Cohesin-dependent loop extrusion is a key active mechanism of genome organization, yet quantitative links between extrusion kinetics and measurable loop statistics remain incomplete. We develop an analytical model that predicts the mean loop scale, full loop-length distributions, state composition, and arm-arm correlations for one-sided versus two-sided extrusion. The theory maps the master equations onto diffusion on a state graph yielding state-resolved loop-length PDFs.

We show that one-sided extrusion yields a universal exponential loop-length distribution, whereas two-sided extrusion generates a sum of exponentials that approaches a gamma-like form at high barrier density. The model also predicts a strictly positive lower bound of 1/4 on arm-arm correlations.

Parameterized with independent measurements for HeLa G1 (cohesin residence and spacing; barrier densities and lifetimes), our model quantitatively accounts for the observed loop size. Also, it reproduces the experimentally measured distribution of CTCF-CTCF loop lengths under the assumption of two-sided extrusion, providing additional evidence that cohesin extrusion in living cells is predominantly bidirectional. Our results provide a compact route to infer biophysical parameters of active extrusion from experimental data.

DY 58: Focus Session: Physics of AI – Part II (joint session SOE/DY)

Time: Friday 9:30–12:45 Location: GÖR/0226

Invited Talk DY 58.1 Fri 9:30 GÖR/0226

What can we learn from neural quantum states? — Brandon Barton[10], Juan Carrasquilla[10], Anna Dawid[9], Antoine Georges[3,6,7,8], Megan Schuyler Moss[1,2], Alev Orfi[3,4], Christopher Roth[3], Dries Sels[3,4], Anirvan Sengupta[3,5], and •Agnes Valenti[3] — [1]Perimeter Institute for Theoretical Physics, Waterloo — [2]University of Waterloo, Waterloo — [3]Flatiron Institute, New York — [4]New York University, New York — [5]Rutgers University, New Jersey — [6]Collège de France, Paris — [7]École Polytechnique, Paris — [8]Université de Genève, Genève — [9]Universiteit Leiden, The Netherlands — [10]ETH Zürich, Switzerland

Neural quantum states (NQS) provide flexible parameterizations of quantum many-body wave-functions that serve as powerful tools for the ground-state search. At the same time, NQS offer something that standard machine-learning tasks and datasets fundamentally lack: a known underlying Hamiltonian and

quantum-physics tools that allow direct examination of the encoded wavefunction. This additional structure makes NQS an interesting platform for probing the behavior of classical neural networks themselves. I will first show how pruning and scaling-law phenomena change when the learning task is the quantum wavefunction itself, and link effects depend on the underlying Hamiltonian. I will then discuss generalization and double descent through the lens of quantum observables, by analyzing how NQS fail at the interpolation threshold. Finally, I will discuss how these results relate back to practical consequences for training and architecture search in the context of the ground state search for quantum many-body systems.

DY 58.2 Fri 10:00 GÖR/0226

The NN/QFT correspondence — •Ro Jefferson — Utrecht University

Exciting progress has recently been made in the study of neural networks by applying ideas and techniques from theoretical physics. In this talk, I will discuss a precise relation between quantum field theory and deep neural networks, the NN/QFT correspondence. In particular, I will go beyond the level of analogy by explicitly constructing the QFT corresponding to a class of networks encompassing both vanilla feedforward and recurrent architectures. The resulting theory closely resembles the well-studied O(N) vector model, in which the variance of the weight initializations plays the role of the 't Hooft coupling. In this framework, the Gaussian process approximation used in machine learning corresponds to a free field theory, and finite-width effects can be computed perturbatively in the ratio of depth to width, T/N. These provide corrections to the correlation length that controls the depth to which information can propagate through the network, and thereby sets the scale at which such networks are trainable by gradient descent. If time permits, I will discuss more recent work incorporating layerwise permutation symmetry. This analysis provides a non-perturbative description of networks at initialization, and opens several interesting avenues to the study of criticality in these models.

DY 58.3 Fri 10:15 GÖR/0226

Online Learning Dynamics and Neural Scaling Laws for a Perceptron Classification Problem — •Yoon Thelge, Marcel Kuhn, and Bernd Rosenow — Institute for Theoretical Physics, University of Leipzig, 04103 Leipzig, Germany

Understanding neural scaling laws and emergence of power law generalisations remains a central challenge in learning dynamics. A natural setting for analysing this behaviour is the online-learning dynamics of a perceptron trained in a teacher*student scenario, where in the thermodynamic limit, the generalisation error exhibits characteristic power-law decay. In realistic classification problems, the teacher is a discrete classifier, while standard gradient-based training requires the student to have continuous outputs. Thus, in practically relevant settings the student is necessarily mismatched to the discrete teacher, a regime that is less well understood. We study this regime for a perceptron with a sign-activation teacher and an error-function student. We derive coupled differential equations for the evolution of the relevant order parameters and verify them via numerical integration and SGD simulations. For fixed learning rates, the generalisation error converges to zero as a power-law with respect to the number of training examples with an exponent of -1/3. The onset of this asymptotic regime shifts with the learning rate, and the generalisation at the onset scales with exponent -1/2, motivating the use of learning-rate schedules to enhance the effective asymptotic decay.

DY 58.4 Fri 10:30 GÖR/0226

Power-Law Correlations in Language: Criticality vs. Hierarchical Generative Structure — •Marcel Kühn[1,2], Max Staats[1,2], and Bernd Rosenow[2] — [1]ScaDS.AI Dresden/Leipzig, Germany — [2]Institute for Theoretical Physics, University of Leipzig, 04103 Leipzig, Germany

Natural language shows power-laws beyond Zipf: the mutual information between words as a function of separation — a two-point correlation — decays approximately as a power-law, a constraint for predictive language models. In autoregressive architectures like transformers, the softmax temperature of the output controls how sharply next-word probabilities concentrate, acting as a thermodynamic knob that might tune correlations. Since phase transitions are a well-known mechanism that generate such scale-free correlations, we ask whether the observed power-law mutual information requires tuning to a critical softmax temperature. Analyzing a Markov (bigram) model, we show that, in a large-system limit, power-law mutual information emerges only at a fine-tuned critical temperature, below correlations decay exponentially. Motivated by the fact that faithful language models must go beyond bigrams and that hierarchical generative processes introducing long range interactions are more representative, we analyze an autoregressive model that perfectly emulates a specific probabilistic context-free grammar. We demonstrate that simple versions of this model preserve power-law mutual information without temperature fine-tuning, and we discuss the generality of this result for variants of the model in which deviations from the grammatical rules may occur.

DY 58.5 Fri 10:45 GÖR/0226

Dynamics of neural scaling laws in random feature regression — •Jakob Kramp[1,2], Javed Lindner[1,2], and Moritz Helias[1,2] — [1]Institute for Advanced Simulation (IAS-6), Computational and Systems Neuroscience, Jülich Research Centre, Jülich, Germany — [2]Department of Physics, RWTH Aachen University, Aachen, Germany

Training large neural networks reveals signs of universality that hold across architectures. This holds also for overparameterized networks which converge to effective descriptions in terms of Gaussian process regression. Those simplified models, already show one ingredient of universality in form of neural scaling laws. An important ingredient are power-law distributed principal component spectra of the training data.

Past work has therefore studied the dynamics of deterministic gradient flow in linear regression with and without consideration of power-law distributed spectra. Previously, dynamics of gradient flow with power law data in a type of linear random feature model were able to mimic effects of feature learning. Our work differs from the former by presenting an approach that holds for Bayesian inference on Gaussian processes obtained by stochastic Langevin training as well as for deterministic gradient flow with or without regularization by weight decay. We obtain interpretability from an effective mean-field theory that requires fewer order parameters than previous works.

15 min. break

Invited Talk DY 58.6 Fri 11:15 GÖR/0226

Creativity in generative AI — •matthieu wyart — JHU & EPFL

Is AI creative? Generative AI such as chatGPT or diffusion models can create new texts or images from a finite training set of examples. I will argue that AI can achieve this magical by learning how compose observed low-level elements into a new whole. I will discuss the type of correlations the model can exploit to do so, how many data are needed for that, and how it relates to a hierarchical construction of latent variables. The analysis is based on the introduction of synthetic languages, and comparison with experiments performed on modern AI architectures trained on real text and images.

DY 58.7 Fri 11:45 GÖR/0226

Understanding Generative Models via Interactions — •Claudia Merger[1,2,3], Alexandre Rene[2,4], Kirsten Fischer[2,3], Peter Bouss[2,3], Sandra Nestler[2,3], David Dahmen[2], Carsten Honerkamp[3], Moritz Helias[2,3], and Sebastian Goldt[1] — [1]SISSA, Trieste, Italy — [2]Jülich Research Centre, Jülich, Germany — [3]RWTH Aachen University, Aachen, Germany — [4]University of Ottawa, Ottawa, Canada

Generative models have become remarkably powerful at reproducing complex data distributions. They can infer the characteristic statistics of a system from comparatively small datasets and even generate new, realistic samples. Yet, our understanding of what these models learn remains limited: which statistics do they capture, and how accurately? To address the first question, we translate the statistics learned by generative models into a central concept of statistical physics: interactions between degrees of freedom that describe how pairs, triplets, and higher-order groups coact to produce the observed statistics of a system. Using invertible neural networks, we extract these interactions directly from trained models, providing a microscopic description of their learned data structure. To assess how accurately these interactions are learned, we use an analytic theory of diffusion models that predicts the precision with which pairwise interactions can be inferred from finite datasets, quantifying how generalization depends on sample size, data hierarchy, and regularization. Together, these results provide a framework grounded in statistical physics to interpret and predict the behavior of modern generative models.

DY 58.8 Fri 12:00 GÖR/0226

From Kernels to Features: A Multi-Scale Adaptive Theory of Feature Learning — •Javed Lindner[1,2], Noa Rubin[5], Kirsten Fischer[1,6], David Dahmen[1], Inbar Seroussi[4], Zohar Ringel[5], Michael Krämer[3], and Moritz Helias[1,2] — [1]Institute for Advanced Simulation (IAS-6), Computational and Systems Neuroscience, Jülich Research Centre, Jülich, Germany — [2]Department of Physics, RWTH Aachen University, Aachen, Germany — [3]Institute for Theoretical Particle Physics and Cosmology, RWTH Aachen University, Aachen, Germany — [4]Department of Applied Mathematics, School of Mathematical Sciences, Tel-Aviv University, Tel-Aviv, Israel — [5]he Racah Institute of Physics, The Hebrew University of Jerusalem, Jerusalem, Israel — [6]RWTH Aachen University, Aachen, Germany

Feature learning in neural networks is crucial for their expressive power and inductive biases, moti- vating various theoretical approaches. Some ap- proaches describe network behavior after train- ing through a change in kernel scale from initial- ization, resulting in a generalization power com- parable to a Gaussian process. Conversely, in other approaches training results in the adapta- tion of the kernel to the data, involving directional changes to the kernel. The relationship and re- spective strengths of these two views have so far remained unresolved. This work presents a theo- retical framework of multi-scale adaptive

feature learning bridging these two views. Using methods from statistical mechanics, we derive analytical expressions for network output statistics which are valid across scaling regimes and in the continuum between them.

DY 58.9 Fri 12:15 GÖR/0226

Statistical physics of deep learning: Optimal learning of a multi-layer perceptron near interpolation — Jean Barbier[1], Francesco Camilli[1], Minh-Toan Nguyen[1], Mauro Pastore[1], and •Rudy Skerk[2] — [1]The Abdus Salam International Centre for Theoretical Physics, Strada Costiera 11, 34151 Trieste, Italy — [2]International School for Advanced Studies, Via Bonomea 265, 34136 Trieste, Italy

We address a long-standing question in statistical physics by analysing the supervised learning of a multi-layer perceptron, beyond narrow models and kernel methods. Crucially, (i) the width scales with input dimension, making the model more prone to feature learning than ultra-wide networks and more expressive than narrow ones; and (ii) we work in the interpolation regime where trainable parameters and data are comparable, forcing task-specific adaptation. In a matched teacher-student setting we establish the fundamental limits for learning random deep-network targets and identify the sufficient statistics that an optimally trained network acquires as data increases. A rich phenomenology appears with multiple learning transitions: with enough data optimal performance arises via model "specialisation", yet practical algorithms can be trapped in theory-predicted suboptimal solutions. Specialisation occurs inhomogeneously across layers, propagating from shallow towards deep ones, but also across neurons in each layer. The Bayesian-optimal analysis thus clarifies how depth, nonlinearity and finite (proportional) width shape feature learning, with implications beyond this idealised setting.

DY 58.10 Fri 12:30 GÖR/0226

Phase Transitions as Rank Transitions: Connecting Data Complexity and Cascades of Phase Transitions in analytically tractable Neural Network Models — •Björn Ladewig, Ibrahim Talha Ersoy, and Karoline Wiesner — Institute of Physics and Astronomy, University of Potsdam, Germany

Tuning the L2-regularization strength in neural networks can result in a cascade of (zero-temperature) phase transitions between regimes of increasing accuracy. This phenomenology was previously numerically observed and linked to a basin structure of the error landscape formed by the underlying data [1]. At the level of analytically tractable models, we (i) establish the existence of cascades of transitions for those models, (ii) give meaning to the transitions in terms of the ordered onset of "learned eigendirections" of the underlying data distribution; and (iii) link the phase transitions and corresponding accuracy regimes to saddle points of the error landscape.

[1] I. Talha Ersoy and Karoline Wiesner. Exploring l2-phase transitions on error landscapes. In ICML, Workshop on High-dimensional Learning Dynamics 2025. https://openreview.net/forum?id=AkQNtAw09u

DY 59: Quantum Chaos and Coherent Dynamics (joint session DY/TT)

Time: Friday 9:30–12:45 Location: HÜL/S186

DY 59.1 Fri 9:30 HÜL/S186

Time reversal invariance breaking in quantum chaotic scattering — •Ahmed Aldabag, Nils Gluth, and Thomas Guhr — Universität Duisburg Essen

A. Aldabag, N. Gluth and T. Guhr, Universität Duisburg-Essen

Scattering theory is a key tool for the investigation of quantum systems. Often, the systems are stochastic or in a broad sense chaotic. Using Random Matrix Theory, our group recently derived the distributions of off-diagonal scattering matrix elements and cross sections with the Supersymmetry Method. We did that for the three Dyson classes which are distinguished by the presence or absence of time-reversal invariance in the system. In some important physics situations, time-reversal invariance is weakly broken. We succeeded in analytically calculating the corresponding effects on the universal behavior of the mentioned distributions. Our results provide new tools to analyze time-reversal invariance breaking in data from scattering experiments.

DY 59.2 Fri 9:45 HÜL/S186

Normalization of resonance states in chaotic scattering systems — •Florian Lorenz, Jan Möseritz-Schmidt, and Roland Ketzmerick — TU Dresden, Institut für Theoretische Physik, Dresden, Germany

The normalization of resonance states in scattering systems poses a challenge due to their divergent asymptotic behavior. As a consequence, they cannot be normalized by the usual norm, but instead, by the overlap between left and right resonance states. For dielectric cavities, we demonstrate that this left-right overlap can be computed efficiently using a boundary integral, avoiding divergent integrands. This result provides a practical numerical tool for resonance state normalization. For example, this allows for exact time evolution of wave packets based on resonance states.

DY 59.3 Fri 10:00 HÜL/S186

How exceptional points conduct mode dynamics in optical microcavities — Tom Simon Rodemund[1], Chang-Hwan Yi[2], Jung-Wan Ryu[2], Síle Nic Chormaic[3], and •Martina Hentschel[1] — [1]Institut für Physik, TU Chemnitz, Germany — [2]PCS, IBS, Daejeon, Korea — [3]OIST, Okinawa, Japan

Optical microcavities confine light through total internal reflection, making them inherently open, non-Hermitian systems. Their resonances have a real and an imaginary part, both of which depend on external parameters such as the resonator geometry or the refractive index. When scanning the parameter space, resonances can coincide and when they do so in their real and imaginary part, they form an exceptional point. We illustrate their occurrence and consequences in mesoscopic optics in two examples. First, we consider two coupled two-dimensional microcavities over coupling distances of several resonance wavelengths. Their mode dynamics is determined by a chain of exceptional points that exhibit a periodicity of approximately the wavelength [1]. The second example is a three-dimensional truncated cone. We investigate the interaction between the two mode polarizations, TE and TM, and find that the mode character changes smoothly, with TE and TM coinciding at exceptional points [2]. We confirm this behavior in phase space by generalizing the concept of Husimi functions to three dimensions. [1] C.-H. Yi, J.-W. Ryu, T.S. Rodemund, and M. Hentschel, Phys. Rev. A 112, L031501 (2025). [2] T.S. Rodemund, S. Li, S. Nic Chormaic, and M. Hentschel, Phys. Rev. A 112, 033528 (2025).

DY 59.4 Fri 10:15 HÜL/S186

Describing the spectral behavior around higher-order exceptional points with "periodic orbits" — •Daniel Grom[1], Julius Kullig[1], Malte Röntgen[2], and Jan Wiersig[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, 39016 Magdeburg, Germany — [2]Laboratoire d'Acoustique de l'Université du Mans, 72085 Le Mans, France

Coupled optical microrings can deliver a simple and robust scheme to generate higher-order exceptional points (EPs), where multiple eigen-values and -modes coalesce. A feature of an EP of order n, is the high sensitivity of the eigenvalues to small perturbations. Two types of perturbations can be classified. The generic behavior, where the eigenvalue response is proportional to the nth root and the non-generic type with a different eigenvalue response.

We present a graph theoretical perspective on the spectral characterization of perturbed higher-order EPs. It turns out that specific "periodic orbits" within the graph picture of the non-chaotic system govern the eigenvalue behavior.

DY 59.5 Fri 10:30 HÜL/S186

Dynamic origin of quantum chaos signatures in the zeros of the Riemann zeta function by means of periodic orbit theory — •Andreas Hötzinger, Sebastian Hörhold, Juan Diego Urbina, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, Germany

In the 90's, Berry and Keating [1] provided a qualitative, semiclassical analogy to the counting function of the nontrivial Riemann zeros, i.e. the zeros of the famous zeta function (ZF) $\zeta(s)$. Similar to Gutzwiller's trace formula they obtain a result in which the primes play the role of periodic orbits and argue that the so-called Riemann dynamics, underlying the primes, should be chaotic. It is speculated that this system is the classical limit of a Hermitian quantum Hamiltonian which has eigenvalues coinciding with the nontrivial zeros of $\zeta(1/2+it_n)$.

Recently, a promising candidate for such a Hamiltonian has been proposed [2], which has the potential to advance research toward a proof of the Riemann hypothesis. Based on these results, we use a related and simpler, yet non-Hermitian Hamiltonian and consider its semiclassical regime by employing methods from periodic orbit theory.

In this talk, we present our progress in the study of the classical limit of this operator and its dynamics in a complexified phase space. Through this, we hope to unveil a deeper relation between quantum chaos signatures of number theory encoded in the ZF with classical phase space structures.

[1] M. V. Berry and J. P. Keating, SIAM Review 41.2 pp. 236-266
[2] E. Yakaboylu, arXiv:2408.15135

DY 59.6 Fri 10:45 HÜL/S186

Semiclassical geometry of entanglement — •Maximilian Kieler and Peter Schlagheck — CESAM research unit, University of Liège, B-4000 Liège, Belgium

We propose a semiclassical perspective on entanglement in the form of a geometric Schmidt decomposition of regular states, e.g., states associated with invariant tori. Utilizing WKB quantization techniques and classical geometry, we derive the Schmidt spectrum and the corresponding Schmidt states. This framework allows for the reduction of the complexity in many-body states by decomposing them into lower-dimensional components.

15 min. break

Invited Talk DY 59.7 Fri 11:15 HÜL/S186

Anyon dynamics in driven topologically ordered quantum systems — •Francesco Petiziol — Technische Universität Berlin, Institut für Physik und Astronomie, Hardenbergstr. 36, 10623 Berlin

Quantum systems with topological order exhibit long-range entanglement and host quasiparticle excitations with unconventional quantum statistics – anyons. These features make them of great interest from both fundamental and quantum-technological perspectives. Recent progress in realizing topological order in quantum simulators highlights the importance and the challenge of understanding the behaviour of such systems under non-equilibrium conditions. Focusing on Kitaev's toric code, I will discuss how external driving, either coherent or incoherent, can impact and alter anyon properties. Examples include the emergence of more complex anyon classes from simpler ones, the dynamics of entanglement under driven anyon proliferation, and opportunities for controlled anyon transport.

DY 59.8 Fri 11:45 HÜL/S186

Floquet engineering in lattice systems with a parametrically modulated parabolic potential — •Usman Ali[1], Martin Holthaus[1], and Torsten Meier[2] — [1]Institut für Physik, Carl von Ossietzky Universität, D-26111 Oldenburg, Germany — [2]Department of Physics, Paderborn University, Warburger Strasse 100, D-33098 Paderborn, Germany

We present a route to Floquet engineering in lattice systems that exploits a parabolic potential to generate tunable slowly varying on-site energies. When a selected level spacing in the spectrum of the combined parabolic lattice is brought into near resonance with an external periodic drive, nonlinear resonances emerge in the classical phase space and reorganize quantum eigenstates into families of near-resonant Floquet states. Using a Mathieu-resonance approximation together with numerical Floquet calculations, we construct these states and demonstrate how resonant trap eigenstates transmute into resonance-induced effective ground states [1]. The long-time population and transport dynamics are strongly sensitive to the initial phase of the drive, providing a phase-dependent control knob for engineered tunneling and coherence. We identify parameter regimes accessible to present-day cold-atom experiments and argue that selectively populating these Floquet ground states provides a clean testbed for driven many-body and Floquet-band phenomena, enabling novel lattice dynamics inaccessible in solid-state materials [2]. References: [1] U. Ali, M. Holthaus, and T. Meier, New J. Phys. 26, 123016 (2024) [2] U. Ali, M. Holthaus, and T. Meier, Phys. Rev. Research 5, 043152 (2023)

DY 59.9 Fri 12:00 HÜL/S186

Transport through two Floquet-engineered Impurities in a One-Dimensional System: Coherent Control of Fano Resonances, BICs and Localization — •Vincenzo Bruno[1,2], Ameneh Sheikhan[1], Roberta Citro[2,3], and Corinna Kollath[1] — [1]Physikalisches Institut, Universität Bonn, Nussallee 12, 53115 Bonn, Germany — [2]Dipartimento di Fisica "E.R. Caianiello", Università degli Studi di Salerno and INFN, Via Giovanni Paolo II, 132, I-84084 Fisciano (Sa), Italy — [3]CNR/SPIN, Fisciano (Sa), 84098, Italy

Floquet engineering has attracted considerable attention due to its ability to coherently control quantum states, finding successful applications across a wide range of fields such as quantum materials, ultracold atoms, and cavity systems. We investigate particle transport through a one-dimensional system containing two periodically driven impurities. Such a configuration is highly relevant for experimental realizations ranging from ballistic semiconductor wires and electron optics to ultracold atoms, and exhibits remarkably rich transmission properties. A central feature of this system is the emergence of Fano resonances-phenomena arising from the quantum interference between a continuum scattering path and discrete quasi-bound states. We demonstrate how drive parameters can be tuned to dynamically control these resonances. Furthermore, we reveal the existence of Bound States in the Continuum (BICs) and explore the interplay between Fano interference and cavity modes. This interplay leads to a localization mechanism where the system can be switched from a fully localized state to a regime of perfect transparency.

DY 59.10 Fri 12:15 HÜL/S186

Ruelle-Pollicott signatures of unitary quantum systems — •Scott Daniel Linz, Jiaozi Wang, Merlin Füllgraf, and Jochen Gemmer — Department of Mathematics/Computer Science/Physics, University of Osnabrück, D-49076 Osnabrück, Germany

Phenomenological observations demonstrate that unitary quantum systems thermalize and equilibrate. While many concepts have been introduced to describe the equilibrium of a quantum system, the route to this state remains an area of ongoing research. A proposed step towards a general description of this behaviour is that correlation functions of chaotic quantum systems can be described by a superposition of relatively few damped oscillations, where each is weighted and assigned a complex frequency. These frequencies will be called Ruelle-Pollicott signatures after the well-understood Ruelle-Pollicott resonances that govern the decay of correlations in classical chaotic systems featuring dissipation. Following this framework, a deterministic fitting method is applied to the correlation functions of numerical simulations of closed unitary quantum systems. This examination will focus on how the number of frequencies needed to reproduce correlation functions relates to other signatures of quantum chaos.

DY 59.11 Fri 12:30 HÜL/S186

Refinements of the Eigenstate Thermalization Hypothesis — •Elisa Vallini[1], Laura Foini[2], and Silvia Pappalardi[1] — [1]University of Cologne, Köln, Germany — [2]Université Paris-Saclay, France

Understanding how isolated quantum many-body systems reach thermal equilibrium is a central question in nonequilibrium physics. The Eigenstate Thermalization Hypothesis (ETH) provides a powerful framework by linking thermalization to the statistical properties of matrix elements of physical observables in the energy eigenbasis.

In this talk, I will present our recent work, in which we revisit and clarify in detail the ideas that have led to the formulation of full ETH, a generalization of the ETH ansatz that captures multi-point correlation functions. Specifically, using tools from free probability, we explore the implications of local rotational invariance, a property that emerges from the statistical invariance of observables under random basis transformations induced by small perturbations of the Hamiltonian.

This approach allows us to analytically characterize subleading corrections to matrix-element correlations, thereby refining the ETH ansatz. Finally, I will show numerical results from non-integrable Floquet systems that support our analytical predictions.

DY 60: Critical Phenomena and Phase Transitions

Time: Friday 9:30–12:00 Location: ZEU/0114

DY 60.1 Fri 9:30 ZEU/0114

Noise-driven transitions and dynamic restoration in a two-state model under stochastic fields — •Raul Toral[1], Sara Oliver-Bonafoux[1], and Amitabha Chakrabarti[2] — [1]IFISC, Institute for Cross-disciplinary Physics and Complex Systems, UIB-CSIC, Palma de Mallorca, Spain — [2]Physics Department, Kansas State University, Manhattan, Kansas, USA

We study a two-state system influenced by both thermal fluctuations and stochastic external fields to explore how randomness affects non-equilibrium transitions and barrier-crossing dynamics. Using the Ising model in a heat bath as a minimal double-well prototype, we introduce spatially uniform, time-dependent random fields and analyze their impact on phase behavior.

The stochastic driving transforms the usual symmetry-breaking transition of the Ising model into a noise-induced transition between soft-paramagnetic and soft-ferromagnetic phases, where magnetization exhibits broad distributions and dynamical symmetry restoration between ferromagnetic states. For small field amplitudes, the transition coincides with the critical point of the undriven system, while at lower temperatures a genuine ferromagnetic phase emerges, marked by spontaneous state selection and diverging switching times.

These results reveal how stochastic forcing modifies phase behavior in bistable systems, providing new insights into noise-driven symmetry breaking and restoration.

DY 60.2 Fri 9:45 ZEU/0114

The frustrated Ising model on the honeycomb lattice: Metastability and universality — •Denis Gessert[1,2,3], Martin Weigel[3], and Wolfhard Janke[2] — [1]Centre for Fluid and Complex Systems, Coventry University, Coventry, CV1 5FB, United Kingdom — [2]nstitut für Theoretische Physik, Universität Leipzig, IPF 231101, 04081 Leipzig, Germany — [3]nstitut für Physik, Technische Universität Chemnitz, 09107 Chemnitz, Germany

We study the Ising model with competing ferromagnetic nearest- and antiferromagnetic next-nearest-neighbor interactions of strengths $J_1 > 0$ and $J_2 < 0$, respectively, on the honeycomb lattice. For $J_2 > -J_1/4$ it has a ferromagnetic ground state, and previous work has shown that at least for $J_2 \gtrsim -0.2J_1$ the transition is in the Ising universality class. For even lower J_2 some indicators pointing towards a first-order transition were reported. By utilizing population annealing Monte Carlo simulations together with a rejection-free and adaptive update, we can equilibrate systems with J_2 as low as $-0.23J_1$. By means of a finite-size scaling analysis we show that the system undergoes a second-order phase tran-

sition within the Ising universality class at least down to $J_2 = -0.23J_1$ and, most likely, for all $J_2 > -J_1/4$. As we show here, there exist very long-lived metastable states in this system explaining the first-order like behavior seen in only partially equilibrated systems.

DY 60.3 Fri 10:00 ZEU/0114

Hardness of the "swap" spin glass ensemble — •Alexander K. Hartmann[1], Leticia Cugliandolo[2], and Marco Tarzia[2] — [1]University of Oldenburg, Germany — [2]Sorbonne University, Paris, France

The "swap" ensemble [1] consist of spin glasses with quenched interaction constants J_{ij}, where the spins $s_i = \sigma_i\tau_i$ with $\sigma_i = \pm 1$ and $\tau_i \in [1 - /\Delta/2, 1 + \Delta/2]$ exhibit varying lengths τ_i. The value $\Delta = 0$ corresponds to the standard Ising case. Inspired by "swap moves" used for simulating structural classes [2], it was observed [1] that when including swaps $\tau_i \leftrightarrow \tau_j$ within Monte Carlo simulations at finite temperature with annealing $T \to 0$, ground states are easier to find. The actual "swap" ensemble samples consist of the bonds $\mathscr{J}_{ij} = J_{ij}\tau_i\tau_j$ obtained at the end of the annealing, respectively. Here, we study for two-dimensional spin glasses, by applying exact ground-state algorithms [3], the probability p_0 that true ground states have been found in the annealing. This allows us to define the hardness of the bond samples. In particular we consider the results as a function of the total number t_{MC} of annealing steps and length variation Δ. Furthermore, by applying domain-wall energy calculations [3], we investigate for various values of Δ and slow annealing ($p_0 \to 1$) whether the $\{\mathscr{J}_{ij}\}$ samples actually behave like spin glasses or rather like ferromagnets.

[1] A. Mirando, L. Cugliandolo and M. Tarzia, Phys. Rev. E **100**, L043301 (2024).
[2] L. Berthier and D. R. Reichman, Nat. Rev. Phys. **5**, 102 (2023).
[3] A.K. Hartmann and A.P. Young, Phys. Rev. B 64, 180404 (2001).

DY 60.4 Fri 10:15 ZEU/0114

Experimental study of dynamic phase transitions in nearly isotropic ferromagnetic films — Juan Marcos Marin Ramirez, Luciano Bravo, and •Andreas Berger — CIC nanoGUNE BRTA, E-20018 Donostia-San Sebastián, Spain

Non-equilibrium phase transitions occur across a wide range of physical systems. A relevant example is the dynamic phase transition (DPT) in ferromagnets, where the time-averaged magnetization Q, the dynamic order parameter, changes sharply under an oscillating field as its amplitude H_0 or period P vary. Hereby, it has also been observed that Q is dependent on the presence of an additional bias field H_b, which turns out to be the conjugate field of Q. Studies of the DPT have yielded important insights into dynamically ordered systems, their phase-space behaviour, and transient properties [1], yet this work has focused almost exclusively on Ising-type systems, restricting our understanding to a single material class [2]. Here, we experimentally investigate the DPT in polycrystalline Co films with very weak anisotropy. Dynamic magnetic states are monitored via real-time magneto-optical Kerr effect measurements across the relevant dynamic phase space. We find that the qualitative features of the dynamic phase diagram closely follow those of uniaxial Ising-type films. However, the metamagnetic anomalies of the paramagnetic dynamic state, ubiquitous in Ising-type films, appear to be significantly weaker in our nearly isotropic films.

[1] P. Riego et al., Phys. B Condens. Matter 549, 13 (2018). [2] M. Quintana and A. Berger, Phys. Rev. Lett. 131, 116701 (2023).

DY 60.5 Fri 10:30 ZEU/0114

Quadrupoling in ferroic materials — •Finja Tietjen and Richard Matthias Geilhufe — Chalmers University of Technology, Gothenburg, Sweden

Quadrupolar ordering has been investigated and characterized experimentally in different materials in recent years, but the theoretical approaches have only focused on special cases so far. We follow a new approach where we describe the quadrupoling as a composite order, arising from the fluctuations of a parent phase. This is in contrast to the conventional approach, where different phases are regarded as competing. We derive a mesoscopic field theory that includes thermal fluctuations. That enables us to find the anisotropy-dependent transition temperature and the free energy of the quadrupolar phase. We identify the phase transition into the quadrupolar phase as first-order and show that it is linked to a tetragonal distortion of the lattice of the material. With this framework, we correctly predict experimental measurements of the distortion in Ba2MgReO6 upon entering its quadrupole phase [1].

[1] D. Hirai, H. Sagayama, S. Gao, H. Ohsumi, G. Chen, T.-h. Arima, and Z. Hiroi, 'Detection of multipolar orders in the spin-orbit-coupled 5d Mott insulator Ba2MgReO6', Physical Review Research 2, 022063 (2020)

DY 60.6 Fri 10:45 ZEU/0114

Out-of-equilibrium intertwining of Landau and time-crystalline orders via collective excitations — •Andras Szabo[1] and Rama Chitra[2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]ETH Zurich, Switzerland

The intertwining of multiple order parameters is a widespread phenomenon in equilibrium condensed matter systems, yet its exploration is often hindered by the complexity of real materials. Here, we present a controlled study of intertwined orders in a minimal and versatile driven-dissipative quantum-engineered platform. We consider a Bose-Einstein condensate at the intersection of two optical cavities, realizing two competing copies of a Z2 symmetry-breaking superradiant phase transition characterized by density wave orders. Using periodic drives that exploit dynamical symmetry reduction, we show that collective excitations can be harnessed to stabilize a variety of novel intertwined orders. Going beyond the conventional phenomenology involving Landau orders, we show the emergence of a larger class of out-of-equilibrium intertwined phases, including intertwining of purely time-crystalline orders, as well as between Landau and time crystal orders. These results should be observable in state of the art experimental setups

15 min. break

DY 60.7 Fri 11:15 ZEU/0114

Nucleation in the Vicinity of the Spinodal — •Sune Kühne and Marcus Müller — Universität Göttingen Institut für Theoretische Physik Friedrich-Hund-Platz 1 37077 Göttingen

Nucleation plays a central role in initiating phase separation across diverse soft-matter systems, from synthetic polymer blends to biomolecular condensates. Near the spinodal, Cahn-Hilliard nucleation theory (CHNT) predicts that the free-energy barrier vanishes while the size and material excess of the critical nucleus diverge. Forming a large cluster significantly delays nucleation even in the absence of a free-energy barrier in analogy to approaching the spinodal from the unstable region. Yet experiments consistently report a finite rate of phase separation even while crossing the spinodal, challenging the classical CHNT scenario. In this work, we investigate the onset of phase separation in the near-spinodal regime and reveal how thermal fluctuations qualitatively modify the nucleation pathway. Using Monte Carlo simulations, we show that fluctuations can locally and transiently push the system beyond the spinodal threshold, enabling the formation of nuclei on a finite length scale well below the system size. This mechanism produces finite nucleation times and naturally explains the experimentally observed smooth crossover from nucleation-dominated to spinodal-like dynamics. By analyzing the free-energy landscape as well as the structure and dynamics of the density fluctuations that eventually become critical, we identify the key physical principles governing phase selection in metastable mixtures.

DY 60.8 Fri 11:30 ZEU/0114

Self-Assembly as a Topological Entropic Transition: Geometry, Connectivity and the Emergence of Molecular Order — •Vicente Domínguez Arca — Biosystem and Bioprocesses Engineering, IIM-CSIC, Spain — Physical and Biophysical Chemistry, Bielefeld University, Germany

Self-assembly in soft-matter systems is traditionally explained through intermolecular forces acting at short metric ranges. Here we propose a radically different view: aggregation emerges from a topological-entropic transition in the geometry of accessible microstates. Using a connectivity-based model of amphiphilic micellization, we show that aggregation reduces the degeneracy of solvent configurations, collapsing a manifold of equivalent states into a confined thermodynamic paraboloid.

This reorganization generates effective forces without invoking pairwise attractions, as entropic gradients arise from the curvature of the configuration manifold itself. The hydrophobic effect thus appears not as a fundamental interaction, but as a solvent-mediated constraint that selects ordered states by maximizing accessible degrees of freedom. This framework explains micellization as a connectivity threshold and rationalizes enthalpy-entropy compensation as a geometric projection of the same curvature tensor. Self-assembly therefore emerges as a topological transition driven by entropy, revealing order as a consequence of state-space geometry rather than microscopic forces.

DY 60.9 Fri 11:45 ZEU/0114

On the adequate and stochastic structure of space in nature and phase transitions in the early universe — •Hans-Otto Carmesin — Universität Bremen, Fachbereich 1, Pf 330440, 28334 Bremen — Studienseminar Stade, Bahnhofstr. 5, 21682 Stade — Gymn. Athenaeum, Harsefelder Str. 40, 21680 Stade

The problem to find an adequate coordinate system (ACS) has been proclaimed by the International Astronomical Union (IAU), and that problem has been solved here. This has far reaching consequences about the structure of space and time: The universal zero of the kinematic time difference δt_{kin} is derived. It corresponds to zero kinetic energy and to the minimum of relativistic energy at a given rest mass. Based on that finding, indivisible volume portions in nature are derived, and homogeneous space is identified as a stochastic average of these indivisible volume portions. With it, gravity and the quantum postulates have been derived. As a consequence, at high density, there occur dimensional phase transitions of space. In the very early universe, there occurred such high densities, and, as a consequence, the corresponding phase transitions took place. This explains the era of 'cosmic inflation', which turns out to be an era of cosmic unfolding.

Carmesin, H.-O. (2025): On the Dynamics of Time, Space and Quanta. Berlin: Verlag Dr. Köster.

Carmesin, H.-O. (2021): Quanta of Spacetime Explain Observations, Dark Energy, Graviton and Nonlocality. Berlin: Verlag Dr. Köster.

DY 61: Brownian Motion and Anomalous Transport

Time: Friday 9:30–11:15 Location: ZEU/0118

DY 61.1 Fri 9:30 ZEU/0118

Quantifying non-Markovianity via entropy production in rotational Brownian motion — •Felix Hartmann[1], Finja Tietjen[2], Matthias Geilhufe[2], and Janet Anders[1,3] — [1]University of Potsdam, Institute of Physics and Astronomy, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany — [2]Department of Physics, Chalmers University of Technology, 412 96 Göteborg, Sweden — [3]Department of Physics and Astronomy, University of Exeter, Stocker Road, Exeter EX4 4QL, UK

Magnetization dynamics is commonly modeled by the stochastic Landau-Lifshitz-Gilbert (LLG) equation, which describes the rotational Brownian motion of a magnetization vector on a spherical surface, and successfully explains and predicts magnetization experiments. On ultrashort timescales (~ a few picoseconds) an extension of the LLG by an inertial term has been theoretically predicted and experimentally measured. More generally ultrafast magnetization experiments are modeled by an open-system LLG equation, which includes a memory kernel and colored noise. It has previously been reported that if classical entropy production rates become negative, the underlying dynamical evolution is non-Markovian. In this talk we employ this to detect and measure non-Markovianity in the evolution of the magnetization dynamics. We analytically show that the inertial LLG and open-system LLG equation may have temporarily negative entropy production rates. We highlight our findings by numerical calculations of the entropy production rates for the three different LLG equations under different initial conditions and field orientations.

DY 61.2 Fri 9:45 ZEU/0118

Resolving hidden barriers and states form time series of projected observables — •Francesco Malcangi and Aljaz Godec — Mathematical Physics and Stochastic Dynamics, Institute of Physics, University of Freiburg

Single molecule experiments, such as FRET, plasmon ruler, and optical tweezers, probe a low- (often one-) dimensional projection of a higher dimensional dynamics. Unless the hidden degrees of freedom relax faster then the observed ones or they are uncoupled, projection induces memory and hides features of the full dynamics, like the presence of hidden states or energy barriers. In this study we show that the higher-order statistics of appropriately chosen functionals of projected paths can reveal some hidden features directly from the time series. In particular, they can unravel and resolve hidden barriers or states.

DY 61.3 Fri 10:00 ZEU/0118

Intensity countoscope: Quantifying dynamics from intensity correlations in real space — •Sophie Hermann and Sophie Marbach — PHENIX, Sorbonne Université/CNRS, Paris, France

Quantifying the dynamics of particle suspensions is of widespread interest in soft matter, including crystalline aggregates and bacterial colonisation. Here, we develop a new technique to learn about these dynamics directly from microscopy images. The intensity countoscope is based on the analysis of intensity correlations in virtual observation boxes of images. Through colloidal experiments, simulations, and theory, we demonstrate how this method determines equilibrium motion properties, such as self-diffusion coefficients and particle drift. By varying the size of the observation boxes, we can probe dynamics across length scales, disentangling contributions of the particle shape and the point spread function (PSF) from those of the particle motion. The intensity countoscope complements the broad range of existing techniques on interpreting images, such as particle tracking, sitting right in between dynamical differential microscopy (DDM), and particle number fluctuations (Countoscope). One strength is its applicability to situations where particle tracking is difficult, e.g. at high densities, with fast dynamics or with poor image resolution. Additionally, the entire analysis is performed in real space, which makes the technique computationally cheap as it does not require Fourier transformations. This also enables to find more intuitively physical meaning behind the obtained signals. This simplicity opens up broad perspectives on the study of collective phenomena and of interparticle interactions.

DY 61.4 Fri 10:15 ZEU/0118

Leveraging Interactions for Efficient Swarm-Based Brownian Computing — •Alessandro Pignedoli, Atreya Majumdar, and Karin Everschor-Sitte — University of Duisburg-Essen, CENIDE Center for Nanointegration Duisburg-Essen

Brownian particles naturally explore a system's configuration space through thermal fluctuations, requiring no external energy input. This intrinsic property makes them an energy-efficient basis for addressing optimisation problems [1]. Inspired by swarm intelligence [2], we show that short-range interactions between Brownian quasiparticles induce dynamic clustering around the global minimum of a complex temperature landscape [3,4]. By varying the interaction strength and particle density, we identify a broad range of physical conditions in which collective behaviour enhances optimization accuracy. Our results highlight that the emergent collective dynamics of interacting Brownian particles provide a scalable, energy-efficient framework for unconventional computing.

[1] C. H. Bennett, Int. J. Theor. Phys. 21, 905 (1982);
[2] Bonabeau, et al, Oxford University Press (1999);
[3] German Patent Application DE 10 2023 131 171, K. Everschor-Sitte, A. Pignedoli, B. Dörschel (2023);
[4] German Patent Application DE 10 2023 131 706, K. Everschor-Sitte, A. Pignedoli, B. Dörschel (2023);

DY 61.5 Fri 10:30 ZEU/0118

Current reversals in periodically driven many-particle colloidal ratchet — •Seemant Mishra[1], David Vorac[2], Artem Ryabov[2], and Philipp Maass[1] — [1]Universität Osnabrück, Institut für Physik, Germany — [2]Charles University, Faculty of Mathematics and Physics, Czech Republic

We study a many-particle colloidal ratchet and demonstrate the occurrence of current reversals under a symmetric, time-periodic driving force. An overcrowding of particles in the potential wells of the ratchet causes the current to be mediated by propagating solitary waves [1,2]. The current reversals arise from distinct modes of these waves. By a mapping onto a quasiparticle dynamics [3] and applying a unit-displacement law [4], we develop an analytic theory for the particle currents as function of the driving parameters and explain the occurrence of the current reversals. We further examine the role of hydrodynamic interactions in the system.

[1] A. P. Antonov, A. Ryabov, P. Maass, Phys. Rev. Lett. 129, 080601 (2022).
[2] E. Cereceda-López, A. P. Antonov, A. Ryabov, P. Maass, and P. Tierno, Nat. Commun. 14, 6448 (2023).
[3] S. Mishra, A. Ryabov, P. Maass, Phys. Rev. Lett. 134, 107102 (2025).
[4] A. P. Antonov, A. Vonhusen, A. Ryabov, P. Maass, Nonlinear Dyn. 113, 31529 (2025).

DY 61.6 Fri 10:45 ZEU/0118

Advection-diffusion processes of Brownian particles in a long corrugated channel: mean first passage time approach — •Xiaohan Huang, Paolo Malgaretti, and Jens Harting — Helmholtz Institute Erlangen-Nürnberg for Renewable Energy, Cauerstr. 1, 91058 Erlangen, Germany

Transport of particles in porous media in micro- and mesoscopic scales is of interest in many applications, such as the catalytic transport and nanoparticles separations. In such scenarios, the time that a particle takes to reach a target for the first time, namely the mean first passage time (MFPT), represents a standard indicator. We model the advection-diffusion of a finite size particle in a diluted suspension through a corrugated channel of N varying cross sections elements. Under the fast transverse equilibrium and the slow longitudinal transport, we encode the geometric effect to an effective entropic potential via the Fick-Jacobs approximation [1]. Together with the lubrication approximation, the 2D equation is reduced to 1D, allowing us to solve the moments of MFPT. The resulting data collapse onto a master curve, enabling us to identify the relevant dimensionless numbers: the MFPT without advection and the particle-sensitive effective advection v. v is the average velocity of a particle in a single element, accounting for advection, geometry and particle-wall interactions. Thus, 1^{st} and 2^{nd} moment of MFPT are expressed as $f(Pe)$, $Pe = \frac{vNL}{D}$ [2]. The model predicts the particle transport in a long channel, enabling fast parameter studies in porous media design.[1] P. Malgaretti et al. Entropy 2023. [2] X.Huang et al. in preparation.

DY 61.7 Fri 11:00 ZEU/0118

Anomalies in first-passage times and survival profiles of the critical Lorentz gas — •Giorgia Marcelli and Felix Höfling — Institute of Mathematics, Freie Universität Berlin

We investigate the non-equilibrium transport in the three-dimensional Lorentz gas, which is a paradigm of tracer motion in crowded environments and heterogeneous porous media [1]. The model exhibits critical slowing down and the emergence of anomalous diffusion as the porosity approaches the percolation threshold, where the void space loses connectivity [2,3]. Based on large-scale molecular dynamics simulations for transport across a finite sample, we discuss the statistics of first-passage times (FPT) covering a wide dynamic window [4]. Upon decreasing the porosity, the tail of the FPT density $p(\tau)$ broadens beyond the diffusive law, $p(\tau) \sim \tau^{-3/2}$, and attains a critical power law.

The picture is complemented by a discussion of the spatially resolved survival probability $\rho(x, t)$, which, at low obstacle densities, varies almost linearly in the distance x to the finish line, as expected for normal diffusion, but develops a broad interior plateau near the threshold.

The hazard rate, quantifying the likelihood of an arrival to occur at the next moment, becomes strongly time dependent, signalling a non-Poissonian statis-

tics. We test the consistency of our results against the well-known subdiffusive scaling of the equilibrium transport.
[1] F. Höfling and T. Franosch, Rep. Prog. Phys. **76**, 046602 (2013).
[2] F. Höfling, T. Franosch, and E. Frey, PRL **96**, 165901 (2006).
[3] M. Spanner et al., PRL **116**, 060601 (2016).
[4] G. Marcelli and F. Höfling, in preparation.

DY 62: Active Matter VI (joint session DY/BP)

Time: Friday 9:30–12:15 Location: ZEU/0160

Invited Talk DY 62.1 Fri 9:30 ZEU/0160

Morphogenesis, transport, and computation in micro-scale swarms — •Akira Kakugo — Division of Physics and Astronomy, Graduate School of Science, Kyoto University, Kyoto, Japan

Collective behavior at the microscale offers a powerful route to creating adaptive and functional materials. In this talk, I present a series of studies in which microtubule/kinesin active matter is treated as an ensemble of active agents, and swarming is engineered through DNA-mediated interactions. By introducing programmable dipole-dipole like binding via designed DNA motifs, we establish tunable microscale swarms with controllable cohesion. First, I describe how external mechanical stimuli trigger diverse modes of morphogenesis within these swarms, leading to the emergence of ordered structures and pattern transformations. Next, I introduce a DNA-programmable transport system in which a swarm of millions of active agents cooperatively captures, carries, and releases microscale cargo, enabling light-controlled, spatiotemporally precise transport. Finally, I demonstrate how such active swarms can function as a physical reservoir, where their high-dimensional, nonlinear dynamics are directly harnessed for computation within an active-matter ensemble.

DY 62.2 Fri 10:00 ZEU/0160

Learning effective hydro-phoretic interactions in active matter — •Palash Bera, Aritra K. Mukhopadhyay, and Benno Liebchen — Technische Universität Darmstadt, Darmstadt, Germany.

In the quest to understand collective behaviors in active matter systems, the complexity of hydrodynamic and phoretic interactions remains a fundamental challenge. Despite the substantial progress in identifying effective models, existing approaches often rely on minimalistic approximations, neglecting many-body interactions and the near-field contributions to the full interaction dynamics. We propose a machine learning-based framework to systematically learn hydrophoretic interactions among active colloids from first principles. By combining high-fidelity simulations with symmetry-preserving descriptors and neural network architectures, our approach captures the effective representations of both near- and far-field interactions. This framework bridges the gap between microscopic continuum models and coarse-grained active matter simulations, enabling scalable many-particle modeling without explicitly resolving the fluid flow or concentration fields. Built on two-body interactions, the coarse-grained model captures clustering phenomena consistent with those observed experimentally in active matter systems. We envision that the principles and tools developed here will have broad applicability across a wide range of active and nonequilibrium systems, including driven colloids, active gels, and field-responsive materials, providing a robust framework for modeling emergent behaviors in living and life-like systems.

DY 62.3 Fri 10:15 ZEU/0160

Interactions between Janus particles in optical tweezers — •Arnaud Compagnie[1], Abhimanyu Nowbagh[2], Ivo Buttinoni[2], and Hartmut Löwen[1] — [1]Institute for Theoretical Physics II, Heinrich Heine University Düsseldorf, Düsseldorf, Germany — [2]Institute for Experimental Physics of Condensed Matter, Heinrich Heine University Düsseldorf, Düsseldorf, Germany

Janus particles, by using their asymmetric properties to self-propel due to phoretic effects, are the most prominent artificial active colloids at the microscale. Their ability to extract energy from their surroundings and to self-assemble are used to perform specific tasks. However, due to the vast amount of types of Janus particles and the complex systems they evolve in, the way they interact with their environment remains poorly understood. Optical tweezers can be used to trap them and control their behaviour. By studying how a trapped Janus particle affects the movements of another one in a separate trap, we aim to identify the main physical phenomena - optics, hydrodynamic fluxes, and phoretic fields - that influence the interactions between them. We establish and simulate physical models in order to derive the characteristic dynamical properties of the Janus particles thanks to the comparison with experimental data.

DY 62.4 Fri 10:30 ZEU/0160

Programmable Hydrodynamic Reconfiguration of Active Particles — •Lisa Rohde, Gordei Anchutkin, and Frank Cichos — Molecular Nanophotonics Group, Peter-Debye-Institute for Soft Matter Physics, University Leipzig, Leipzig, Germany

Self-propelled microparticles generate hydrodynamic flow fields that govern their interactions with boundaries and neighbouring particles. The long-range behavior of the flow patterns classifies them as either pushers, pullers or neutral swimmers - each exhibiting fundamentally different collective behaviours. In nature, some microorganisms can adaptively switch between swimming modes in response to their environment. However, in synthetic matter, the hydrodynamic signature is fixed during fabrication constraining our ability to study how switching between modes might enable new emergent behavior. Here, we demonstrate a novel approach for real-time switching of the hydrodynamic character of the microswimmer. By illuminating the particle with a structured light field, we create tailored temperature gradients that drive controllable slip flows on the particle*s surface. This effectively allows control over the swimmer*s flow field and enables mode switching by dynamically changing the illumination pattern on demand. The ability to alter the propulsion characteristics established a versatile platform for experimentally investigating swimming efficiency, adaptivity, and collective behavior.

DY 62.5 Fri 10:45 ZEU/0160

From Passive to Active: Active Particles in Coatings Formulation and Film Formation — •Jan Cammann[1], Karnika Singh[1], Luka Burduli[1,2], Edgar Espinosa Rodriguez[3], Franck D'Agosto[3], Muriel Lansalot[3], and Ignacio Martin-Fabiani[1] — [1]Loughborough University — [2]Constructor University Bremen — [3]Universite Claude Bernard Lyon

Coatings are widely used in protective and functional applications but are fundamentally limited by the passive nature of their formulation ingredients. This leads to a critical lack of control over the spatial distribution of ingredients and prevents the optimization of key functional properties. Addressing this challenge, we propose a paradigm shift towards active coatings formulation. We introduce active Janus particles in coatings formulations and demonstrate how they overcome sedimentation and chemical gradients to accumulate at both the top and bottom coating interfaces. To achieve this programmable microstructure, we balance the timescales of active particle fuel depletion and evaporation induced assembly. We find that Janus particles at the top coating surface have an orientational bias, with the sub-equatorial orientation being the most common. This work lays the foundation for future studies developing functional coatings with programmable microstructures and dual functionalities enabled by orientation-biased active particles.

15 min. break

DY 62.6 Fri 11:15 ZEU/0160

Critical Dynamics of Active, Isotropic Systems — •Emir Sezik and Gunnar Pruessner — Imperial College London

A central result of field theory and renormalisation group (RG) is the concept of universality classes. Systems with different microscopic properties display the same physics near a continuous phase transition as they share the same symmetries. In equilibrium critical dynamics, where systems relax to a thermal steady state, Hohenberg and Halperin have provided the authoritative catalogue, which however, does not immediately extend to critical active matter systems. As they display exciting and new phases by their breaking of detailed balance, we have every reason to attempt to identify the relevant terms and to catalogue these non-equilibrium, critical systems. Motivated by this, in this work, we study an active version of Model A by including the relevant terms that are allowed by symmetry in the coarse-grained description. We show that this universality class encompasses diverse systems including spins with vision-cone interactions and Malthusian flocks. Finally, using field-theoretic RG, we perform a 1-loop calculation, approaching the critical point from the disordered regime, and elucidate the effects of activity on the Wilson-Fisher fixed point.

DY 62.7 Fri 11:30 ZEU/0160

Conservation laws and slow dynamics determine the universality class of interfaces in active matter — •Raphael Maire[1], Andrea Plati[1], Leonardo Galliano[2,3], Frank Smallenburg[1], Ludovic Berthier[2], and Giuseppe Foffi[1] — [1]Université Paris-Saclay, Laboratoire de Physique des Solides, 91405 Orsay, France — [2]Gulliver, ESPCI Paris, PSL Research University, 75005 Paris, France — [3]Dipartimento di Fisica, Università di Trieste, Strada Costiera 11, 34151, Trieste, Italy

While equilibrium interfaces display universal large-scale statistics, interfaces in phase-separated active and driven systems are predicted to belong to distinct non-equilibrium universality classes. Yet, such behavior has proven difficult to

observe, with most systems exhibiting equilibrium-like fluctuations despite their strongly non-equilibrium microscopic dynamics.

We introduce an active hard-disk model that is far from equilibrium but lacks self-propulsion. Contrary to self-propelled models, it displays clear non-equilibrium interfacial scaling and allows the first observation of the $|\boldsymbol{q}|$KPZ and wet-$|\boldsymbol{q}|$KPZ universality classes while revealing a new, previously overlooked universality class arising in systems with slow crystalline or glassy dynamics. We also show that hyperuniformity in the bulk suppresses accordingly the fluctuations of the interface. These distinct classes are selected by conservation laws and slow hydrodynamic modes.

Our model can be experimentally realized in vibrated granular systems and offers a new route to study far from equilibrium interfaces.

DY 62.8 Fri 11:45 ZEU/0160

Spontaneous emergence of solitary waves in active flow networks — Rodrigo García[1], •Gonçalo Antunes[2,3], Jens Harting[2,4], Holger Stark[3], Chantal Valeriani[1], Martin Brandenbourger[5], Juan Mazo[1], Paolo Malgaretti[2], and Miguel Ruiz-García[1] — [1]Universidad Complutense de Madrid, Madrid, Spain — [2]Helmholtz-Institut Erlangen-Nürnberg für Erneuerbare Energien (IET-2), Erlangen, Germany — [3]Technische Universität Berlin, Berlin, Germany — [4]Friedrich-Alexander-Universität Erlangen-Nürnberg, Nürnberg, Germany — [5]Aix Marseille Université, Marseille, France

Flow networks like animal/plant vasculature and power distribution grids can encode, transmit, and transform information embodied in the spatial and temporal distribution of their flows. To study these emergent dynamics, we focus on a minimal yet physically grounded system which supports information transmission. The system is composed of a one-dimensional network of active units that pump fluid via phoresis and elastic units that store volume. We coarse-grain the elastohydrodynamics to an active flow network model. We show that the pressure field can develop solitary waves, resulting in the spontaneous creation and transmission of localized packets of information stored in the physical properties of the flow. We show how the shape and speed of these waves depend on the physical parameters. When the elastic units are coupled to their neighbors, a critical size emerges, below which the solitary waves have a finite lifetime.

DY 62.9 Fri 12:00 ZEU/0160

Instabilities and turbulence in extensile swimmer suspensions — •Purnima Jain[1], Navdeep Rana[3], Roberto Benzi[4,5], and Prasad Perlekar[2] — [1]Leibniz-Institut für Polymerforschung Dresden, Germany — [2]Tata Institute of Fundamental Research, Hyderabad, India — [3]Max Planck Institute for Dynamics and Self-Organization (MPIDS), Göttingen, Germany — [4]Hangzhou International Innovation Institute, Beihang University, Hangzhou, China — [5]Department of Physics and INFN, Tor Vergata University of Rome, Via della Ricerca Scientifica 1, Rome, Italy

Swimmers moving in the same direction form an ordered state of living matter. However, this ordered state is not always stable to ambient disturbances. This may lead to chaotic flows characterized by the presence of topological defects, a phenomenon known as active turbulence. The ordered state of microswimmers can be destroyed by an instability created by their swimming stresses. For slightly larger swimmers, where viscous and inertial forces are comparable, an instability due to the fluctuations in the concentration of swimmers destroys the order [1].

In this talk, I will discuss about the instabilities and turbulence in weakly inertial suspensions of extensile swimmers, where the defect turbulent state transitions to the concentration-wave turbulent state. These findings reveal new ways in which living matter may get organized in nature.

[1] P. Jain et. al., Phys. Rev. Lett. 133, 158302 (2024). [2] P. Jain et. al., Phys. Rev. Fluids 10, 114602 (2025).

DY 63: Nonlinear Stochastic Systems

Time: Friday 11:30–12:45 Location: ZEU/0118

DY 63.1 Fri 11:30 ZEU/0118

Stochastic Dynamics of Noisy Oscillators under Eigenfunction Transformation — •Georg Podhaisky[1,2], Alberto Pérez-Cervera[3], and Benjamin Lindner[1,2] — [1]Bernstein Center for Computational Neuroscience, Berlin, Germany — [2]Humboldt University, Berlin, Germany — [3]Universitat d'Alacant, Alicante, Spain

Stochastic oscillations are observed for a wide range of systems in biology and physics. Although their dynamics may vary drastically, a simple approach for a unified description exists. As recently demonstrated by Pérez-Cervera et al. (PNAS 120, 2023), the first non-trivial eigenfunction $Q_1^*(\mathbf{x})$ of the Kolmogorov backward operator, which is obtained from the adjoint Fokker-Planck equation, can be used as a particularly useful transformation rule: This eigenfunction maps the trajectories of a given stochastic oscillator to a complex-valued domain. In this domain the autocorrelation statistics as well as the system's linear response are characterized by simple and qualitatively universal functions, regardless of the original dynamics. Here we study the stochastic dynamics in the $Q_1^*(\mathbf{x})$ domain, specifically, a number of two-dimensional systems including the Stuart-Landau oscillator and the harmonic oscillation with damping and thermal noise.

DY 63.2 Fri 11:45 ZEU/0118

Impact of heavy-tailed synaptic strength distributions on self-sustained activity in networks of spiking neurons — •Ralf Tönjes — Humboldt Universität, Berlin, Deutschland

We analyze states of stationary activity in randomly coupled quadratic integrate-and-fire neurons using stochastic mean-field theory. Specifically, we consider the two cases of Gaussian random coupling and Cauchy random coupling, which are representative of systems with light- or with heavy-tailed synaptic strength distributions. For both, Gaussian and Cauchy coupling, bistability between a low activity and a high activity state of self-sustained firing is possible in excitable neurons. In the system with Cauchy coupling we find analytically a directed percolation threshold, i.e., above a critical value of the synaptic strength, activity percolates through the whole network starting from a few spiking units only. The existence of the directed percolation threshold is in agreement with previous numerical results in the literature for integrate-and-fire neurons with heavy-tailed synaptic strength distribution. However, we have found that the transition can be continuous or discontinuous, depending on the excitatory-inhibitory imbalance in the network. Networks with Gaussian coupling and networks with Cauchy coupling and additional additive noise lack the percolation transition in the thermodynamic limit.

DY 63.3 Fri 12:00 ZEU/0118

Stochastic thermodynamics of bifurcations in all-to-all interacting systems — •Ankita Gupta[1] and Aljaž Godec[1,2] — [1]Mathematical Physics and Stochastic Dynamics, Institute of Physics, University of Freiburg, 79104 Freiburg im Breisgau, Germany — [2]Mathematical bioPhysics Group, Max Planck Institute for Multidisciplinary Sciences, Am Fassberg 11, 37077 Göttingen, Germany

All-to-all interacting systems provide a fundamental framework for understanding cooperative behavior and synchronization. Here, we examine the stochastic thermodynamics of such systems in continuous space as they are driven across bifurcation. Our analysis centers on the total entropy production rate (tEPR), which quantifies the thermodynamic cost of maintaining or transitioning between different dynamical phases. Focusing on the microscopically reversible Desai-Zwanzig model and irreversible Bonilla-Casado-Morillo models, we investigate how the tEPR depends on microscopic parameters-including interaction strength, temperature, and external driving. Leveraging recent advances on the Onsager-Machlup functional for McKean-Vlasov stochastic differential equations, we study path measures and characterize dynamical fluctuations near criticality. Through a combination of phase-plane methods and numerical simulations, we reveal the structure and nature of the bifurcations across a range of parameter regimes.

DY 63.4 Fri 12:15 ZEU/0118

Estimation of typical time scales in a Langevin-type model for wind turbine power conversion — •Martin Wagner and Joachim Peinke — Carl von Ossietzky Universität Oldenburg, School of Mathematics and Science, Institute of Physics, ForWind - Center for Wind Energy Research, Küpkersweg 70, 26129 Oldenburg, Germany

In the recent years, a data-driven and computationally efficient Langevin approach has been successfully used to detect physically reasonable fixed points in the short-term power conversion dynamics of wind turbines [1]. In our contribution, we aim to use this model to describe the multi-body interaction and possible synergy effects of the power production of many turbines in a wind farm. Additionally to the fixed points, this requires the extraction of the typical inertial time scales of the power conversion from the stochastic model. We find that this is difficult, since the model does not fulfil the Markov property due to a projection that induces a memory kernel to the stochastic differential equation according to the Mori-Zwanzig formalism [2]. Nevertheless, we show that upper boundary estimates for the typical inertial time scales of a wind turbine can be extracted from the stochastic model. In the future, this is a first step towards the stochastic modelling of many turbines, e.g. to model a grid-supportive power production of a whole wind farm.

[1] Milan P, et al. Phys Rev Lett. 2013;110(13):138701.

[2] Zwanzig R. Nonequilibrium Statistical Mechanics. Oxford University Press; 2001. p. 149 ff.f.

DY 63.5 Fri 12:30 ZEU/0118

Universal Kardar-Parisi-Zhang scaling in non-equilibrium magnon condensates — •Alexander Wowchik and Achim Rosch — Institute for Theoretical Physics, University of Cologne, Zülpicher Str. 77, 50937 Köln, Germany

Extensive studies in the past decade have unveiled how driven-dissipative condensates in one and two dimensions can form a unique non-equilibrium phase of matter characterized by a Kardar-Parisi-Zhang (KPZ) equation for the emergent Goldstone modes. We investigate whether the condensation of magnons, as demonstrated in Yttrium Iron Garnet (YIG) films when driven with microwave radiation, is a suitable candidate to study such phenomena. Via micromagnetic simulations of a corresponding system, we show that, after strong initial pumping, the dynamical autocorrelation function of the magnon field exhibits the universal scaling exponent predicted by the KPZ equation.

DY 64: Closing Talk (joint session CPP/BP/DY)

Time: Friday 13:15–14:00 Location: HSZ/0002

Invited Talk DY 64.1 Fri 13:15 HSZ/0002

Biomolecular Condensates: Challenges for Polymer Physics — •Jens-Uwe Sommer — Leibniz-Insitut für Polymerforschung Dresden, Bereich Theorie der Polymere,Hohe Straße 6, 01069 Dresden, Germany — TU Dresden, Insitut für Theoretische Physik, Zellescher Weg 17, D-01069 Dresden, Germany

Biomolecular condensates (BMCs) constitute an emerging paradigm in the understanding of biological functions. They shift the focus from individual biochemical processes toward the collective behavior of biopolymers, in which phase-separation mechanisms and intrinsically disordered proteins lacking canonical enzymatic roles play central and often decisive functions. Consequently, universal principles of complex (bio)polymer solutions gain relevance, and several classical questions in the physics of living matter can now be revisited from this polymer-physics perspective. In this talk, I will discuss theoretical approaches and concepts that are based on universal principles, with a particular emphasis on current challenges in the field.

Functional Materials Division
Fachverband Funktionsmaterialien (FM)

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Overview of Invited Talks and Sessions

(Lecture halls BEY/0138 and BEY/0E40; Poster P4)

Invited Talks

FM 4.1	Mon	15:00–15:30	BEY/0138	**(Anti)Ferroelectric HfZrO2: from non volatile memory to energy storage applications** — •Bertrand Vilquin, Gregoire Magagnin, Jordan Bouaziz, Martine Le Berre, Sara Gonzalez, Ingrid Canero Infante, Brice Gautier, Kevin Alhada-Lahbabi, Damien Deleruyelle
FM 6.1	Tue	9:30–10:00	BEY/0138	**Robust Data Generation, Heuristics and Machine Learning for Materials Design** — •Janine George
FM 9.1	Tue	14:00–14:30	BEY/0138	**Thin film combinatorial studies of functional magnetic materials** — •Nora Dempsey
FM 12.1	Wed	9:30–10:00	BEY/0138	**Shedding Light on Polar Topological Textures** — •Salia Cherifi-Hertel
FM 17.1	Thu	9:30–10:00	BEY/0138	**Piled higher, probed deeper: X-ray insights into ferroelectric devices** — •Martina Müller
FM 18.1	Thu	10:15–10:45	BEY/0138	**Stabilizing antiferroelectricity in PbZrO3 thin films using epitaxial tensile strain** — •Vincent Garcia
FM 18.2	Thu	10:45–11:15	BEY/0138	**Strain effects in free-standing membranes of antiferroelectric Lead Zirconate** — •Umair Saeed, Huazhang Zhang, David Pesquera, Philippe Ghosez, Nini Pryds, Jose Santiso, Felip Sandiumenge, Gustau Catalan
FM 22.1	Fri	9:30–10:00	BEY/0138	**Topological thermoelectrics for solid state cooling** — •Yu Pan, Claudia Felser
FM 23.1	Fri	9:30–10:00	BEY/0E40	**Mapping topological textures in compensated magnets with X-rays** — •Claire Donnelly

Invited Talks of the joint Symposium SKM Dissertation Prize 2026 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	HSZ/0002	**Stochastic-Calculus Approach to Non-equilibrium Statistical Physics** — •Cai Dieball
SYSD 1.2	Mon	10:00–10:30	HSZ/0002	**Nonuniform magnetic spin textures for sensing, storage and computing applications** — •Sabri Koraltan
SYSD 1.3	Mon	10:30–11:00	HSZ/0002	**Anomalous Quantum Oscillations beyond Onsager's Fermi Surface Paradigm** — •Valentin Leeb
SYSD 1.4	Mon	11:00–11:30	HSZ/0002	**Coherent Control Schemes for Semiconductor Quantum Systems** — •Eva Schöll
SYSD 1.5	Mon	11:30–12:00	HSZ/0002	**On stochastic thermodynamics under incomplete information: Thermodynamic inference from Markovian events** — •Jann van der Meer

Invited Talks of the joint Symposium Beyond Transistors: Material-Based Edge Computing Paradigms (SYBT)

See SYBT for the full program of the symposium.

SYBT 1.1	Wed	9:30–10:00	HSZ/AUDI	**Finding Neuromorphic Advantage with Magnetism** — •Johan Mentink
SYBT 1.2	Wed	10:00–10:30	HSZ/AUDI	**Accelerating Neural Networks Computation with Ferroelectric Oxides** — •Laura Bégon-Lours, Nikhil Garg, Alexandre Baigol, Anwesha Panda, Nathan Savoia, Alexander Flasby
SYBT 1.3	Wed	10:30–11:00	HSZ/AUDI	**a photonic approach to probabilistic computing** — •Wolfram Pernice
SYBT 1.4	Wed	11:15–11:45	HSZ/AUDI	**Tackling Reliability and Scalability in Neuromorphic Computing via Noise-aware Learning** — •Eleni Vasilaki
SYBT 1.5	Wed	11:45–12:15	HSZ/AUDI	**Bayesian nanodevices for trustworthy artificial intelligence** — •Damien Querlioz

Sessions

FM 1.1–1.5	Sun	16:00–18:15	HSZ/0002	**Hands-on Tutorial: HyperSpy – Multidimensional data analysis using Python (joint session FM/TUT)**
FM 2.1–2.7	Mon	9:30–11:30	BEY/0138	**Energy Materials**
FM 3.1–3.6	Mon	9:30–12:00	POT/0151	**Focus Session: Novel mechanisms of ferroic switching (joint session MA/FM)**
FM 4.1–4.9	Mon	15:00–17:45	BEY/0138	**Focus Session: (Anti)ferroic states – Non-conventional states I**
FM 5.1–5.11	Mon	15:00–18:00	BEY/0E40	**Focus Session: Holistic structural and safety assessment of battery materials and cells**
FM 6.1–6.11	Tue	9:30–12:45	BEY/0138	**Focus Session: Materials Discovery I – Material informatics**
FM 7.1–7.8	Tue	9:30–11:45	BEY/0E40	**Crystal Defects and Real Structure Physics in Diamond and Functional Materials I**
FM 8.1–8.11	Tue	9:30–12:30	POT/0112	**Multiferroics and Magnetoelectric Coupling (joint session MA/FM)**
FM 9.1–9.5	Tue	14:00–15:30	BEY/0138	**Focus Session: Materials Discovery II – High throughput searches for functional magnetic materials (joint session FM/MA)**
FM 10.1–10.5	Tue	14:00–15:30	BEY/0E40	**Crystal Defects and Real Structure Physics in Diamond and Functional Materials II**
FM 11.1–11.38	Tue	18:00–20:30	P4	**Poster Session Functional Materials**
FM 12.1–12.11	Wed	9:30–13:00	BEY/0138	**German-French Focus Session: Materials Research in Polar Oxides – From Domain Engineering to Photonic and Electronic Devices I**
FM 13.1–13.5	Wed	10:15–11:30	SCH/A251	**Topical Session: Dislocations in Functional Materials I (joint session MM/FM)**
FM 14.1–14.4	Wed	15:00–16:00	BEY/0138	**Focus Session: Materials Research in Polar Oxides – From Domain Engineering to Photonic and Electronic Devices II**
FM 15.1–15.3	Wed	15:00–15:45	BEY/0E40	**Nanoscale Probing of Functional Properties**
FM 16.1–16.5	Wed	15:45–17:15	SCH/A251	**Topical Session: Dislocations in Functional Materials II (joint session MM/FM)**
FM 17.1–17.1	Thu	9:30–10:00	BEY/0138	**Highlighted Talk: Piled higher, probed deeper: X-ray insights into ferroelectric devices (Martina Müller)**
FM 18.1–18.8	Thu	10:15–12:45	BEY/0138	**German-French Focus Session: (Anti)ferroic states – ferroelectrics, ferroelastics and antiferroelectrics II**
FM 19.1–19.9	Thu	10:15–12:45	BEY/0E40	**Advanced Microscopy and Tomography for Functional Materials**
FM 20	Thu	13:30–17:00	Infineon	**Excursion and Network-Event at Infineon Dresden AG (joint session FM/HL)**
FM 21	Thu	18:00–18:45	BEY/0138	**Members Assembly**
FM 22.1–22.11	Fri	9:30–12:45	BEY/0138	**Focus Session: Materials Discovery III – New materials and functionalities by general principles**
FM 23.1–23.6	Fri	9:30–11:30	BEY/0E40	**Focus Session: (Anti)ferroic states – Magnetic and magnetoelectric III (joint session FM/MA)**

Members' Assembly of the Functional Materials Division

Thursday 18:00–18:45 BEY/0138

Sessions

– Invited Talks, Topical Talks, Tutorials, Contributed Talks, and Posters –

FM 1: Hands-on Tutorial: HyperSpy – Multidimensional data analysis using Python (joint session FM/TUT)

HyperSpy is a community-developed, open-source library providing a framework to facilitate interactive analyses of multidimensional datasets – in particular spectrum images – in an easy and reproducible fashion. It facilitates the application of analytical procedures operating on individual spectra/images to a multi-dimensional dataset and gives easy access to tools that exploit the multi-dimensionality of the dataset. Born out of the electron microscopy scientific community and building on the extensive scientific Python environment, HyperSpy provides tools to efficiently explore, manipulate, and visualize complex datasets of arbitrary dimensionality, including those larger than a system's memory. The HyperSpy ecosystem includes Python packages that provide dedicated routines for many electron microscopy-based measurement techniques, but also for luminescence spectroscopy and other fields. Through the library RosettaSciIO, the reading and writing of a large range of file formats is supported.

Please bring your laptop. There will be limited power outlets in the room, so come with a fully charged battery.

Materials will be made available from 01.03.2026 via a dedicated GitHub repository. Participants are encouraged to download them ahead of time, set-up Python on their computer following the instructions and run the jupyter notebooks presented during the tutorials on their laptops:

https://github.com/LumiSpy/DPG2026-Tutorial

Organized by Jonas Lähnemann (PDI Berlin), Benedikt Haas (HU Berlin), Aidan Campbell (PDI Berlin), Hannah C. Nerl (HU Berlin) and Magnus Nord (NTNU Trondheim).

Time: Sunday 16:00–18:15 Location: HSZ/0002

FM 1.1 Sun 16:00 HSZ/0002

Introduction to HyperSpy — •Jonas Lähnemann[1], Aidan F. Campbell[1], Hannah C. Nerl[2], Magnus Nord[3], and Benedikt Haas[2] — [1]Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany — [2]Department of Physics, Humboldt Universität, Berlin, Germany — [3]Department of Physics, Norwegian University of Science and Technology, Trondheim, Norway

The session begins with a brief introduction to HyperSpy that with its 2.0 release has grown to an ecosystem of Python packages that provide dedicated routines for electron microscopy-based measurement techniques such as EELS, EDX, 4DSTEM, holography, tomography and CL, but also for luminescence spectroscopy. In general, it can be useful for any measurement, where a signal is mapped over multiple dimensions (position, time, angle, ...).

Tutorial FM 1.2 Sun 16:15 HSZ/0002

Hands-On Session 1: General usage HyperSpy/RosettaSciIO — •Jonas Lähnemann — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

In the initial tutorial, we will show how to easily read in data from a variety of formats and introduce the basic data structure of HyperSpy. General data operations, artefact removal and plotting functionalities as a basis of reproducible data analysis workflows will be covered as well.

Tutorial FM 1.3 Sun 16:45 HSZ/0002

lumiSpy for luminescence spectroscopy — •Aidan Campbell — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

This session will focus on tools ideal for analysing data recorded with cathodoluminescence, photoluminescence or related spectroscopy techniques. We will demonstrate convenience functions for rapid spectroscopy data analysis, model fitting, and visualisation. Luminescence spectroscopy may also lead to more complicated data sets with spectral, spatial and time dimensions for which we showcase interactive tools for navigating and understanding this data.

Tutorial FM 1.4 Sun 17:15 HSZ/0002

Hyperspy for Electron Energy-loss Spectroscopy — •Hannah Nerl — Humboldt Universität zu Berlin, Berlin, Germany

This hands-on session demonstrates a complete electron energy-loss spectroscopy (EELS) analysis workflow using HyperSpy and its exSpy extension. Participants will work through practical examples covering essential preprocessing steps including spectral alignment and drift correction, followed by quantitative analysis techniques such as model-based peak fitting and automated peak tracking across multidimensional datasets. The tutorial emphasizes reproducible analysis pipelines, showcasing how to leverage principal component analysis (PCA) for noise reduction in low-signal regimes. All examples use real EELS datasets and focus on practical workflows applicable to both core-loss and low-loss spectroscopy of 2D materials and nanostructures. Participants will gain hands-on experience with Jupyter notebooks that can be directly adapted to their own research data.

Tutorial FM 1.5 Sun 17:45 HSZ/0002

Using pyXem for magnetic and structural analysis of 4D-STEM data — •Magnus Nord — Norwegian University of Science and Technology, Trondheim, Norway

pyXem is an extension of HyperSpy with a focus on data processing of 4D-STEM data: from crystallographic analysis using Scanning Precession Electron Microscopy (SPED), to magnetic imaging with Scanning Transmission Electron Microscopy - Differential Phase Contrast (STEM-DPC). In this tutorial, we will show how one can study the crystal structure and domain structure in a nanostructured magnetic material.

FM 2: Energy Materials

Chair: Anna Grünebohm (Ruhr Universität Bochum, DE)

Time: Monday 9:30–11:30 Location: BEY/0138

FM 2.1 Mon 9:30 BEY/0138

Fundementals of elctrochemical hydrogen charging of MAX phases and their storage potential — •Rebeca Miyar, Adam C. Miles, Manoj Prabhakar, Lilian Vogl, Gerhard Dehm, Yug Joshi, Barak Ratzker, and Maria Jazmin Duarte — Max Planck institute for Sustainable Materials, Düsseldorf, Germany

Hydrogen storage remains a central challenge in the transition to renewable energy systems, as current technologies face limitations in scalability, safety, and efficiency. MAX phases, a class of nanolaminated carbides and nitrides composed of an early transition metal, an A-group element, and carbon or nitrogen, are perspective candidates for solid-state hydrogen storage due to their layered structure, which provides potential interstitial trapping sites. Although many theoretical studies discuss their hydrogen trapping behaviour, experimental evidence remains limited and previous work has focused only on gas-phase hydrogenation. Here, we present the first systematic study of electrochemical hydrogen charging and desorption in Ti2AlC and Ti3AlC2, which differ in their metal/ceramic

layer ratio. Hydrogen trapping and release were analysed using thermal desorption spectroscopy, Kelvin probe measurements, and electrochemical methods. Two dominant trap types were identified in both materials, with their relative contributions reflecting the layer ratio. These results provide new insight into hydrogen permeation and trapping in MAX phases.

FM 2.2 Mon 9:45 BEY/0138

Multilayer Na intercalation in bilayer graphene — •Mahdi Ghorbani-Asl and Arkady V. Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany.

The intercalation of atomic and molecular species into layered materials has emerged as a powerful route for creating novel encapsulated two-dimensional systems with tunable physical properties. Among these, alkali-metal intercalation in graphitic carbon has been widely explored for energy-storage applications. However, sodium (Na) intercalation into bulk graphite is predicted to be energetically unfavorable, making it particularly challenging to realize experimentally. In this work, we combine first-principles calculations with scanning transmission electron microscopy (STEM) to investigate Na intercalation into bilayer graphene. Using DFT simulations, we analyze the energetics and atomic structures of Na intercalants in single-layer and multilayer configurations, and evaluate how charge transfer between graphene and the Na atoms affects their stability. Our simulations reveal that the lowest-energy structure is an fcc trilayer with an A-B-C stacking sequence, whose projected atomic arrangement is fully consistent with the STEM observations. These findings provide new insight into Na intercalation mechanisms and may support the development of future sodium-ion battery technologies.

FM 2.3 Mon 10:00 BEY/0138

The Role of Lone Pairs in Fast Oxide Ion Conduction in $Bi_{0.8}Pr_{0.2}O_{1.5}$ — •Marcin Kryński — Warsaw University of Technology

Elucidating the microscopic processes that enable rapid oxide-ion transport is key to advancing solid electrolyte design. In this study, we integrate total neutron scattering with reverse Monte Carlo modelling and ab initio molecular dynamics to dissect the structural and electronic mechanisms underlying a pronounced conductivity increase observed across the order/disorder phase transition. Our results reveal that this transition is driven not by changes in the cation framework, but by a collective reorganization of oxide ions and local coordination environments. Specifically, oxide ions shift from the edges of fluorite-like blocks into the van der Waals gap, where they gain access to extended, predominantly two-dimensional diffusion pathways. Concurrently, BiO_4 units undergo a subtle yet systematic reorientation linked to the stereochemical activity of Bi^{3+} lone pairs. Although the local coordination of Bi remains largely preserved, the orientation of these lone pairs evolves in tandem with the redistribution of oxide ions, suggesting a dynamic coupling reminiscent of a paddle-wheel-type mechanism. This interplay between lone-pair-driven asymmetry and anion mobility provides a unified mechanistic picture of how structural flexibility and electronic degrees of freedom cooperate to enhance high-temperature oxide-ion transport. The insights gained here establish general principles for designing fast-ion conductors in systems where active lone pairs play an essential role.

Coffee break

FM 2.4 Mon 10:30 BEY/0138

Metal Poisoning of Nafion Proton Exchange Membrane — •Souvik Mitra[1], Jialiang Liu[1], Kristina Fröhlich[1], Simone Köcher[1,2], Christoph Scheurer[2,1], and Rüdiger-A. Eichel[1] — [1]IET-1, Forschungszentrum Jülich GmbH, 52425 Jülich, DE — [2]Fritz-Haber-Institute der MPG, 14195 Berlin, DE

Metal-ion contamination of Nafion proton-exchange membranes (PEMs) remains a persistent durability and performance issue in PEM fuel cells. Metal cations originating from insufficiently deionized feed water, coolant leaks, or corrosion of metallic cell components can exchange with protons at the sulfonate groups (SO_3^-) of Nafion, thereby reducing proton conductivity and overall cell performance.

In this work, we combine atomistic molecular dynamics simulations with in-plane conductivity measurements to build a consistent picture of how a broad series of mono-, di-, and trivalent cations affect transport in Nafion under comparable conditions. For monovalent ions (Li^+, Na^+, and K^+), our study reveals a reversal of the familiar mobility trend of these cations in the presence of Nafion membrane compared to bulk water, reflecting the competition between ion hydration and specific binding to the SO_3^- groups of Nafion. Our study also shows that, as cation charge increases from +1 to +2 to +3, their mobility drops significantly, correlating with longer residence times at sulfonate sites and increasingly multidentate SO_3^- coordination.

Our study highlights the strengths of simulations in elucidating the atomistic origin of diffusivity trends, but also their challenges in making reasonable physical approximations.

FM 2.5 Mon 10:45 BEY/0138

Synchrotron X-ray Characterization of Irradiated Ag/PVA Polymer Electrolyte — Mohamed Salah Soliman Asser and •Mohamed Salah Soliman Asser — Polymer Chemistry Department, National Center for Radiation Research and Technology, Egyptian Atomic Energy Authority, Cairo, Egypt.

Polymer electrolyte membrane thin films were developed and characterized for potential use in electroconductive applications. Polymer composites of polyvinyl alcohol (PVA), sulfuric acid, ethanol, and silver nitrate were prepared using both casting and dip-coating techniques. For the dip-coating method, glass slides were first cleaned by immersion in acetone, rinsed with isopropanol, and dried. The prepared polymer composite solutions were then dip-coated onto the glass substrates. The coated slides were irradiated at three doses: 62 J/cm2 (low), 251 J/cm2 (medium), and 502 J/cm2 (high) using the DXRL beamline. High-resolution X-ray diffraction (HR-XRD) analyses were performed at the Elettra Synchrotron Laboratory, Trieste, Italy, using the MCX beamline at a glancing angle of 1°. The X-rays had an energy of 12 keV (λ = 1.033 Å). Diffraction patterns were recorded in the 2θ range of 1*80° with a step size of 0.01° and an exposure time of 1 s per step for the Ag*PVA samples.

FM 2.6 Mon 11:00 BEY/0138

Tailoring Electrochemical Functionality of Transition-Metal Glycerolates for Next-Generation Energy Storage Devices — •Ali Hyder[1,2], Irlan S Lima[2], Zahid ullah Khan[2], Ayaz Ali Memon[1], and Lucio Angnes[2] — [1]National Centre of Excellence in Analytical Chemistry, University of Sindh, Jamshoro 76080, Pakistan — [2]Departament de Química Fundamental, Institute de Química, University of São Paulo, Av. Prof. Lineu Prestes, 748 * 05508-000, São Paulo, SP, Brazil

Abstract Metal glycerolates are emerging as promising precursors and active materials for electrochemical energy-storage systems due to their tunable coordination chemistry, oxygen-rich structures, and flexible architectures. In this study, transition-metal glycerolates (Mn, Co, Ni, Cu, Fe) were synthesized via a controlled solvothermal method to explore how formation and nanoscale morphology influence electrochemical performance. Structural analyses show that the resulting M*O*C networks form layered or clustered architectures that enhance ion diffusion and electron transport. Used as electrode materials either directly mild thermal treatment the glycerolates exhibit strong pseudo capacitance, improved redox kinetics, and good stability. Metal glycerolytes deliver the highest capacitance due to synergistic redox activity and accessible surfaces. Overall, the results demonstrate the potential of metal glycerolates as low-cost, versatile candidates for advance hybrid energy-storage devices.

FM 2.7 Mon 11:15 BEY/0138

Thermoelectric properties of In-doped Bi2Te3 crystalline bulk alloys — •Alaa Adam[1] and E. Ibrahim[2] — [1]Sohag University — [2]Sohag university

Influence of indium doping on the structure, morphology and thermoelectric properties of bulk Bi2Te3 is investigated in the current work. Bi2Te3 and Bi2-xInxTe3 crystalline bulk samples have been fabricated using a simple mono-temperature melting method. Analyses employing X-ray diffraction (XRD) and scanning electron microscopy (SEM) techniques proved the existence of the concerned phases. In addition, morphology and internal structure have been examined via the scanning electron microscopes and the energy dispersive X-ray (EDX) spectroscopy. Thermoelectric properties were determined in a temperature range between 300*700 K. The electrical conductivity (σ) against the temperature showed metallic-like behavior. Carrier concentration has increased with in-doping. The Seebeck coefficients (S) of the synthesized alloys proved the domination of n-type conduction due to consistently negative S values. The largest Seebeck coefficient was recorded at 203.5 *V/ K which was observed at 700 K for the pristine Bi2Te3 sample. The highest power factor was found at PF = 5.46 mWm-1K-2, obtained for Bi2Te3 at room temperature. Thermal conductivity was measured and studied against temperature elevation. It was found that the thermal conductivity of the In-doped Bi1.98In0.02Te3 alloys are significantly reduced compared with that of the pure Bi2Te3 material.

FM 3: Focus Session: Novel mechanisms of ferroic switching (joint session MA/FM)

This focus session highlights recent advances in ferroic switching across ferroelectric, multiferroic, ferroaxial and magnetic systems. Topics include topologically protected order-parameter dynamics, ultrafast non-thermal switching, and complex domain-wall phenomena revealed by atomistic modeling, ultrafast optics and advanced imaging. Contributions span machine-learning-based simulations of domain kinetics, optical control of ferroaxial and structural orders, multiferroic multi-cell memory concepts, and theoretically predicted unidirectional domain-wall motion with time-crystal behavior. Together, these works uncover new switching pathways and robust functional mechanisms, offering promising routes toward energy-efficient memory and quantum devices.

Organizer: Andrei Pimenov, andrei.pimenov@tuwien.ac.ac

Time: Monday 9:30–12:00 Location: POT/0151

See MA 4 for details of this session.

FM 4: Focus Session: (Anti)ferroic states – Non-conventional states I

chair: Nives Strkalj (University of Zagreb, HR)

This focus session explores recent advances in understanding and control of (anti)ferroic states. Emphasis will be placed on theoretical modelling, advanced characterization techniques, and the engineering of emergent properties for use in nano-electronic devices. The session aims to bridge fundamental research with emerging device-relevant functionalities, bringing together experimental, and theoretical perspectives on ferroic materials.

Time: Monday 15:00–17:45 Location: BEY/0138

Invited Talk FM 4.1 Mon 15:00 BEY/0138

(Anti)Ferroelectric HfZrO2: from non volatile memory to energy storage applications — •Bertrand Vilquin[1], Gregoire Magagnin[2], Jordan Bouaziz[3], Martine Le Berre[1], Sara Gonzalez[2], Ingrid Canero Infante[2], Brice Gautier[1], Kevin Alhada-Lahbabi[1], and Damien Deleruyelle[1] — [1]INSA Lyon, Ecole Centrale de Lyon, CNRS, Universite Claude Bernard Lyon 1, CPE Lyon, INL, UMR5270, 69621 Villeurbanne, France — [2]CNRS, INSA Lyon, Ecole Centrale de Lyon, Universite Claude Bernard Lyon 1, CPE Lyon, INL, UMR5270, 69621 Villeurbanne, France — [3]Ecole Centrale de Lyon, INSA Lyon, CNRS, Universite Claude Bernard Lyon 1, CPE Lyon, INL, UMR5270, 69621 Villeurbanne, France

Fluorite-structured HfZrO2 and ZrO2 thin films are promising for both non-volatile memory and energy storage applications. Antiferroelectric (AFE) capacitors were fabricated by PE-ALD and annealed using BEOL-compatible thermal budgets. All devices exhibit AFE double hysteresis loops, with polarization strongly dependent on film thickness and annealing temperature. Phase-field modeling reveals thickness-driven phase transitions enabling low-voltage, high-polarization operation. These characteristics are relevant for future AFE FET. Energy storage performances of linear dielectric (LD), ferroelectric (FE), and AFE films are compared. While FE films show high energy density but large losses, LDs offer high efficiency with low storage density. AFE ZrO2 provides an optimal balance, reaching up to 84 J/cm3 with 75% efficiency. These results position HfZrO2 as a multifunctional platform bridging memory and energy storage technologies.

FM 4.2 Mon 15:30 BEY/0138

From metal to oxide: Oxygen vacancy evolution in HfO_2 controlled by PLD — •Berk Yildirim[1], Oliver Rehm[1], Philipp Gebauer[1], Marc Neumann[1], Andrei Gloskovskii[3], Christoph Schlueter[3], Lutz Baumgarten[2], Ron Tenne[4], and Martina Müller[1] — [1]FB Physik, U Konstanz — [2]FZ Jülich — [3]DESY, Hamburg — [4]Technion, Haifa, Israel

Hafnium dioxide (HfO_2) has emerged as a ferroelectric material for non-volatile memory applications. The ferroelectric phase is linked to the presence and amount of oxygen vacancies (OVs), but their direct experimental observation is challenging. In this work, a combination of in situ soft X-ray and ex situ hard X-ray photoelectron spectroscopy is used to trace the evolution of OVs. To systematically control the oxidation and OV concentration in HfO_2, 120 nm films are grown from stoichiometric targets by pulsed laser deposition (PLD) without oxygen supply, but varying the $SrTiO_3$ (001) substrate temperature T. With increasing T, the amount of metallic Hf is systematically reduced, while the oxide fraction increases. The evolution of Hf 4f spectral features is evaluated as the indirect signature of the T-dependent OV concentration through the Hf^{3+}/Hf^{4+} spectral weight. In addition, photoluminescence measurements confirm the presence and T-dependent variation of OVs. In situ RHEED, ex situ AFM and XRD validate T-driven changes in morphology and structure, linking Hf oxidation state, vacancy concentration and film properties. These results demonstrate that T-controlled oxidation enables a systematic control of OVs and helps clarify how defects influence the formation of ferroelectric HfO_2.

FM 4.3 Mon 15:45 BEY/0138

Influence of Different Transition-Metal defect Dipoles on Polarization Rotation in $BaTiO_3$ — •Aldo Raeliarijaona[1], Ronald E. Cohen[2], and Anna Grünebohm[1] — [1]Ruhr-Universität, Bochum,Germany — [2]Carnegie Institution for Science, Washington D.C., U.S.A

Ferroelectric materials are an important class of materials for various technological applications such as non-volatile random-access memory mainly due to spontaneous electric polarization. Key ferroelectric property is the switching mechanism induced by an electric field. However, defect dipoles in ferroelectrics can act like a bias field or restoring forces to rotation of the polarization after an electric field has been applied and then removed. Using first-principles molecular dynamics, we compare polarization rotation induced by defect dipoles, in which divalent transition metal dopants on the perovskite B-site couple with neighboring oxygen vacancies, in the archetypical ferroelectric BaTiO3. We compare the effects of Cu^{2+}, Mn^{2+}, and Fe^{2+} dopants. We find that copper is much more efficient at enhancing electromechanical coupling or restoring polarization direction, over manganese or iron. We relate this effect of chemistry to the shape and bonding of the transition metal cations.

FM 4.4 Mon 16:00 BEY/0138

Reentrant relaxor behaviours in Ba(Ti0.85Zr0.15)O3-Bi(Zn2/3Nb1/3)O3 — •Vladimir Shvartsman[1], Eva Kröll[1], Boriana Mihailova[2], Vadzim Haronin[3], Juras Banys[3], and Doru Lupascu[1] — [1]University Duisburg-Essen, Essen, Germany — [2]University of Hamburg, Hamburg, Germany — [3]Vilnius University, Vilnius, Lithuania

Upon decreasing temperature, thermodynamic systems usually transform from a disordered high symmetry phase to a more ordered phase with lower symmetry. However, in some cases an unusual phase sequence is observed, where after this *normal* transition, an ordered system reenters a disordered phase. We observed the reentrant behavior in the relaxor ferroelectrics (1-x)Ba(Ti0.85Zr0.15)O3-xBi(Zn2/3Nb1/3)O3 (x = 0 - 0.15) by analysis of temperature dependences of the dielectric permittivity. Namely, a frequency-independent maximum associated with the ferroelectric phase transition is followed by a frequency-dependent anomaly at lower temperatures, which is typical of relaxors. Raman spectroscopy revealed a competition between polar and antiferrodistortive modes. Softening of the polar mode related to correlated B-cation displacements leads to the ferroelectric phase transition. On the other hand, correlated antiferrodistortive rotations of the oxygen octahedra give rise to nanometer size clusters of antipolary shifted A-site cations distributed within the polar matrix. Slowing down the dynamics of these clusters leads to the low-temperature dielectric anomaly and reentrant relaxor behavior.

FM 4.5 Mon 16:15 BEY/0138

Time-domain thermoreflectance for monitoring thermal conductivity switching in ferroelectric thin film — •Wasim Akram[1], Stefan Dilhaire[2], Thomas Maroutian[3], and Guillaume F. Nataf[1] — [1]GREMAN UMR7347, CNRS, Université de Tours, France — [2]CNRS-LOMA/UMR5798, Université de Bordeaux, France — [3]C2N, CNRS, Université Paris-Saclay, France

Ferroelectric materials that exhibit thermal conductivity switching under external stimuli could serve as promising candidates for thermal conductivity

switches [1,2]. To integrate these switches into miniaturized devices, nanoscale ferroelectric films are essential. In this work, we aim to study ferroelectric thin films and propose to manipulate their thermal conductivity by applying an electric field. To monitor the thermal conductivity, we employ time-domain thermoreflectance (TDTR). In TDTR, the sample surface is periodically heated with a far-infrared pump laser through a metallic transducer, and the resulting thermoreflectance response is probed using a delayed probe laser. The probe reflectivity change is directly related to the temperature evolution at the sample surface. The analysis relies on multilayer heat-transfer models that incorporate the substrate, film, and transducer. However, modelling is sensitive to several experimental constraints, including non-uniform interface properties and interfacial thermal resistance. Here, we address these challenges by optimizing both data-acquisition and sample-preparation methods. We use a home-made software based on Thermal Quadrupole model to fit the signal received by the photodetector [3]. Additionally, we propose to apply an electric field to ferroelectric films to modulate their domain structures, with the goal of achieving multiple fold switching of thermal conductivity. This approach could pave the way toward a device-compatible ferroelectric thermal conductivity switch. [1] Ihlefeld et al. Nano Letters 15 (3), 1791-1795 (2015). [2] Nataf et al. Nature Reviews Materials 9, 530 (2024). [3] Dilhaire et al. J. Appl. Phys. 110, 114314 (2011).

Coffee break

FM 4.6 Mon 16:45 BEY/0138

Correlated domain and crystallographic orientation mapping in uniaxial ferroelectric polycrystals by interferometric vector piezoresponse force microscopy — •Ruben Dragland[1], Jan Schultheiss[1], Ivan Ushakov[1], Roger Proksch[2], and Dennis Meier[1,3,4] — [1]NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]Asylum Research an Oxford Instruments Company, Santa Barbara, USA — [3]University of Duisburg-Essen, Duisburg, Germany — [4]Research Alliance Ruhr, Bochum, Germany

Advances in scanning probe microscopy techniques are expanding the possibilities for nanoscale characterization of functional materials, giving new opportunities for correlated studies of their local properties. Here, we apply a recent extension of piezoresponse force microscopy (PFM) for simultaneous mapping of polarization domains and local crystallographic orientation in a uniaxial ferroelectric. By shifting the laser beam position on the cantilever, direction-dependent piezoresponse signals are acquired analogous to classical vector PFM, but without the need to rotate the sample. Using polycrystals of the uniaxial ferroelectric $ErMnO_3$ as a model system, we demonstrate that the reconstructed piezoresponse vectors correlate one-to-one with the crystallographic orientations of the micrometer-sized grains, carrying grain-orientation and domain-related information. We establish a versatile platform for rapid, multimodal characterization of polycrystalline uniaxial ferroelectrics, enabling automated, high-throughput reconstruction of polarization, and grain orientations with nanoscale precision.

FM 4.7 Mon 17:00 BEY/0138

Optical control of ferroelectric polarization in epitaxial lead titanate thin films — •Valentine Gillioz, Manfred Fiebig, and Morgan Trassin — ETH Zurich, Switzerland

In this work, we use light as an active tool for remotely and dynamically controlling ferroelectricity in epitaxial $PbTiO_3$-based thin films and heterostructures. The exposure to above-bandgap ultraviolet (UV) light enables the manipulation of charge-screening dynamics via the accumulation of photo-induced charge carriers at the bottom electrode/ferroelectric Schottky interface. A transient light-induced enhancement (or suppression) of spontaneous polarization is observed using second-harmonic generation (SHG) in films with a pristine upward (or downward)-oriented polarization. Here, we explore the impact of $PbTiO_3$ growth conditions on the photoresponse of the films in more depth. Importantly, we show a robust and improved cyclability of the optical modulation of the ferroelectric polarization in films grown at low oxygen partial pressure ($\sim 10^{-2}$mbar) pointing to the role of oxygen vacancies in the light-induced polarization change. In addition, we combine our ability to monitor the polarization dynamics during the thin-film growth process using in-situ SHG with the UV light exposure to balance the depolarizing-field contribution and the light-induced polarizing effect in our heterostructures. We report a strong on/off ratio in the optical manipulation of ferroelectric polarization between a fully depolarized state in dark conditions and a polarized state under UV light exposure. Our work, hence, constitutes a critical step towards all-optical control of ferroelectricity in functional thin films.

FM 4.8 Mon 17:15 BEY/0138

Ferroelectricity in organic - inorganic TMCM-BCl3 (B=Mn, Fe, Zn) materials — •Mwanaidi Mauwa Namisi and Anna Grünebohm — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Germany

Ferroelectric materials have switchable polarization in external electric field and play a central role in sensors, memory devices and dielectrics. Although oxide ceramics have been the main focus, they have limited chemical flexibility [1]. In contrast, hybrid organic-inorganic perovskites combine multiple degrees of freedom of both inorganic and organic frameworks enhancing structural versatility [2]. Their phase transition mechanisms and origin of ferroelectricity however remain underrepresented in literature. Here, we investigate the class of TMCM-BCl3 (B=Mn, Fe, Zn) hybrids using DFT methods and discuss these open questions. Furthermore, by B site compositional tuning, we explore the structure-property relations and how the choice of transition metal affects polarization, electronic properties and magnetism.

[1] Y-M You et al., Science 357, 6348 (2017). [2] Ghosh et al., Phys. Rev. Lett. 125, 207601, (2020).

FM 4.9 Mon 17:30 BEY/0138

Tuning the Properties of the Organic Supramolecular Ferroelectric BTA by Dipole Engineering — •Sophia Klubertz[1], Florian Behrendt[2], Johannes Brendel[2], and Martijn Kemerink[1] — [1]IMSEAM, Heidelberg University, Germany — [2]Bayreuth University, Germany

Benzene-1,3,5-tricarboxamide (BTA) has become the paramount example of an organic supramolecular ferroelectric. To widen the property space of these compounds, and to gain insight into the underlying structure-property relations, this work examines the impact of a stepwise replacement of BTA's three amide groups by urea groups, as well as of the anchoring point of the dipolar group. We investigate BTA-C6/2 analogues, where one (BUDA), two (BDUA), or three (BTU) amide groups are substituted by urea groups. The compounds were newly synthesized in their C-centered and N-centered versions, regarding the amide connectivity. True ferroelectric behavior was experimentally demonstrated for C- and N-centered BUDA and BDUA through temperature- and time-dependent electrical switching measurements. By investigating remnant polarization values and double structures in the switching currents, we can draw conclusions about the switching behavior of urea groups in comparison to amide groups of either connectivity. Moreover, we find orders-of-magnitude differences in key properties like retention time, which we rationalize through molecular dynamics simulations. Overall, the results show how chemical structure translates into (ferroelectric) properties.

FM 5: Focus Session: Holistic structural and safety assessment of battery materials and cells

chairs: Carlos Ziebert (Karlsruhe Institute of Technology, DE), Philipp Finster (KIT, DE)

The focus session is dedicated to the characterization of microstructure, electrochemical, thermal and safety properties of Lithium-ion and Post-Lithium cells and their individual active and passive materials. This is required to obtain quantitative and reliable data, which are necessary to improve the current understanding in order to design and develop better and safer materials and cells. Potential topics include, but are not limited to electrochemical characterization techniques , thermal characterization techniques, safety testing, development of safer materials and cell designs, thermodynamic modelling of materials, modelling of thermal runaway and propagation.

Time: Monday 15:00–18:00 Location: BEY/0E40

FM 5.1 Mon 15:00 BEY/0E40

Hot-pressing enhances mechanical strength of PEO solid polymer electrolyte for all-solid-state sodium metal batteries — •Lanqing Zhao[1,2], Huaping Zhao[1], Feng Liang[2], and Yong Lei[1] — [1]Institut für Physik & IMN MacroNano* (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany — [2]Faculty of Metallurgical and Energy Engineering, Kunming University of Science and Technology, 650093, Kunming, China

A PEO-based composite polymer electrolyte (CPE) was successfully prepared using an emerging solvent-free hot-pressing method, with Na3Zr2Si2PO12 (NZSP) and NaClO4 incorporated to improve ionic conductivity. Benefiting

from its good mechanical strength and interfacial contact with the electrodes, the Na||Na3V2(PO4)3@C all-solid-state sodium metal battery (ASSSMB) delivers a high-capacity retention of 97.1% after 100 cycles at 0.5 C and 60 °C. Furthermore, the ASSSMB with an electrolyte thickness of approximately 20 μm also demonstrates excellent cycling stability. This study provides a promising strategy for designing stable polymer-ceramic composite electrolytes through hot-pressing to realize high-energy-density sodium metal batteries.

FM 5.2 Mon 15:15 BEY/0E40

Suppressing Li movement in solid-state electrolyte via Cryo EM Workflows: LLZO case study — •yuqi liu[1], yuwei zhang[1], Jazmin Durate[1], Yug Joshi[1], and Baptiste Gault[2] — [1]Max Planck Institute for Sustainable Materials, 40237 Düsseldorf, Germany — [2]Univ Rouen Normandie, CNRS, INSA Rouen Normandie, Groupe de Physique des Matériaux, UMR 6634, F-76000 Rouen, France

Focused Ion Beam-Scanning Electron Microscopy (FIB-SEM) is widely used to examine solid-state battery materials and prepare site-specific samples for advanced techniques such as Electron Backscatter Diffraction (EBSD), Transmission Electron Microscopy (TEM), and Atom Probe Tomography (APT). However, the electron beam can induce irreversible damage particularly in lithium-containing systems by driving lithium displacement and expulsion, thereby compromising data reliability.

In this work, we investigate how cryogenic conditions mitigate beam-induced damage in LLZO, with an emphasis on lithium expulsion under varying beam parameters. We demonstrate that lithium mobility is significantly suppressed at cryogenic temperatures, leading to a marked reduction in beam-driven lithium redistribution. Based on a comprehensive set of cryogenically prepared EBSD and APT datasets, we show that cryo-enabled workflows are essential for obtaining structurally and chemically artefact-free characterization of LLZO and, more broadly, for reliable analysis of solid-state battery materials.

FM 5.3 Mon 15:30 BEY/0E40

Synthesizing the Solid-State Electrolyte LLZO via the Mixed-Oxide Route: The Li loss - Reality or Fiction? — •Daniel Wagner, Torsten E.M. Staab, and Dominik Boras — LCTM/IFB, Julius-Maximilians Universität Würzburg, D-97070 Würzburg, Röntgenring 11

The solid-state electrolyte LLZO is discussed for applications in all solid-state batteries. Undoped and Fe-doped LLZO ($Li_7La_3Zr_2O_{12}$) samples have been synthesized via the mixed-oxide route, i.e. grinding of the educt's powders followed by calcination at 950°C for 6h and a second grinding before pressing into pellets and finally sintering them at 1200°C. The excess Li content and the restrictiveness for atmospheric gas exchange during the synthesis has been varied through usage of lidded crucibles. The samples were characterized by thermogravimetric analysis (TG), mass spectroscopy of its decomposition gas (TG/MS), X-Ray-diffraction (XRD) in reflection geometry and scanning electron microscopy (SEM).The formed phases (cubic and tetragonal) were identified by XRD. The phase fraction showed a clear influence of a varying lithium-excess and/or usage of a restricted gas exchange capability. Lattice defects were investigated by the method of positron annihilation lifetime spectroscopy (PALS). PALS showed clear differences after calcination and at different stages of sintering for both undoped and Fe-doped samples. One option may be increasingly filled Li-lattice sites after the calcination step or a formation of amorphous Li containing phases. No traces of Li were found in the decomposition gases.

FM 5.4 Mon 15:45 BEY/0E40

Microstructure of Metal Anodes used in Solid-State Batteries and Strategies for Its Control — •Till Fuchs — Center for Materials Research & Institute of Experimental Physics I, Justus-Liebig-University Giessen

The microstructure of materials fundamentally dictates their mechanical, electrochemical, and transport properties. Electron backscatter diffraction (EBSD) enables direct microscopic visualization of these microstructural features, providing quantitative insight into crystallographic orientation, grain morphology, and defect structures. This technique has become essential for understanding how processing pathways and operational conditions shape functional materials.

In a series of recent studies on lithium metal, we demonstrated how its microstructure can be visualized and conceptualized in detail, how it evolves depending on electrochemical cycling and charging conditions, and how it can be deliberately modified or controlled through the use of engineered interlayers. These findings highlight the interplay between microstructure and performance, and show how EBSD-guided analysis can inform strategies for guiding the growth morphology of alkali metal anodes during operation.

The principles established in lithium metal research are then extended to a broader class of energy materials, including nickel-rich layered oxides (NCM) and solid electrolytes. These systems exhibit their own characteristic microstructural challenges, from anisotropic degradation to cracking and dendrite formation in solid electrolytes.

FM 5.5 Mon 16:00 BEY/0E40

Decoding Complex Solid Electrolyte Architectures by an NMR Simulation Approach — •Javier Valenzuela Reina[1], Vera Barysch[2,3], Simone Köcher[2,1], Josef Granwehr[2,3], and Christoph Scheurer[1,2] — [1]Fritz-Haber-Institute der MPG, Berlin — [2]IET-1, Forschungszentrum Jülich — [3]RWTH Aachen

Advancing next-generation lithium batteries requires a detailed understanding of hybrid electrolytes and the complex organic-ceramic interfaces they contain. Nuclear magnetic resonance (NMR) spectroscopy provides a non-destructive, highly sensitive probe of interfacial structure and ion transport, which however is challenging to interpret unambiguously.

In this work, we combine different NMR experiments with theoretical modeling and high-throughput density-functional theory (DFT) simulations to investigate the structural chemistry of Al-doped lithium lanthanum zirconium oxide (LLZO), a leading hybrid electrolyte candidate. By integrating ^{27}Al, ^{7}Li, and ^{1}H NMR measurements with first-principles calculations and simulated NMR parameters, we resolve key features of the Al-doping mechanism and elucidate both bulk and surface environments within the material.

Our results illustrate how a tightly coupled experimental-computational strategy can reveal interfacial behavior that is otherwise difficult to access, and highlight its promise for guiding the design and optimization of hybrid electrolytes with complex interfaces.

Coffee break

FM 5.6 Mon 16:30 BEY/0E40

The Inclusive Investigation of Defect Thermodynamics for Cl-Ion Battery Materials using Grand Canonical Diagrams — •Johannes Döhn[1] and Axel Gross[1,2] — [1]Institute of Theoretical Chemistry, Ulm University, Germany — [2]Helmholtz Institute Ulm, Germany

In our contribution we use the example of chloride perovskites to discuss the crucial role of defect thermodynamics for electrode and solid electrolyte materials in Cl-ion batteries. In this regard, the energetic relation between the pristine compound, the formation of defects and the conversion into other materials under varying electrochemical conditions is of great importance, though still underexplored.

Here, we suggest an analysis based on grand canonical approaches which is frequently applied using the concepts of ab initio thermodynamics or the computational hydrogen electrode. Grand canonical diagrams contain in a compact form information on the relative stability of the pristine and defective materials as well as potential decomposition products at varying potentials and loadings. Thus they can help to predict whether topotactic or conversion reactions are to be expected during chlorination/dechlorination. Furthermore, relevant properties as the open circuit voltage or the electrochemical stability window can be read off directly from the diagrams.

We demonstrate that this inclusive investigation of all relevant thermodynamic properties presented here enables a comprehensive and intuitive access to the eludication of materials properties which can hardly be gained otherwise.

FM 5.7 Mon 16:45 BEY/0E40

Polaron Calculations at Scale via a DFT-Based Landau-Pekar Model — •Daria Ustimchuk, Karsten Reuter, and Christian Carbogno — Fritz-Haber-Institut der MPG, Berlin

Polarons are of ubiquitous importance in material science, be it for charge retention in energy materials or as charge reservoirs in heterogeneous catalysis. While perturbation theory allows for an accurate and efficient assessment of isolated polarons in perfect crystals [1], addressing higher concentrations in complex, disordered compounds typically requires costly hybrid density-functional theory calculations in many, extended supercells. To facilitate such investigations, we here present several strategies to accelerate the required calculations. In line with Landau-Pekar schemes, we model the mechanisms underlying polaron formation at different levels of theory, e.g., using the harmonic approximation or machine-learning potentials for describing lattice distortions and Madelung or Born effective charges for electrostatic screening effects. We discuss the pros & cons of these techniques by carefully benchmarking their accuracy and reliability for polaron formation in MgO and $BiVO_4$. Furthermore, we apply them to lithium titanium oxide (LTO), a prototypical anode material hosting elevated polaron concentrations. We demonstrate how the proposed approaches allow to semi-quantitatively predict the relevant energetics and geometric distortions, and thereby substantially accelerate the exploration of the humongous phase space associated with polaron formation in disordered energy materials.

[1] W.H. Sio *et al.*, Phys. Rev. Lett. **122**, 246403 (2019).

FM 5.8 Mon 17:00 BEY/0E40

Grain-Boundary-Driven Activity Enabled by Grain Size Engineering in Iron-Air Batteries — •Adam Cohen Miles[1], Yujun Zhao[1], Yan Ma[1,2], Dierk Raabe[1], and Yug Joshi[1] — [1]Max Planck Institute for Sustainable Materials, Max Planck Str. 1, 40237 Düsseldorf — [2]Department of Materials Science & Engineering, Delft University of Technology, Mekelweg 2, Delft 2628 CD, the Netherlands

Iron-air batteries are gaining renewed attention as cost-effective candidates for long-duration energy storage. While research to date has focused on improving anode performance through surface area enhancement or chemical additives, the role of iron microstructure in dictating electrochemical behavior remains unexplored. Here, we systematically isolate and examine the effect of grain size on the electrochemical activity of high-purity iron anodes by eliminating confounding factors such as porosity, dopants, and additives. The results reveal a strong inverse correlation between grain size and electrochemical performance, with ultrafine-grained anodes exhibiting substantially higher current densities and diffusive contributions than coarser grained counterparts. This enhancement is attributed to the increased grain boundary density, which promotes charge transfer and mitigates surface passivation. These findings represent the first direct demonstration of grain-size-controlled electrochemical activity in iron-air systems and establish microstructural engineering as a powerful design lever for performance optimization.

FM 5.9 Mon 17:15 BEY/0E40

Bismuth telluride (Bi2Te3) incorporated on 3D-printed carbon electrode for rechargeable aqueous ammonium-ion battery — •Sunny Nandi[1] and Martin Pumera[2] — [1]NTC, University of West Bohemia in Pilsen, Pilsen, Czech Republic — [2]NTC, University of West Bohemia in Pilsen, Pilsen, Czech Republic

Lithium-ion batteries are leading the battery market but there are ever growing concerns over the sustainability of Li-based batteries due to paucity and escalating cost of Li-resources. Therefore, it become increasingly important to develop a low cost and easily processable novel energy storage technologies in the future. Hence, ammonium-ion battery based on aqueous electrolyte hold great potential owing to their low cost, high safety and excellent electrochemical characteristics. In an effort to develop such NH4+ ion based rechargeable electrochemical cells. Herein, for the first time, we report here the working of a rechargeable aqueous ammonium (NH4+) ion battery by integrating a topological insulator, bismuth telluride (Bi2Te3), onto a 3D printed nanocarbon electrode as anode and copper hexacyanoferrate (CuHCF) as the cathode. Taking advantage of the 3D porous framework and the non-metallic nature of NH4+ ions, the ammonium-ion cell delivers a high energy density of 134.8 Wh kg*1 and a power density of 1800 W kg-1 in 1 M (NH4)2SO4, outperforming previously reported studies. Furthermore, ex-situ characetrization clearly explain the plausible storage mechanism of NH4+ insertion. We show immense promise of the system by recycling and reusing the used 3D printed nanocarbon electrode for next-generation energy storage systems.

FM 5.10 Mon 17:30 BEY/0E40

Investigation of Degradation Mechanisms in High-Nickel NMC Cathodes for Lithium-Ion Batteries — •Yosra Dammak — Max Planck Institute for Sustainable Materials, Düsseldorf, Germany

High-nickel layered oxides like NMC955 are attractive cathode materials for lithium-ion batteries. However, their long-term use is often hindered by structural and mechanical degradation during cycling.

This study examined the influence of electrode microstructure and cycling parameters on the performance and degradation of NMC955 cathodes, comparing two average grain sizes: NMC-1.0 (1 micrometer) and NMC-0.5 (0.5 micrometer). The finer-grained NMC-0.5 consistently outperformed NMC-1.0, showing higher specific capacity, better capacity retention, and superior rate capability. Post-mortem analysis indicated that NMC-1.0 suffered from extensive intergranular cracking, while NMC-0.5 particles mostly remained intact. Microstructural analysis (SEM and EBSD) revealed that the coarser NMC-1.0 accumulated higher, heterogeneously distributed strain, especially at the grain boundaries, which promoted fracture. Conversely, the finer NMC-0.5 accommodated strain through more distributed deformation, facilitated by faster grain boundary diffusion. Both grain sizes maintained their layered structure as confirmed by XRD.

In summary, the enhanced electrochemical and microstructural stability of the finer-grained NMC-0.5 is attributed to its ability to manage strain more effectively, contrasting with the strain-induced cracking observed in the coarser NMC-1.0.

FM 5.11 Mon 17:45 BEY/0E40

Sodium Contamination Impact on Performance of Lithium-Ion Battery Cells — •Slaheddine Jabri[1], Krum Banov[2], Anita Röstek[3], Wibke Dempwolf[4], Olaf Rienitz[3], Petr Novák[2], Markus Etzkorn[1], and Uta Schlickum[1] — [1]Institute of Applied Physics Mendelsohnstraße 2, 38106 Braunschweig, Germany — [2]Institute of Energy and Process Systems Engineering, Langer Kamp 19b, 38106 Braunschweig, Germany — [3]Physikalisch-Technische Bundesanstalt (PTB), Bundesallee 100, 38116 Braunschweig, Germany. — [4]Institut für Technische Chemie, Hagenring 30, 38106 Braunschweig, Germany

Sodium impurities can enter battery materials through several contamination sources, particularly when NaCl or NaOH are used in the recycling processes. Residual sodium is difficult to eliminate completely, and due to its high solubility, it easily dissolves into the electrolyte, where it may influence the cell performance. In this work, the electrochemical testing of high power NMC881-Graphite cells was studied using LP572 electrolyte containing sodium Na+ impurities with various concentrations. It was found that the discharge capacity decreased drastically and increase of impedance compared to Na+ free electrolyte. The Na+ ion sodium could intercalate between the Graphen layers like Li+ and due to its big ionic radius and higher charge density modify the C-C bonding and lattice parameters. The degradation effects could be found with 3 ppm Na level as impurity in electrolyte.

FM 6: Focus Session: Materials Discovery I – Material informatics

chairs: Anna E. Böhmer (Ruhr Universität Bochum, DE), Suguru Yoshida (Kyoto University, JP)

Discovering new functional materials is crucial to advance today's technologies, ranging from caloric cooling via catalysis to next-generation energy conversion and storage, such as thermoelectric, ferroelectric, and ionic conductor materials. New materials also form the basis for potential applications in quantum information technologies. This session provides a platform to highlight functional materials discoveries and how they come about. Notably, systematic searches with high-throughput synthesis approaches, as well as predictions from materials informatics, have helped to go beyond serendipitous discoveries in recent years. However, intuition guided by general principles remains an important factor. In this session, we particularly welcome contributions that showcase the discovery of new functional materials with original approaches. Diverse material systems - from well-established to emerging and niche classes across condensed-matter and materials physics - will be featured. Bringing together diverse discoveries in a single session will help delineate general principles and inspire future work.

Time: Tuesday 9:30–12:45 Location: BEY/0138

Invited Talk FM 6.1 Tue 9:30 BEY/0138

Robust Data Generation, Heuristics and Machine Learning for Materials Design — •Janine George — BAM Berlin, Germany — University of Jena

Machine learning (ML) offers new routes to overcome the limitations of density functional theory (DFT) for advanced materials. We present data-generation strategies and workflows for ML interatomic potentials, including large-scale quantum-chemical bonding analysis.[1,2,3] Incorporating bonding descriptors into ML models enables prediction of phononic properties and validation of correlations between bonding strength, force constants, and thermal conductivity.[3] We introduce autoplex, an automated framework for training ML potentials, supporting general-purpose and phonon-focused workflows.[4] These developments provide a basis for fine-tuning foundation models for thermal transport at reduced cost.[5] For properties such as magnetism or synthesizability, we discuss complementary approaches, comparing ab initio methods with chemical heuristics and experimental data-driven ML models.[6,7] Our work advances scalable, accurate simulations for materials discovery.

[1] M. K. Horton, et al. Nat. Mater. 2025, 24, 1522*1532. [2] A. M. Ganose, et al., Digit. Discov. 2025, 4, 1944*1973. [3] A. A. Naik, et al. Sci. Data 2023, 10, 610. [4] Y. Liu, et al. Nat. Commun. 2025, 16, 7666. [5] J. Bustamante, et al. 2025, DOI 10.48550/arXiv.2510.23133. [6] S. Amariamir, et al. Digit. Discov. 2025, 4, 1437*1448. [7] K. Ueltzen, et al. 2025, DOI 10.26434/chemrxiv-2025-xj84d.

FM 6.2 Tue 10:00 BEY/0138

Data-driven Discovery of 2D Non-van der Waals Materials and Design of Their Heterostructures — Anastasiia Nihei[1,2], Tom Barnowsky[1,2], and •Rico Friedrich[1,2] — [1]TU Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf

Two-dimensional (2D) materials and their heterostructures are a platform to realize advanced electronic and magnetic functionalities at the nanoscale. With traditional 2D systems extracted from weakly van der Waals (vdW) bonded bulk layered compounds, the experimental fabrication of semiconducting non-vdW 2D materials obtained from non-layered crystals [1] came as a surprise.

In our recent data-driven investigations [2], we discover several dozens of new candidates exhibiting appealing electronic, optical, and magnetic properties owing to the (magnetic) cations at their active surfaces. The electronic and magnetic properties of these next generation 2D compounds are also demonstrated to be controllable by a surface chemistry approach employing for instance hydrogen passivation [3]. Eventually, their chemically bonded interfaces in non-vdW heterostructures [4] give rise to qualitatively new properties and potential functionalities including hybrid interface bands, strong magnetic coupling, and characteristic strong moiré property variations upon twisting.

[1] A. Puthirath Balan *et al.*, Nat. Nanotechnol. **13**, 602 (2018).
[2] R. Friedrich *et al.*, Nano Lett. **22**, 989 (2022).
[3] T. Barnowsky *et al.*, Nano Lett. **24**, 3974 (2024).
[4] A. Nihei *et al.*, submitted, arXiv:2503.12209 (2025).

FM 6.3 Tue 10:15 BEY/0138

Exfoliation and Cleavage of Crystals from a Universal Potential — •Tom Barnowsky[1,2], Carsten Timm[3], and Rico Friedrich[1,2] — [1]Theoretical Chemistry, TU Dresden — [2]Institute of Ion Beam Physics and Materials Research, HZDR — [3]Institute of Theoretical Physics, TU Dresden

Two-dimensional (2D) materials display unique electronic, optical, and mechanical features that differ from their three-dimensional bulk counterparts. Most known 2D materials are derived from layered crystals but recent experiments reveal that even non-layered compounds can give rise to stable so called non-van der Waals (vdW) 2D sheets [1]. Current models, however, provide limited guidance for such materials: existing descriptors and computational approaches are largely tailored to vdW layered systems [2].

We present a computational framework that predicts crystal cleavage and exfoliable 2D sheets directly from arbitrary bulk structures [3]. At its core is a universal interatomic potential enabling rapid, large-scale screening of diverse materials. Two complementary algorithms detect weakly bonded planes and iteratively isolate connected 2D subunits. Applying this approach, we identify several thousand candidate 2D materials from non-layered bulk crystals, opening a systematic route to explore and design new low-dimensional materials with unprecedented chemical and structural diversity.

[1] R. Friedrich *et al.*, Nano Lett. **22**, 989 (2022)
[2] N. Mounet *et al.*, Nat. Nanotechnol. **13**, 246 (2018)
[3] T. Barnowsky, C. Timm, & R. Friedrich, Submitted (2025)

FM 6.4 Tue 10:30 BEY/0138

Research data management for high-throughput DFT calculations using NOMAD Oasis — •Vikrant Chaudhary[1,2], Fu Li[2], Yue Zhao[2], Joseph F. Rudzinski[1], Nathan Daelman[1], and Hongbin Zhang[2] — [1]Physics Department and CSMB, Humboldt-Universität zu Berlin, Germany — [2]Institute of Materials Science, Technical University of Darmstadt, Darmstadt, Germany

NOMAD Oasis is an open-source, locally installable version of the central NOMAD software [nomad-lab.eu] [1]. Importantly, it allows users to add custom extensions such as data schemas and workflows. In this work, we showcase two representative cases implemented in our local NOMAD Oasis: (I) high-throughput spin Hall conductivity calculations for 4486 2D materials [2], and (II) medium-throughput bulk-photovoltaic effect in 549 experimentally available two-dimensional hybrid perovskites. In both cases, data generation relies on complex computational workflows involving multiple software packages, including VASP, Wannier90, and WannierBerri. We implement a customized parser for Wannier90, and a locally developed parser for WannierBerri, with the resulting data organized based on NOMAD's built-in workflow functionalities. These examples show how NOMAD Oasis can simplify large-scale computational data management with custom parsers, automated workflows, unrestricted storage and uploads, and enhanced privacy. It also ensures compliance with the FAIR principles, making data Findable, Accessible, Interoperable, and Reusable.

[1] M. Scheidgen et al., JOSS 8, 5388 (2023).
[2] Li, F. et al., arXiv:2509.13204 (2025).

FM 6.5 Tue 10:45 BEY/0138

Finding interoperable datasets in diverse databases via provenance and similarity analysis — •Martin Kuban, Alvin Noe Ladines, Thea Denell, Lauri Himanen, Joseph F. Rudzinski, Claudia Draxl, and FAIRmat team — Physics Department and CSMB, Humboldt-Universität zu Berlin, Germany

Collecting data from different sources has the potential to significantly increase the amount of available data for data-driven discovery. However, different producers of data use distinct methods and setups, e.g., approximations and parameters used in computational data, to achieve the best data quality for the properties that are studied in a specific project. Bringing these data together requires to understand the impact of the method and setup on the accuracy and precision of the produced data. In order to do so, two key requirements must be fulfilled: First, the provenance and metadata of each data point need to be recorded. This can be achieved by leveraging the NOMAD infrastructure[1, 2], an ecosystem of parsers, schemas, and workflow tools, to extract rich metadata and provenance information. Second, using this information, similarity metrics can be used to identify data that achieve similar precision besides distinct computational setups[3]. We showcase our approach on different examples using data from NOMAD.

[1] Draxl and Scheffler, MRS Bulletin **9** (2018), 676-682.
[2] Scheidgen *et al.*, Journal of Open Source Software **8** (2023), 5388.
[3] Kuban *et al.*, MRS Bulletin **47** (2022), 991-999.

Coffee break

FM 6.6 Tue 11:15 BEY/0138

Search for thermodynamically stable ambient-pressure superconducting hydrides in GNoME database — Antonio Sanna[1,2], Tiago F. T. Cerqueira[3], Ekin Dogus Cubuk[4], Ion Errea[5,6,7], and •Yue-Wen Fang[6] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]nstitut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [3]CFisUC, Department of Physics, University of Coimbra, Rua Larga, 3004-516 Coimbra, Portugal — [4]Periodic Labs, San Francisco, CA, USA — [5]Fisika Aplikatua Saila, Gipuzkoako Ingeniaritza Eskola, University of the Basque Country (UPV/EHU), Europa Plaza 1, 20018 Donostia/San Sebastián, Spain — [6]Centro de Física de Materiales (CFM-MPC), CSIC-UPV/EHU, Manuel de Lardizabal Pasealekua 5, 20018 Donostia/San Sebastián, Spain — [7]Donostia International Physics Center (DIPC), Manuel de Lardizabal Pasealekua 4, 20018 Donostia/San Sebastián, Spain

There are very few ambient-pressure hydride superconductors in experiment, and their critical temperatures (T_c) are typically < 10 K. Herein, by combining machine learning techniques with ab initio methods, we have identified 25 cubic thermodynamically stable hydrides with T_c beyond the boiling point of liquid helium (4.2 K) from the GNoME database. These cubic hydrides all crystallize in double-perovskite-like or fluorite-like structures, and most of them demonstrate T_c lower than 10 K. Our study provide more candidates for the study of ambient-pressure superconductivity in the hydrides that can be very likely to be synthesized in experiment despite the low T_c.

FM 6.7 Tue 11:30 BEY/0138

Exploration of high-entropy alloys for key electrochemical reactions: a comparative study for the solid solution systems X-Pd-Pt-Ru (X=Cu, Ir, Ni) — •Jan Lukas Bürgel[1], Rico Zehl[1], Felix Thelen[1], Ridha Zerdoumi[1,2], Olga A. Krysiak[2], Benedikt Kohnen[1], Ellen Suhr[1], Wolfgang Schuhmann[2], and Alfred Ludwig[1] — [1]Chair for Materials Discovery and Interfaces, Institute for Materials, Faculty of Mechanical Engineering, Ruhr University Bochum, Bochum, Germany — [2]Analytical Chemistry - Center for Electrochemical Sciences (CES), Faculty of Chemistry and Biochemistry, Ruhr University Bochum, Bochum, Germany

Developing new electrocatalysts is essential for green energy technologies such as hydrogen production, fuel cells, and environmental remediation. Compositionally complex solid solutions offer vast opportunities for catalyst discovery due to their tunable surface sites, but exploring their large compositional spaces requires optimised strategies. Using a high-throughput approach, the electrocatalytic activity of the three quaternary systems X-Pd-Pt-Ru (X = Cu, Ir, Ni) was screened for four reactions in alkaline media: oxygen evolution, oxygen reduction, hydrogen evolution, and nitrate reduction reaction. Thin-film materials libraries were synthesised and characterised to identify composition-activity relationships, while also considering relevant information on crystal structure and surface morphology. The resulting multidimensional dataset reveals clear trends, similarities, and distinct activity maxima, demonstrating the effectiveness of this approach for navigating complex multinary systems.

FM 6.8 Tue 11:45 BEY/0138

Phase formation and stability of transition-metal solid solutions containing volatile elements — Martin Kostka[1], Luqman Mustafa[1], Jill Fortmann[2], Aurelija Mockute[2], Alan Savan[2], Susanne Kunzmann[3], Anna Grünebohm[3], Alfred Ludwig[2], Andreas Kreyssig[1], and •Anna E. Böhmer[1] — [1]Experimental physics IV, Ruhr University Bochum, 44801 Bochum, Germany — [2]Materials Discovery and Interfaces, Institute for Materials, Ruhr University Bochum, 44801 Bochum, Germany — [3]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr University Bochum, 44801 Bochum, Germany

In the combinatorial synthesis of thin films, multiple elements are simultaneously deposited to achieve well-defined composition gradients and create a materials library. However, including volatile elements directly into the combina-

torial synthesis is a challenge. Here, we use instead a two-step synthesis process combining combinatorial cosputtering with a separate ex-situ reaction step with the volatile elements Se and Sb. In particular, we investigate the phase formation and stability of the (Fe,Ni)Sb_2 and (Fe,Cr)Sb_2 solid solutions in the orthorhombic marcasite structure. Further, we study the (Fe,Co)Se_2 solid solution, which is on the brink of transformation from orthorhombic marcasite to cubic pyrite structure. Our preparation route with a separate low-temperature synthesis step permits detailed studies of solid solutions and phase diagrams at well-defined temperatures.

FM 6.9 Tue 12:00 BEY/0138

AI for Complex Catalytic Systems: C2 Catalysis — •Haobo Li — Nanyang Technological University, Singapore

AI-driven big data set analysis offers opportunities for theoretical research on systems that combine complex catalyst materials with intricate catalytic reactions. In this study, we explore high-entropy alloys (HEAs) as potential electrocatalysts for the electrochemical semihydrogenation of acetylene. HEAs provide a variety of surface active sites due to the diverse combination of constituent elements, while the presence of bidentate dicarbon species further complicates surface interactions. By integrating density functional theory computations, geometric optimizer development, and graph neural network-based machine learning predictions, we efficiently compile a comprehensive database of 52,900 adsorption properties for AgAuCuNiPd HEA surfaces. Lasso regression and t-SNE projection reveal the distinct influences of the five metal components on adsorption and reaction properties. Using Cu as a reference, logistic regression assesses the potential for other components to surpass Cu in terms of catalytic activity and selectivity toward ethylene. Our findings suggest that, while HEAs can enhance the reaction, the ternary AgAuCu alloy achieves optimal results, indicating that high entropy is not essential. This research methodology can be extended to other complex catalytic systems, providing valuable insights into catalytic mechanisms and facilitating experimental endeavors.

FM 6.10 Tue 12:15 BEY/0138

Compositional and Structural Impact on the Hydrogen Evolution Reaction Activity across Noble-Metal-Based Compositionally Complex Solid Solutions Thin Film Libraries — •Natalia Pukhareva[1], Moonjoo Kim[2], Felix Thelen[1], Geovane Arruda de Oliveria[2], Rico Zehl[1], Wolfgang Schuhmann[2], and Alfred Ludwig[1] — [1]Materials Discovery & Interfaces, Ruhr University Bochum — [2]Analytical Chemistry - Center for Electrochemical Sciences (CES), Ruhr University Bochum

Compositionally complex solid solutions (CCSS) stabilize multielement alloys and allow tuning of surface chemistry for the hydrogen evolution reaction (HER). Three quinary libraries (Ir-Pd-Pt-Rh-Ru, Ag-Au-Pd-Pt-Ru, Ag-Au-Cu-Pd-Pt) were prepared by sputtering and mapped across 342 positions each. Energy-dispersive X-ray spectroscopy (EDX) confirmed smooth composition gradients, and X-ray diffraction (XRD) showed fcc solid solutions with minor hcp fractions in Rh-Ru-rich regions and no detectable phase effect on HER. X-ray photoelectron spectroscopy (XPS) with Gaussian-process regression revealed composition-dependent surface segregation and distinct surface compositions. HER activity, measured by scanning electrochemical cell microscopy (SECCM), followed Ir-Pd-Pt-Rh-Ru > Ag-Au-Pd-Pt-Ru > Ag-Au-Cu-Pd-Pt. In the Ag-containing libraries Pd-rich compositions outperformed Pt-rich ones, and in Ag-Au-Cu-Pd-Pt Ag-rich regions exceeded Cu-rich regions despite Cu's higher intrinsic activity, consistent with segregation limiting surface Pt and Pd and indicating that HER in these CCSS is dominated by multielement interactions.

FM 6.11 Tue 12:30 BEY/0138

Soft Degradable Magnetic Microcarriers for Encapsulation and Guided Transport of Drugs and 3D Spheroids — •Lulu Song, Xinne Zhao, Xuan Peng, Željko Janićijević, Lin Guo, Denys Makarov, and Larysa Baraban — Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Soft microrobots hold strong promise for next-generation biomedical applications, including targeted drug delivery, tissue engineering, and minimally invasive therapies. However, their translation remains limited by challenges in scalable fabrication, controlled biodegradation, and insufficient co-encapsulation and transport of diverse cargos. Here, we present degradable hydrogel microcarriers fabricated via droplet-based microfluidics and UV photopolymerization, enabling scalable production with tunable properties. These microcarriers can co-encapsulate therapeutic molecules, superparamagnetic particles, and living cell spheroids, supporting multifunctional delivery strategies. Their motion is precisely actuated under externally applied gradient magnetic fields, allowing guided navigation in microchannels for targeted delivery. Importantly, the microcarriers exhibit programmable degradation under physiological conditions, providing temporary mechanical integrity, controlled release, and safe post-treatment clearance, with complete degradation at 37 °C within several days. Overall, this platform offers a robust and biocompatible soft microrobotic system for targeted therapies, micro-tissue transport, and diagnostic monitoring, representing a promising step toward clinical translation.

FM 7: Crystal Defects and Real Structure Physics in Diamond and Functional Materials I

chair: Theo Scherer (Karlsruhe Institute of Technoloy, DE)

Time: Tuesday 9:30–11:45 Location: BEY/0E40

FM 7.1 Tue 9:30 BEY/0E40

Fluorescence lifetime measurements of NV- and NV0 color center ensembles at room temperature and 4K in HPHT, CVD and nanodiamond samples — •Kai Kühnlenz, Kevin Lauer, Phillip Kellner, Mario Bähr, Andreas T. Winzer, and Thomas Ortlepp — CiS Forschungsinstitut für Mikrosensorik GmbH, Konrad-Zuse-Str. 14, 99099 Erfurt, Deutschland

Nitrogen vacancy (NV) centers in diamond are key solid-state quantum emitters whose photophysical properties depend on their charge state and the surrounding diamond lattice. We analyze diamond samples made of chemical vapor deposition- (CVD), high-pressure-high-temperature- (HPHT) or nanodiamond material by exciting them with a 513nm green laser and detecting the fluorescence light via time resolved photoluminescence (TRPL). This work presents measurements of the fluorescence lifetime of NV-ensembles. Hereby a monochromator is employed to detect 20nm wide spectral bands centered at the NV- phonon sideband (710nm) and the zero-phonon-lines of NV- and NV0 (638nm and 575nm) to differentiate between the charge states. Measurements are performed at both room temperature (293K) and 4K. The influence of varying excitation laser power and of the selected spectral detection window is investigated and compared with established reference values. The measurement approach allows a systematic comparison of NV-diamond materials and provides a baseline for quantitative lifetime-based characterization of NV ensembles.

FM 7.2 Tue 9:45 BEY/0E40

Diamond windows for microwave application: numerical analyses and characterization by microscope and Raman measurements — •Gaetano Aiello, Andreas Meier, Theo Scherer, Sabine Schreck, and Dirk Strauss — Karlsruhe Institute of Technology, Institute for Applied Materials, 76021 Karlsruhe, Germany

Electron cyclotron heating and current drive systems in nuclear fusion devices feature optical quality polycrystalline diamond windows for the transmission of microwave beams of 1 to 2 MW power. The windows consist of diamond disks of 1 to 2 mm thickness integrated into a metallic housing. Numerical analyses verify the performance of such windows with respect to temperature and stress limits. In this work, examples of analyses are provided with reference to a Brewster-angle window design featuring a first-of-its-kind manufactured diamond disk with 180 mm diameter. For the first time, instead of a single constant value, the entire map of the loss tangent measured over the disk has been given as input to the analysis. In addition, examples of microscope and Raman investigations of the disks are shown with reference to dark microfeatures and residual stresses generated by the chemical vapour deposition process.

FM 7.3 Tue 10:00 BEY/0E40

Investigation of irradiation effects in artificial diamond — •Theo Andreas Scherer and Francesco Mazzocchi — Karlsruhe Institute of Technology KIT-IAM-AWP 76344 Eggenstein-Leopoldshafen

Diamond is used as window material for high power microwave transmission to heat plasmas and to perform diagnostics in nuclear fusion devices like ITER, Wendelstein 7X or ASDEX-UG. In such environments neutron and gamma radiation has a quite important influence on dielectric and thermal properties of diamond. Spectroscopic investigations, like RAMAN, cathode luminescence or EPR can detect all the defects produced by irradiation. Swift heavy ion and neutron irradiation was us to study defect chemistry and physics in diamond (single crystalline and polycrystalline diamond samples). Newest results of this investigation are presented.

FM 7.4 Tue 10:15 BEY/0E40

EC Heating systems for present and future fusion experiments and power plants — •Peter Späh — KIT, Institute for Applied Materials, Karlsruhe, Germany

CVD diamond windows are an essential component in Electron Cyclotron (EC) plasma heating and stabilisation systems for nuclear fusion reactors. Beside the characterisation and qualification of CVD diamond disks and the design and

analysis of CVD diamond window assemblies, the Institute for Applied Materials (IAM) at Karlsruhe Institute of Technology (KIT) also contributes to concept findings, layout, design and integration of EC heating systems for several fusion experiments and power plant studies.

Experimental fusion devices and future fusion power plants with magnetic confinement require powerful heating systems for plasma core heating, plasma disruption mitigation, breakdown of gas, plasma ramp-up and -down, impurity control and to counteract thermal instabilities. Electron Cyclotron Resonance Heating (ECRH) is one of these heating systems. Microwave beams in the frequency range of 80 to 240 GHz are generated by gyrotrons and subsequently transmitted via waveguides and an antenna into the plasma chamber, where they interact with the electrons.

This talk gives an overview on the design status of the EC heating antennas for the EU DEMO fusion power plant and for the Volumetric Neutron Source (VNS) which is a conceptual study of a beam-driven Tokamak, serving as test-bed for full-sized breeding blanket modules.

coffee break

FM 7.5 Tue 10:45 BEY/0E40

Application of Raman and Photoluminescence Spectroscopy to MgO-C Refractories — •Julia Richter[1], Felix Drechsler[1], Till Stadtmüller[2], Cameliu Himcinschi[1], Christos Aneziris[2], and Jens Kortus[1] — [1]Technische Universität Bergakademie Freiberg - Institut für Theoretische Physik, Leipziger Straße 23, 09599 Freiberg, Germany — [2]Technische Universität Bergakademie Freiberg - Institut für Keramik, Feuerfest und Verbundwerkstoffe, Agricolastraße 17, 09599 Freiberg, Germany

By applying Raman and photoluminescence (PL) spectroscopy in the visible and near-infrared range to MgO, magnesia-carbon (MgO-C) refractory bricks - partially produced from recycled magnesia - are examined in hardened and coked state, and compared with nominally pure MgO powder as a reference. Two sharp, high-intensity PL signals (699 nm and 871 nm), each accompanied by symmetrical sidebands, are investigated by varying the excitation wavelength (532, 633, and 785 nm). The 699 nm PL feature observed for both brick and reference arises from Cr^{3+} impurities within the MgO lattices, whereas the 871 nm signal, associated with V^{2+}, appears only in the brick-derived MgO. To elucidate the origin of the symmetrical sidebands, temperature-dependent spectroscopic measurements from 100 to 295 K are performed, monitoring the intensity ratio of the higher-energy (anti-Stokes) and lower-energy (Stokes) sidebands. The results confirm phonon participation in both the MgO:Cr^{3+} and MgO:V^{2+} emission processes. Together, these findings connect fundamental defect physics with practical considerations in refractory material science.

FM 7.6 Tue 11:00 BEY/0E40

Creation of Color Centers in Magnesium Fluoride Single Crystals by Irradiation with MeV Heavy Ions — •Ayman El-Said — Physics Department and Interdisciplinary Research Center for Advanced Materials, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia

The irradiation of ionic halide single crystals with MeV heavy ions can lead to the creation of various types of color centers [1]. Here, MgF2 single crystals were irradiated with MeV heavy ions of different energies and fluence [2]. UV-Vis spectroscopic measurements demonstrate the existence of F1-, F2-, and F3-centers due to ion irradiation. The type, concentration and creation efficiency of the observed color centers are studied in terms of ion fluence and energy loss. The results are not only of high importance for understanding the creation mechanism of the induced color centers but also for the degradation of optical materials in high-altitude and space environments.

Acknowledgements: Parts of this research were carried out at the Ion Beam Center at the Helmholtz-Zentrum Dresden-Rossendorf e. V., a member of the Helmholtz Association. Ayman S. El-Said acknowledges the support by KFUPM, Saudi Arabia (Project: ISP24236).

[1] K. Schwartz, C. Trautmann, A.S. El-Said, R. Neumann, M. Toulemonde, W. Knolle, Phys. Rev. B 70, 184104 (2004). [2] A.S. El-Said, Rad. Phys. and Chem. 227, 112369 (2025).

FM 7.7 Tue 11:15 BEY/0E40

Oxygen vacancies in vanadium dioxide: A DFT+*V* study — •Oskar Leibnitz[1,2], Peter Mlkvik[1], Nicola A. Spaldin[1], and Claude Ederer[1] — [1]Materials Theory, Department of Materials, ETH Zurich, Switzerland — [2]Present address: Multifunctional Ferroic Materials, Department of Materials, ETH Zurich, Switzerland

We present a density-functional theory study of the effects of oxygen vacancies on the structural and electronic properties of vanadium dioxide (VO_2). Our motivation is the reported suppression of the metal-insulator transition by oxygen vacancies and the lack of a clear consensus on its origin. We use the DFT+*V* method with a static intersite vanadium-vanadium interaction term, *V*, to calculate the properties of the oxygen-deficient metallic rutile and insulating monoclinic M1 phases of VO_2 on the same footing. We find that oxygen vacancies induce local distortions in the M1 phase, but do not destroy the dimerization usually associated with the insulating behavior. In spite of this, we find that the M1 phase becomes metallic as a result of the partial filling of the conduction band due to a rigid-band-like doping effect.

FM 7.8 Tue 11:30 BEY/0E40

Distortion tensor around dislocations in GaN studied by electron backscatter diffraction and cathodoluminescence spectroscopy — •Domenik Spallek, Vladimir Kaganer, Oliver Brandt, Thomas Auzelle, and Jonas Lähnemann — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

The effect of elastic distortion in the vicinity of a threading dislocation (TD) in GaN on its luminescence has been shown previously [1]. However, quantifying this distortion and its components remains a challenge. Therefore, we investigate individual TDs by correlated high-resolution electron backscatter diffraction (HR-EBSD) and cathodoluminescence (CL) spectroscopy. The sample is a high-purity, homoepitaxial GaN layer grown by molecular beam epitaxy with a low TD density.

A cross-correlation analysis with the software CrossCourt from BLG Vantage is used to determine the spatially-resolved components of the distortion tensor from the HR-EBSD results [2]. Signatures of the TDs are resolved in the elastic strain and rotation components. Through reference measurements, we explore the resolution limit of this analysis and its dependence on the material and measurement conditions. Hyperspectral CL maps show a reduced intensity as well as a shifted emission wavelength around the TD. With additional modeling of the distortion around a TD, these correlated measurements are related to the Burger's vector of the dislocation, determining its type.

[1] Kaganer *et al.*, Phys. Rev. Appl. **12**, 054038 (2019).
[2] Wilkinson *et al.*, Ultramicroscopy **106**, 307 (2006).

FM 8: Multiferroics and Magnetoelectric Coupling (joint session MA/FM)

Time: Tuesday 9:30–12:30 Location: POT/0112

See MA 17 for details of this session.

FM 9: Focus Session: Materials Discovery II – High throughput searches for functional magnetic materials (joint session FM/MA)

chairs: Jan Schultheiß (Norwegian University of Science and Technology, NO), Hiroki Taniguchi (Nagoya University, JP)

Discovering new functional materials is crucial to advance today's technologies, ranging from caloric cooling via catalysis to next-generation energy conversion and storage, such as thermoelectric, ferroelectric, and ionic conductor materials. New materials also form the basis for potential applications in quantum information technologies. This session provides a platform to highlight functional materials discoveries and how they come about. Notably, systematic searches with high-throughput synthesis approaches, as well as predictions from materials informatics, have helped to go beyond serendipitous discoveries in recent years. However, intuition guided by general principles remains an important factor. In this session, we particularly welcome contributions that showcase the discovery of new functional materials with original approaches. Diverse material systems - from well-established to emerging and niche classes across condensed-matter and materials physics - will be featured. Bringing together diverse discoveries in a single session will help delineate general principles and inspire future work.

Time: Tuesday 14:00–15:30 Location: BEY/0138

Invited Talk FM 9.1 Tue 14:00 BEY/0138

Thin film combinatorial studies of functional magnetic materials — •Nora Dempsey — Institut NEEL, CNRS/UGA, Grenoble, France

Combinatorial studies based on the preparation and characterisation of compositionally graded thin films are being used for the screening and optimization of a range of functional materials [1]. When combined with Machine Learning (ML), such high-throughput film-based studies hold much potential to guide data driven design of new materials [2,3]. In this talk I will outline our work at Institut Néel on high throughput fabrication and characterisation of functional magnetic materials as well as our recent developments concerning data handling and analysis. I will then show examples from on-going studies of the effect of composition and fabrication conditions on both structural and magnetic properties of hard magnetic and magnetocaloric materials. I will finish up by briefly outlining preliminary results from ML-driven data analysis for the accelerated development of functional magnetic materials with reduced dependence on critical elements, carried out in the framework of various collaborations. [1] ML Green et al., J. Appl. Phys. 113 (2013) 231101 [2] A.G. Kusne et al. Sci. Rep. 4 (2014) 6367 [3] A. Ludwig, npj Comput. Mater. 5 (2019) 70

FM 9.2 Tue 14:30 BEY/0138

Potentially magnetic platinum oxides obtained by computationally guided high-pressure synthesis — •Yasuhito Kobayashi[1], Akitoshi Nakano[2], Shunsuke Kitou[3], Tomasz Klimczuk[4], Hidefumi Takahashi[1,5], and Shintaro Ishiwata[1,5] — [1]Division of Materials Physics, The University of Osaka, Japan — [2]Department of Physics, Nagoya University, Japan — [3]Department of Advanced Materials Science, The University of Tokyo, Japan — [4]Advanced Materials Center, Gdansk University of Technology, Poland — [5]Institute for Open and Transdisciplinary Research Initiatives, The University of Osaka, Japan

The exploration of Pt-based oxides has remained significantly limited, primarily due to the high chemical inertness of platinum and the typically nonmagnetic d^6 or d^8 electronic configurations. Here, we report the discovery of a new layered homologous series of Pt-based ternary oxides, $Na(PtO_2)_{2n+1}$ (n = 1, 2), synthesized through a combination of highly oxidizing high-pressure techniques and density functional theory (DFT) calculations. This series features unprecedented layered structural motifs composed of rutile-based PtO_6 octahedra and one-dimensional PtO_4 square-planar chains, distinct from the perovskite-based Ruddlesden-Popper oxides. We discuss the possibility that this layered homologous series represents the first realization of a magnetic Mott insulator within Pt-based oxides, where $NaPt_3O_6$ (n = 1) exhibits localized spin behavior with an effective spin S = 1/2, likely arising from the unusual d^7 electronic configuration of square-planar Pt^{3+} along with one-dimensional antiferromagnetic interactions.

FM 9.3 Tue 14:45 BEY/0138

Magnetism and electrical and thermal transport in the natural $Fe_{1-x}Mn_xWO_4$ (x=0.2) mineral from Potosí, Bolivia — •Skachko Dmytro[1], Bohdan Kundys[2], Volodymyr Levytskyi[1], Esteban Zuñiga-Puelles[1], Andreas Leithe-Jasper[3], and Roman Gumeniuk[1] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg, 09596 Freiberg, Germany — [2]Université de Strasbourg, CNRS, Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504, Strasbourg F-67000, France — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany

The natural ferberite single crystal of $Fe_{0.8}Mn_{0.2}WO_4$ composition with the monoclinic $NiWO_4$-type structure ($P2/c$) [a = 4.74751(6) Å, b = 5.71335(7) Å, c = 4.96847(5) Å, β = 90.15(1)°] reveals multiple magnetic transitions at T_{N1} = 67(1) K, T_{N2} = 28(3) K, T_{N1}^{cp} = 66(1) K and T_{N2}^{cp} = 8(1) K. The reduced magnetic entropy of ≈ Rln3 observed near T_{N1} indicates the simplified LS-coupling scheme to fail in the description of complex magnetic behavior of the studied ferberite. The temperature dependence of electrical resistivity [$\rho(T)$] shows a semiconducting exponential decay saturating at ≈ 300 K. The activation energy of the decay is found to be ≈310 meV. Temperature dependence of thermal conductivity [$\kappa(T)$] is characterized by a well defined maximum at ≈68 K, which is described by the Debye-Callaway model, pointing to the dominance of phonon scattering on defects and *umklapp* processes. Despite revealing relatively low $\kappa(T)$ and high Seebeck coefficient $Fe_{0.8}Mn_{0.2}WO_4$ is rather poor thermoelectric material because of enhanced $\rho(T)$.

FM 9.4 Tue 15:00 BEY/0138

Ab initio-based phase diagrams for compositionally complex ThMn12-type alloys — •Sourabh Kumar[1], Semih Ener[2], and Tilmann Hickel[1] — [1]Bundesanstalt für Materialforschung und -prüfung, 12489 Berlin — [2]Technische Universität Darmstadt, 64289 Darmstadt

The structural and chemical stability of rare-earth-based transition-metal (such as Nb, Ce, and Sm) alloys is critical in determining the performance of modern hard magnets (HMs), particularly their coercivity and thermal robustness. This study examines the intrinsic phase competition in (Sm/Ce)-(Fe/Co)-Ti systems, focusing on how Ti additions influence the thermodynamic stability of high-temperature HMs. Two compositional pathways were examined: one dominated by Sm/Ce-Fe/Co binary chemistry and the other influenced by (Sm/Ce)-(Fe/Co)-Ti ternary interactions. We employed ab initio calculations to investigate the finite-temperature stability of ordered, disordered, and metastable phases, thereby guiding experiments. Based on the computed energetics, we analyzed how Ti incorporation alters local bonding environments and stabilizes magnetically desirable motifs. Furthermore, we constructed an ab initio phase diagram to reveal the interplay between rare-earth metals and transition metals across a broad temperature range. We have revealed that Ti addition promotes the formation of a more robust Sm-rich phase by strengthening the local Sm-Fe-Ti matrix. This stabilization enhances alloy coercivity and provides insights into the thermodynamic and chemical factors driving phase evolution, enabling the design of better permanent HMs.

FM 9.5 Tue 15:15 BEY/0138

Molecular orbital degeneracy lifting in NbSeI — •Keita Kojima[1], Hayato Takano[1], Youichi Yamakawa[2], Shunsuke Kitou[3], Ryutaro Okuma[1], and Yoshihiko Okamoto[1] — [1]Institute for Solid State Physics, University of Tokyo, Kashiwa 277-8581, Japan — [2]Department of Physics, Nagoya University, Nagoya 464-8602, Japan — [3]Department of Advanced Materials Science, University of Tokyo, Kashiwa 277-8581, Japan

The breathing pyrochlore lattice, composed of alternating small and large tetrahedra, hosts molecular orbitals within the smaller tetrahedra that strongly influences its physical properties. Such molecular-orbital and frustration-driven effects have led to diverse electronic states in related compounds. We investigated NbSeI, a MoSBr-type material with a particularly large breathing distortion whose physical properties remain unexplored despite previous synthesis reports. We synthesized single crystals and conducted x-ray diffraction, physical property measurements, and first-principles calculations. While the calculations predict metallic flat bands originating from Nb 4d orbitals, magnetic and transport measurements reveal a nonmagnetic insulating state below 300 K. NbSeI also undergoes a structural transition at Ts = 106 K. Our structural studies demonstrate local atomic displacements above Ts and a trimer-like molecular transformation below Ts. Our results show that the combination of strong breathing distortion and flat-band*derived electronic structure stabilizes molecular-orbital degrees of freedom, advancing orbital physics beyond single-ion descriptions toward cluster-based electronic phenomena.

FM 10: Crystal Defects and Real Structure Physics in Diamond and Functional Materials II

chair: Theo Scherer (Karlsruhe Institute of Technoloy, DE)

Time: Tuesday 14:00–15:30 Location: BEY/0E40

FM 10.1 Tue 14:00 BEY/0E40

Identification of defects in iron molybdate catalysts via first principles calculations — •Young-Joon Song and Roser Valentí — Institut für Theoretische Physik, Goethe-Universität, 60438, Frankfurt am Main, Germany

Iron molybdate ($Fe_2(MoO_4)_3$) is well known as a commercial catalyst for oxidative dehydrogenation. Recently, L. Schumacher et al. reported an experimental reduction in Raman intensity at 782 cm^{-1} during catalytic processes. The authors attribute this decrease to oxygen migration from the bulk to the surface during the reaction, in contrast to the conventional understanding that oxygen atoms are supplied only near the surface. To identify the types of defects responsible for the observed reduction in Raman intensity, we performed DFT electronic and phononic structure calculations for $Fe_2(MoO_4)_3$. Our findings reveal that optical phonon modes involving oxygen dominate the spectrum at around 790 cm^{-1}, with a small contribution from Mo, corresponding to asymmetric MoO_4 stretching modes. In the Raman calculations, a major peak appears at 789.68 cm^{-1} with a small shoulder-like feature and a minor peak at 972.05 cm^{-1}, consistent with the experimental observations. By selectively freezing specific phonon modes, we introduced an effective method to incorporate defect effects into Raman calculations without explicitly creating oxygen vacancies. Using this approach, we found that oxygen vacancies play a dominant role in the reduction of Raman intensity. Finally, we discuss the relaxed structure containing explicit oxygen vacancies. This research was supported by the German Research Foundation for funding through CRC 1487.

FM 10.2 Tue 14:15 BEY/0E40

Exsolution of metal nanoparticles by control of point defects — •Andreas Rosnes[1], Bo Jiang[2], Holger von Wenckstern[1], Øystein Prytz[1], and Jonathan Polfus[2] — [1]Department of Physics, Centre for Materials Science and Nanotechnology, University of Oslo, PO Box 1048 Blindern, NO NO-0316 Oslo, Norway — [2]Department of Chemistry, Centre for Materials Science and Nanotechnology, University of Oslo, PO Box 1033 Blindern, NO-0315 Oslo, Norway

Exsolution involves redox precipitation of metal nanoparticles from metal oxides, resulting in materials that exhibit excellent electrocatalytic properties and hold great promise for novel types of nanoscale heterostructures. However, a coherent understanding of the phenomenon is lacking. Here, exsolution is described by three point defect equations involving the reduction of the host oxide, reduction and exsolution of the transition metal, and annihilation of host unit cells. Guided by their predictions, significantly enhanced exsolution in terms of molar amount, rate, and nucleation density is shown by acceptor substitution to the system $La_{0.2}Ca_{0.7}Ti_{0.95}Cu_{0.05}O_{3-\delta}$ through atomic scale imaging and in situ X-ray diffraction and spectroscopy. It is demonstrated that the oxygen stoichiometry of the parent oxide increases upon exsolution despite oxygen loss in the reducing environment. Furthermore, strain in both the host oxide and the exsolved metal can constitute an additional thermodynamic barrier for exsolution beyond the availability of the required point defects.

FM 10.3 Tue 14:30 BEY/0E40

Machine-Learning Potentials Reveal Defect Segregation at Grain Boundaries in Lithium Solid Electrolytes — •Waldemar Kaiser[1], Hyunwon Chu[2], Jennifer L.M. Rupp[1,2], and David A. Egger[1] — [1]TUM School of Natural Sciences, Technical University of Munich — [2]Department of Materials Science and Engineering, Massachusetts Institute of Technology

Grain boundaries (GB) play a central role in ionic and electronic transport in polycrystalline solid electrolytes [1, 2], yet their local defect chemistry remains difficult to resolve. Their structural complexity and chemical heterogeneity introduce a wide distribution of possible defect configurations that are computationally demanding to characterize with first-principles methods. As a result, the origins of variations of ionic and electronic transport often remain unclear.

Here, machine-learning potentials (MLPs) are applied to representative Σ5 and Σ3 GB structures to investigate ionic defects in lithium lanthanum zirconate (LLZO). The MLPs enable the systematic and efficient mapping of lithium- and oxygen-vacancy formation energies, revealing reductions of up to 1 eV within GB cores relative to bulk sites. Structural analysis further identifies locally Zr-deficient coordination environments as preferred incorporation sites for lithium vacancies, and experiments show that Ta-doping fills these bottlenecks and enhances the material's stability.

[1] B. Gao et al., Adv. Energy Mater. 12, 2102151, 2021 [2] Y. Zhu et al., Nat. Rev. Mater. 6, 313-331, 2021

coffee break

FM 10.4 Tue 15:00 BEY/0E40

2 - Dimensional hybrid perovskite as a promising semiconductor for large area electronics — •Tomasz Marszalek, Shuanglong Wang, Zhitian Ling, Denis Andrienko, Hai Wang, Paul W.M. Blom, and Wojciech Pisula — Max Planck Institute for Polymer Research, Mainz, Germany

Two-dimensional (2D) perovskites with bulky spacer cations are promising candidates for field-effect transistors due to the suppressed ion movement caused by large size insulating ligands. However, the relationship between the chemical nature of organic cations and film morphology, crystallinity, molecular organisation and charge carrier transport in 2D layered perovskites is not yet fully understood, which significantly limits the development of 2D perovskite FETs.

This report presents a distinct odd-even effect in 2D Sn-based perovskite semiconductors for the first time, incorporating monovalent phenylalkylammonium-based organic cations with alkyl side chains of different lengths containing either an odd or an even number of carbon atoms. An odd-even oscillation of charge carrier transport was revealed using optically pumped terahertz spectroscopy and transistor devices. By combining density functional theory calculations with simulated grazing-incidence wide-angle X-ray scattering, we demonstrate that organic ligands featuring odd carbon atoms exhibit a disordered crystal lattice and tilted inorganic octahedra. This results in a larger effective mass and inferior charge mobilities compared to perovskites with an even number of carbon atoms in the organic cations. (J. Am. Chem. Soc. 2024, 146, 19128, Mater. Horiz., 2024,11, 1177)

FM 10.5 Tue 15:15 BEY/0E40

On the origin of the strange metal Hall effect in BaFe2(As1-xPx)2 — •Augusto Ghiotto[1], Darian Hall[1], Yuanqi Lyu[1], Kohtaro Yamakawa[1], John Singleton[2], and James Analytis[1] — [1]University of California, Berkeley, USA — [2]National High Magnetic Field Laboratory's Pulsed Field Facility at Los Alamos, USA

BaFe2(As1-xPx)2 is an unconventional superconductor in which the antiferromagnetic, nematic and structural order is suppressed by isovalent P substitution, leading to a quantum critical point at x = 0.31. It has been shown that the Hall effect of the overdoped series contains an anomalous contribution arising from the correlations within the strange metal, whose behavior emanates from a quantum critical point and, in the zero-temperature limit, decays together with the superconducting critical temperature. Here, we present new data on the underdoped series taken at pulsed high magnetic fields. To achieve a large signal to noise ratio and an accurate measurement of the Hall coefficient, we microstructured the crystals into well-defined Hall bars. In this talk, we will draw parallels between the Hall effect in the ordered state and in the strange metal.

FM 11: Poster Session Functional Materials

chairs: Jan Schultheiß (NTNU, NO), Anna Grünebohm (Ruhr Universität Bochum, DE)

Time: Tuesday 18:00–20:30 Location: P4

FM 11.1 Tue 18:00 P4

Structural and Optical Characterization of FeGaInS* Layered Crystals — •Zeynab Addayeva and Mustafa Muradov — Baku State University, Baku , Azerbaijan

FeGaInS4 layered crystals were synthesized using the Bridgman technique, and their crystal structure was investigated via powder X-ray diffraction (XRD). FeGaInS4 is a quaternary complex metal chalcogenide that belongs to the class of layered, quartz-like A-B-C-X4 type compounds. The material crystallizes in the rhombohedral system and adopts the R3m (No. 160) space group, according to the International Union of Crystallography (IUCr) classification. The refined lattice parameters (a = b = 5.406 Å, c = 10.708 Å) confirm the presence of a highly symmetric and anisotropic layered crystal structure. Within the structure, Fe, Ga, and In atoms occupy different coordination environments and form tetrahedral bonds with sulfur (S) anions, resulting in a complex three-dimensional network. These bonding interactions directly influence the material's electronic structure and related functional properties, including electrical conductivity, op-

tical absorption, dielectric response, and thermal stability. Due to its anisotropic layered architecture, FeGaInS4 exhibits natural cleavage along specific crystallographic directions. This property renders it suitable for exfoliation into few-layer or monolayer nanosheets, making it a promising candidate for the fabrication of two-dimensional (2D) materials and high-performance composite systems. The optical band gap of FeGaInS4 is approximately 1.46 eV.

FM 11.2 Tue 18:00 P4

An Atom Probe Tomography Study of the Bond Breaking Behavior of Transition Metal Chalogenides — •Sophia Schreinemacher[1], Jan Köttgen[1], Elias Hildebrnad[1], Felix Hoff[1], Christian Stenz[1], Vicky Hasse[3], Yuan Yu[1], and Matthias Wuttig[1,2] — [1]I. Institute of Physics (IA), RWTH Aachen University, Germany — [2]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany — [3]Max Planck Institute for Chemical Physics of Solids 01187 Dresden, Germany

Chemical bonds are a vital subject in materials science, as they are one of the central factors that define the properties of a material. Transition metal chalcogenides are a group of materials characterized by the bonding between the chalcogenide p-orbitals and the metal d-orbitals, which exhibit unique electronic, optical, and magnetic properties. The main bonding indicator in this study is the probability of multiple events (PME) obtained during atom probe tomography (APT) acquisition.

The results show a medium PME (40-60%), highlighting the unique bond-breaking behavior that transition metal chalcogenides display during APT evaporation. In a plot of the PME against the electrical conductivity, the studied materials cluster at the border between the metavalent and covalent materials. These findings expose a clear connection between transition metal chalcogenides, their d- and p-orbital interaction, and their bonding characteristics, thereby broadening our understanding of metavalent materials.

FM 11.3 Tue 18:00 P4

Epitaxial Growth and Optimization of LiNbO3 Thin Films on LiTaO3 and Al2O3 by Pulsed Laser Deposition Using Machine Learning — •Hyeyeon Cho, Milena Petkovic, Steffen Ganshow, and Jutta Schwarzkopf — Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, 12489 Berlin, Germany

Lithium niobate (LiNbO3) thin films are widely used in electro-optical and electro-acoustic devices due to their excellent ferroelectric, piezoelectric, and nonlinear optical properties, offering broader bandwidths at higher frequencies and reduced operational voltages compared to bulk materials. The development of high-quality, phase-pure, and smooth LiNbO3 films is essential for achieving superior device performance. Pulsed Laser Deposition (PLD) offers precise control over growth parameters, enabling the fabrication of epitaxial LiNbO3 layers with tunable structural properties. In our work, we investigated the epitaxial growth of LiNbO3 thin films on LiTaO3 and Al2O3 substrates using PLD. The influence of various PLD growth conditions and substrate materials was systematically investigated with regard to phase formation and structural ordering by x-ray diffraction and surface roughness by atomic force microscopy. Furthermore, a four-step machine learning workflow, including Artificial Neural Network (ANN) and Random Forest (RF) models, was employed to analyze the nonlinear relationships between PLD parameters and structural film properties. This combined experimental and computational approach accelerates development and provides deeper insight into LiNbO3 thin film growth for advanced photonic and optoelectronic applications.

FM 11.4 Tue 18:00 P4

Ferroelectricity in spin-liquid candidate $TbInO_3$ — •Andrea Tobiassen[1], Elvia Chavez[1], Jiali He[1], Dennis Meier[1,2], and Jan Schultheiss[1] — [1]NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]University of Duisburg-Essen, Duisburg, Germany

Hexagonal rare-earth oxides exhibit a variety of intriguing physical phenomena, ranging from rich magnetism to improper ferroelectricity. Among them, $TbInO_3$ has recently been proposed as a spin-liquid candidate, where magnetic frustration suppresses long-range magnetic order at low temperatures. The ferroelectric properties of $TbInO_3$ remain largely unexplored.

In this work, we synthesize $TbInO_3$ polycrystals via a solid-state route. Phase purity is confirmed by X-ray diffraction (XRD), while Scanning Electron Microscopy (SEM) and Piezoresponse Force Microscopy (PFM) reveal a pronounced domain contrast, evidencing a topological ferroelectric domain structure typical for hexagonal oxides. High-temperature XRD indicates a Curie temperature (T_C) of approximately 1630 K, corresponding to the polar $P6_3cm$ to non-polar $P6_3/mmc$ phase transition. Understanding the ferroelectricity in $TbInO_3$ provides a foundation for engineering its domain structure and exploring potential magnetoelectric coupling effects.

FM 11.5 Tue 18:00 P4

Localized High-Concentration High-Entropy Electrolytes for Superior Lithium Metal Anodes via Solvation Cluster Regulation — •Haixuan Luo and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany

The practical deployment of high-energy-density lithium metal batteries (LMBs) is severely hindered by the thermodynamic instability of the lithium metal anode, which precipitates dendritic growth and poor Coulombic efficiency. Although localized high-concentration electrolytes (LHCEs) have emerged as a promising solution, optimizing their cluster configurations to maximize interfacial durability remains a challenge. Herein, we propose a groundbreaking localized high-concentration high-entropy electrolyte (LHCHEE) strategy that leverages the high-entropy effect to tailor solvation structures at the molecular level. Our systematic investigation reveals that the introduced configurational entropy promotes the formation of uniform, anion-rich solvation clusters while suppressing solvent decomposition. This unique solvation environment facilitates the construction of a robust, inorganic-dominated solid electrolyte interphase (SEI) on the lithium metal. Consequently, the LHCHEE enables exceptional stability, while Li||Cu cells demonstrate significantly improved Coulombic efficiency. Furthermore, full cells paired with high-voltage cathodes exhibit remarkable capacity retention. This work not only demonstrates the superiority of LHCHEEs but also establishes entropy engineering as a critical dimension for designing advanced electrolyte systems.

FM 11.6 Tue 18:00 P4

Ferroelectric switching at edge dislocations in $BaTiO_3$ modelled at the atomic scale — •Himal Wijekoon[1,2], Pierre Hirel[3], and Anna Grünebohm[1,2] — [1]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) and Center for Interface-Dominated High Performance Materials (ZGH), Ruhr-University Bochum, Universitätsstr 150, 44801 Bochum, Germany — [2]Faculty of Physics and Astronomy, Ruhr-University Bochum, Universitätsstr 150, 44801 Bochum, Germany — [3]Univ. Lille, CNRS, INRAE, Centrale Lille, UMR 8207 - UMET - Unité Matériaux et Transformations, F-59000 Lille, France

Domain nucleation and switching largely govern the functional properties of ferroelectric perovskites. Consequently, one can utilize defects to tailor domain switching and thereby tune the functional properties of these materials. While previous studies have mainly focused on switching in pristine pervoskite materials, the influence of defects, particularly dislocations, on domain nucleation and switching remains insufficiently understood. Using molecular static simulations, we show that ⟨100⟩ edge dislocations cores in barium titanate can serve as domain nucleation sites. By applying an external electric field in three different orientations relative to the Burgers vector and dislocation line, we show how domain nucleation and subsequent growth occurs in dislocations-induced strain variations. Our simulations reveal that the coupling between electric field and polarization is strongest when the field is applied parallel to the Burgers vector.

FM 11.7 Tue 18:00 P4

Topology and Bonding: A bonding-based approach to topological insulators via Atom Probe Tomography — •Elias Hildebrand[1], Jan Köttgen[2], Yuan Yu[1], and Matthias Wuttig[1,2] — [1]I. Institute of Physics (IA), RWTH Aachen University, Germany — [2]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany

Ever since the discovery of the quantum Hall effect, interest in topological phases of matter has steadily increased. Initially attributed to spin-orbit coupling, the underlying guiding principle causing these topological phases of matter has been a topic of ongoing discussion.

Here, we want to propose a bonding-based approach to explain nontrivial topological states. The experimental foundation for this connection is established through Atom Probe Tomography (APT). While APT is primarily employed for microstructural analysis, it has recently been proposed as a tool capable of identifying different bonding mechanisms.

Within this method, most topologically nontrivial materials also exhibit distinct bond-breaking behaviour corresponding to their characteristic bonding mechanisms. Here, different materials are investigated regarding their topological nature and behaviour in the APT.

Consequently, APT can be established as an experimental method for identifying topological phases of matter and as an empirical argument highlighting the significance of bonding in understanding the fundamental principles governing topological materials.

FM 11.8 Tue 18:00 P4

Strain-driven phonon instabilities in BaSnO3 — •Benyao Sun and Anna Grünebohm — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Germany

The perovskite BaSnO3(BSO) has attracted extensive research interest due to its favorable properties, including non-toxicity, high thermal stability, and distinctive electronic characteristics. However, bulk BSO is generally non-ferroelectric, limiting its applications. Fortunately, strain engineering can induce ferroelectricity by tuning the perovskite structure. For example, strain-induced tetragonality leads to a large dipole moment and, consequently, to a high polarization in strained ferroelectrics [1]. BSO exhibits ferroelectric polarization under applied epitaxial strain [2]. Strain-induced ferroelectricity in BSO has been studied, but phonon-spectrum analyses under sustained strain remain limited. In our work, we carry out a systematic study of the phonon instabilities of BSO under compressive strain. We calculate the critical compressive strain at which soft modes

appear in the phonon dispersion of BSO, analyze the contributions of the polar mode and the antiferrodistortive mode to the ferroelectricity as well as the couplings between different soft modes, and also discuss the effect of an external electric field on these soft modes.

[1] Zeches,R.J.et al.Science 2009, 326,977-980.
[2] Zhang,Y.et al.Phys.Chem.Chem.Phys.2017,19, 26047-26055.

FM 11.9 Tue 18:00 P4

Virtual Characterization Lab: A Python Toolkit for Material Characterization from Molecular Dynamics — •Vahid Jamebozorgi[1,2] and Christian Schröder[1,2] — [1]HSBI, Bielefeld, Germany — [2]Bielefeld University, Bielefeld, Germany

Material discovery using traditional experimental methods is a slow and costly process, often limited by the sampling process, characterization condition constraints, and the requirement for expensive equipment. While computational tools have transformed materials research by accelerating the investigation of material properties, a significant gap remains in connecting high-fidelity simulations with established experimental characterization techniques. We present the Virtual Characterization Lab (VCL), a unified, open-source Python toolkit designed to bridge this gap. The VCL streamlines the entire workflow from molecular dynamics simulations, enabling researchers to generate and analyze key characterization data, such as X-ray Diffraction (XRD), Selected Area Electron Diffraction (SAED), and Vibrational Density of States (VDOS), all within a single, intuitive environment. By integrating every step from initial structure preparation to final data visualization, the VCL accelerates materials discovery by making virtual characterization more efficient, accessible, and directly comparable to experimental results.

FM 11.10 Tue 18:00 P4

Structural Factors Governing Stability and Electronic Transport in Future Neuromorphic Memristor Technologies — •Wiktoria Szopa[1,2,3], Marcin Krynski[1], Attila Cangi[2,3], and Piotr Wisniewski[4] — [1]Faculty of Physics, Warsaw University of Technology, 00-662 Warsaw, Poland — [2]Center for Advanced Systems Understanding, 02826 Görlitz, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [4]Centre for Advanced Materials and Technologies CEZAMAT, Warsaw University of Technology, 02-822 Warsaw, Poland

With the rapid rise of artificial intelligence, the demand for technologies that enable its development and application is high, as AI is now widely used across science, industry, and everyday life. Neuromorphic materials may offer a promising solution to the increasingly complex hardware requirements posed by next-generation, high-throughput AI.

Silicon-oxide-based memristors may operate as adjustable weights within hardware neural networks, enabling more efficient, neuromorphic computation. The electronic component contains two electrodes separated by a thin amorphous silicon oxide layer, within which charge transport occurs through filamentary silicon chains that form conductive pathways.

In this project, we investigate how the local atomic structure influences electronic transport. To this end, we generated hundreds of memristor models and identified their most stable configurations, with high structural robustness and defined conduction pathways by using a combination of DFT calculations and machine learning modeling.

FM 11.11 Tue 18:00 P4

Computational modelling of phonon, elastic, and electronic properties of layered quantum crystalline materials — •Zoya Eremenko[1], Yuri Savin[2], and Vladimir M. Fomin[1] — [1]IFW Dresden, Germany — [2]O.Ya. Usikov Institute for Radiophysics and Electronics, National Academy of Sciences of Ukraine, Kharkiv, Ukraine

We present a comparative computational study of the phonon, elastic, and electronic properties of several crystalline quantum materials $NbSe_2$, FeSe, MoS_2, and BSCCO using density functional theory (DFT) and COMSOL Multiphysics. For each material, we analyze the primitive-cell geometry, symmetry, the resulting vibrational and mechanical responses extracted from both the first-principles calculations and the available experimental references. Layered transition-metal dichalcogenides $NbSe_2$, and MoS_2, show significantly anisotropic elastic responses, consistent with their quasi-2D bonding. MoS_2 shows elastic constants aligned with experimental values. Properties of the tetragonal iron-based chalcogenide FeSe are modelled using its primitive cell and the electronic band structure. By leveraging elastic constants obtained from the available experimental and theoretical studies, the BSCCO phonon frequencies are calculated with COMSOL Multiphysics. The close agreement between our simulated phonon frequencies and the experimental data for BSCCO validates our multi-scale approach, providing a solid foundation for future studies of the electron-phonon interactions and structural effects in complex quantum materials. We thank Dr. Golam Haider for providing us with the experimental data for verification of the simulated Raman frequencies.

FM 11.12 Tue 18:00 P4

First-Principles Modeling and ESR Identification of an Intrinsic Radical Spin Center in UiO-66-NH_2 Metal-Organic Framework — •Timur Biktagirov[1], Anastasiia Kultaeva[2], Daniel Klose[3], Eugenio Otal[4], and Wolf Gero Schmidt[1] — [1]Physics Department, University of Paderborn, 33098 Paderborn, Germany — [2]Experimental Physics 6, Julius-Maximilian University of Würzburg, 97074 Würzburg, Germany — [3]ETH Zurich, 8093 Zurich, Switzerland — [4]Institute for Aqua Regeneration (ARG), Shinshu University, 4-17-1 Wakasato, Nagano 380-8553, Japan

Metal-organic frameworks (MOFs) are emerging as tunable platforms for sensing, photocatalysis, and energy conversion, where charge transfer, spin interactions, and defect states play key roles. Here, we identify and characterize a native NH· radical defect intrinsic to the aminoterephthalate linker in UiO-66-NH_2 MOF. Combining density functional theory (DFT) modeling with multi-frequency electron spin resonance (ESR) spectroscopy, we elucidate the radical's electronic structure, spin density distribution, formation pathway, and spin-coherence properties. Our findings reveal the radical's exceptional stability and highlight its relevance for both photocatalytic charge separation and quantum-enhanced sensing in MOFs.

FM 11.13 Tue 18:00 P4

Efficient Discovery of Intermediate-Temperature Proton Conductors via Ion Exchange Strategy with Machine Learning Potential — •Yun An, Karsten Reuter, and Christoph Scheurer — Fritz Haber Institute of the Max Planck Society, 14195 Berlin, Germany

Proton-conducting solid-oxide fuel cells (H-SOFCs) are promising for direct ammonia-fed SOFC applications, as they eliminate NO_x emissions compared to conventional oxide-ion-conducting solid-oxide fuel cells. However, current proton-conducting electrolytes operate at high temperatures and suffer from leakage currents. Known suitable materials remain rare, calling for systematic investigations into novel proton conductor classes. We present a framework that combines machine-learning techniques with high-throughput computation to screen and design efficient proton conductors at intermediate temperatures. Through an ion-exchange strategy applied to known alkaline-ion conductor classes, we identify a database of potential proton-conducting materials. Machine learning molecular dynamics simulations are employed to assess stability and diffusion barriers, enabling the selection of top-performing candidates. The screened proton conductors contain cations that span from monovalent to pentavalent, including Rb^+, Ba^{2+}, Ca^{2+}, B^{3+}, Zr^{4+}, and Nb^{5+}, and predominantly feature SO_4^{2-} and PO_4^{3-} polyanion groups. Proton transport in these materials follows the Grotthuss mechanism. The strength of hydrogen bonds increases after ion-exchange engineering, thereby enhancing proton transfer.

FM 11.14 Tue 18:00 P4

Dual Strategy Engineering of Zn4Sb3: Indium Doping and ZnO Coating for High zT — •Abhishek Pandey[1], Amin Bahrami[2], and Kornelius Nielsch[3] — [1]Leibniz Institute for Solid State and Materials Research, Helmholtzstraße 20, Dresden 01069, Germany — [2]Leibniz Institute for Solid State and Materials Research, Helmholtzstraße 20, Dresden 01069, Germany — [3]Leibniz Institute for Solid State and Materials Research, Helmholtzstraße 20, Dresden 01069, Germany

Zn4Sb3 is one of the promising thermoelectric materials due to its very low thermal conductivity and favorable electronic properties for high TE performance. However, its practical application to TE device is limited by structural instability and Zinc-ion migration, which lead to the formation of zinc whiskers and degradation of TE performance. In this work, a dual-strategy approach has been adopted to enhance and stabilize Zn4Sb3, (1) Indium doping, and (2) ZnO surface coating of powder. Indium substitution within the Zn4Sb3 lattice is shown to increase the figure of merit (zT). In parallel the bulk modification, ZnO coating on Zn4Sb3 particles acts as a diffusion barrier that mitigates zinc migration and whisker formation, which improves the structural robustness during prolonged thermal cycling.

FM 11.15 Tue 18:00 P4

Towards Quantification of Convergent Beam Electron Diffraction Patterns — •Jimmy Steinweh[1], Daniel Wolf[1], and Axel Lubk[1,2] — [1]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [2]Institute of Solid State and Materials Physics, TU Dresden, Germany

Convergent beam electron diffraction (CBED) is a transmission electron microscopy (TEM) method, that utilizes a convergent electron beam to investigate the symmetry of crystalline samples at the nanoscale. A method for quantifying discrete rotational and mirror symmetries in CBED patterns is presented, involving a quantification algorithm for both simulated and experimental CBED patterns. This approach is used to investigate the influence of probe shifts, beam tilts, and thermal lattice vibrations on the symmetry of simulated CBED patterns of silicon to identify crystal structure related asymmetries. It is found that for a semi-convergence angle of $\alpha = 1.7$ mrad, the asymmetry introduced by probe shifts is barely detectable in simulations, whereas beam tilt effects are significant at beam tilt angles as low as 0.1 mrad. Consequently, precise alignment

of the beam in zone axis is crucial. We find furthermore that consideration of lattice vibrations within the frozen lattice approximation also slightly breaks the symmetry and discuss the origin of this effect. These results aim to establish a foundation for further development of CBED as a quantitative tool for probing crystal symmetries at the nanoscale.

FM 11.16 Tue 18:00 P4

Correlated Imaging of Thermal Conductivity and Ferroelectric Domains in $PbTiO_3$ Using Scanning Probe Microscopy — •Ciara Ward, Lindsey Lynch, and Raymond McQuaid — Queen's University Belfast, Belfast, UK

Perovskite ferroelectrics are an attractive platform for realising thermal conductivity switching through voltage configuration of domain microstructure. Reported mechanisms involve thermal conductivity modulation through structural re-orientation (anisotropy) [1,2] or phonon scattering by domain wall defects [3-5], both of which can be controlled through sample geometry and applied fields. Heat flow measurements and thermoreflectance investigations have quantitatively benchmarked thermal switching ratios but, in some cases, a lack of direct thermal mapping introduces ambiguity as to the relative role played by the two mechanisms. We are using Scanning Thermal Microscopy to explicitly map the local thermal conductance in samples of archetypal ferroelectric $PbTiO_3$ to clarify the underlying mechanisms that enable modulation of thermal transport. In tandem, we are using domain engineering and electric-field poling techniques to demonstrate the maximum achievable contrast in thermal conductance in this system.

[1] J. Seijas-Bellido *et al. Appl. Phys. Lett.* 115, 192903 (2019). [2] L. Féger *et al. Phys. Rev. Mater.* 8, 094403 (2024). [3] Ihlefeld *et al. Nano Lett.* 15, 1791 (2015). [4] E. Langenberg *et al. Nano Lett.* 19, 7901 (2019). [5] R. Belrhiti-Nejjar *et al. Adv. Sci.* 12, e06931(2025).

FM 11.17 Tue 18:00 P4

Impurity-Driven Vacancy Evolution in Irradiated Tungsten Revealed by Positron Annihilation Spectroscopy and Multiscale Modeling — •Zhiwei Hu[1,2], Qigui Yang[3], Jintong Wu[4], François Jomard[5], Thomas Jourdan[6], and Marie-France Barthe[2] — [1]HZDR, Dresden, Germany — [2]CEMHTI-CNRS, Orléans, France — [3]KTH, Stockholm, Sweden — [4]University of Helsinki, Finland — [5]GEMAC; Versailles; France — [6]CEA,Gif-sur-Yvette, France

Thermonuclear fusion demands plasma-facing materials that withstand extreme heat and irradiation. Tungsten, selected for ITER, develops microstructural evolution. Predicting defects behavior is therefore crucial. Using Positron Annihilation Spectroscopy, TEM, atomistic modeling, and DFT, irradiation-induced defects were examined. A new PAS data-inversion method using quadratic programming and two-component DFT was created. This method reconstructs full vacancy-cluster distributions from PAS data. Results show small vacancy clusters dominate after high-temperature irradiation. These clusters remain invisible to TEM yet strongly affect microstructure. Room-temperature electron irradiation showed reduced pure vacancy fractions. Unexpected positron traps were observed. SIMS and DFT identified these traps as oxygen-vacancy complexes. Cluster-dynamics simulations confirmed oxygen interacts with Frenkel pairs. Such interactions significantly modify defect evolution. Comparative irradiations of varying-purity tungsten were performed, PAS and TEM together revealed impurity effects.

FM 11.18 Tue 18:00 P4

Phase Transitions and Ferroic Properties in Organic*Inorganic Hybrid Halide TMCM-Mn*-*Fe*Cl* Crystals — •Chithra Kandappanthodi, Boris Slautin, Sobhan M Fathabad, Daniil Lewin, Doru Lupascu, and Vladimir Shvartsman — University of Duisburg-Essen

Organic*inorganic hybrid halides have garnered significant attention in materials science due to their eco-friendly, cost-effective synthesis, and outstanding optoelectronic properties. We report the properties of Fe-substituted trimethyl chloromethyl ammonium manganese trichloride TMCM-Mn1-xFexCl3 single crystals. The samples were obtained via the solvent evaporation seed assisted crystal growth method. Temperature-dependent X-ray diffraction and differential scanning calorimetry measurements confirm a sequence of structural phase transitions: from a monoclinic P121 phase at 302 K to monoclinic Cc, and subsequently to a hexagonal P6*/mmc phase at 408K for the pure TMCM-MnCl3 sample. Dielectric permittivity measurements indicate the improper ferroelectric transition at 408 K. Piezoresponse force microscopy further identifies well-defined ferroelastic domains at room temperature, which vanish upon heating above 304 K, as also observed using polarized light microscopy. Fe-substituted TMCM*Mn***Fe*Cl* samples exhibit a new intermediate phase transition near 328 K. UV*vis absorption spectra also demonstrate that increasing Fe content tunes the electronic bandgap. This comprehensive characterizations highlights TMCM-MnCl3, and TMCM-Mn1-xFexCl3 as a promising candidate for multifunctional applications.

FM 11.19 Tue 18:00 P4

Polymorph Stability and Mo Substitution in WO_3 — •Hiran Kankanamge[1], Susanne Susanne[2,1,3], and Anna Grünebohm[1] — [1]Scale-bridging simulations of functional composites, Interdisciplinary Centre For Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Universitätsstr. 150, 44801 Bochum, Germany — [2]Applied Quantum Materials, Institute for Energy and Materials Processes (EMPI), Faculty of Engineering, University of Duisburg*Essen, Forsthausweg 2, 47057 Duisburg, Germany — [3]Research Center Future Energy Materials and Systems (RC FEMS), University of Duisburg*Essen, Forsthausweg 2, 47057 Duisburg, Germany

Mixed molybdenum-tungsten oxides offer tunable electrochromic and catalytic properties [1]. Pure WO_3 exhibits several polymorphs separated by only a few meV·atom^{-1} [2], leaving the structural trends in $Mo_xW_{1-x}O_3$ insufficiently resolved. As a baseline for substitution, we use first-principles calculations to reassess the stability of the main WO_3 polymorphs and recover the characteristic low-energy grouping of the β, γ, and ε phases.

Building on these optimized structures, the focus of this work is to introduce molybdenum across all phases and trace how composition modifies the energy landscape, octahedral tilting, and relative phase preferences. The resulting trends are compared with experimental observations on mixed Mo-W oxides [1] to evaluate their consistency and refine the microscopic picture of phase competition within the Mo-W-O system.

[1] H.-J. Lunk and H. Hartl, ChemTexts 9, 5 (2023).
[2] H. Hamdi et al., Phys. Rev. B 94, 245124 (2016).

FM 11.20 Tue 18:00 P4

Mechanistic Origin of Charge Separation and Enhanced Photocatalytic Activity in D-π-A-Functionalized UiO-66-NH_2 MOFs — •Anastasiia Kultaeva[1], Timur Biktagirov[2], Volodymyr Vasylkovskyi[1], Andreas Sperlich[1], Eugenio Otal[3], Wolf Gero Schmidt[2], and Vladimir Dyakonov[1] — [1]Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany — [2]Physics Department, Paderborn University, D-33098 Paderborn, Germany — [3]Institute for Aqua Regeneration, Shinshu University, Nagano 380-8553, Japan

Donor-π-acceptor (D-π-A) functionalization of MOF linkers offers a promising route to enhance visible-light photocatalysis, yet the underlying photophysical mechanisms remain insufficiently resolved. Here we investigate UiO-66-NH_2 modified via diazo coupling with anisole, diphenylamine (DPA), and N,N-dimethylaniline (NNDMA) dyes. Optical measurements and first-principles calculations show that all donor groups introduce new occupied states near the valence-band edge, enabling dye-to-framework charge transfer and red-shifted absorption. EPR and transient photoluminescence reveal that anisole uniquely promotes efficient intersystem crossing to a long-lived triplet charge-transfer state, whereas bulkier donors such as DPA and NNDMA can also generate defect-associated traps that enhance recombination. These results clarify how donor structure dictates electronic-state formation, triplet pathways, and defect behavior, providing mechanistic guidelines for tailoring charge dynamics and photocatalytic activity in D-π-A-modified MOFs.

FM 11.21 Tue 18:00 P4

Isovalent exchange of Al, Mg and Zr in strontium hexagallate ($SrGa_{12}O_{19}$) — •Finn Bietz[1], Christian Rhode[2], and Simone Sanna[1,3] — [1]Institut für Theoretische Physik, Justus-Liebig-Universität Gießen, Gießen 35392, Germany — [2]Leibniz Institut für Kristallzüchtung, Max Born Straße 2, 12489 Berlin — [3]Center for Materials Research (ZfM), Justus Liebig University Gießen, Gießen 35392, Germany

Strontium hexagallate ($SrGa_{12}O_{19}$) can be used as a substrate for the growth of barium hexaferrite ($BaFe_{12}O_{19}$), a ferrimagnetic and a quantum paraelectric material. The lattice parameters of $SrGa_{12}O_{19}$ can be adjusted by substitution of Ga by Al or Mg and Zr, respectively, for the lattice-matched growth and strain engineering of ($BaFe_{12}O_{19}$) thin films. Unfortunately, a microscopic picture of the doping mechanisms, as well as of their effect on the lattice parameters, is still missing. In this contribution, we report on first-principles calculations performed to determine the lattice site of Al, Mg and Zr atoms in the $SrGa_{12}O_{19}$ structure, and support corresponding experiments performed at the IKZ in Berlin. Thereby the defect formation energies of Al, Mg and Zr atoms incorporated in the dilute limit at different lattice sites were calculated within density functional theory (DFT). The atomistic models reveal that Mg populates the so called $Ga^{(3)}$ position, Al prefers the $Ga^{(1)}$ site, but also populates the $Ga^{(4)}$ and $Ga^{(5)}$ sites, and that the Zr is incorporated at the $Ga^{(4)}$ site. A substitution at the Sr site is energetically unfavorable for all dopants, instead. The calculated formation energies are in good agreement with the experimental results.

FM 11.22 Tue 18:00 P4

Ferroelectric domain shapes in LiNbO3 and LiTaO3 from a revised Ising model — •Jonas Paul[1], Leonard Verhoff[2], and Simone Sanna[1] — [1]Justus-Liebig-Universität Giessen, Giessen, Germany — [2]Technische Universität Wien, Wien, Austria

Lithium niobate (LN) and lithium tantalate (LT) are both ferroelectric materials whose domains can be influenced by external electric fields. While both crystal-

lize within the same symmetry group (R3c), congruent LN and LT form different domain shapes as experimentally observed [1]. DFT calculations could explain the domain shapes of LN and LT via calculations of the domain wall energy [2], however, knowledge about build-up of domain shapes in mixed lithium niobate-tantalate (LNT) mixed crystals is still lacking.

In this contribution, we demonstrate that the domain build-up in LNT can be modeled with a modified Ising model and performed Monte Carlo and Greedy calculations to simulate the domain growth. We show that an additional interaction term in the Ising model determines the characteristic domain shape. Furthermore, we employ Greedy simulations for different parameters, obtaining a phase diagram for the domain shape transition. In consequence, we predict domain shapes for LN, LT, and LNT mixed crystals.

[1] D. A. Scrymgeour et al., Phys. Rev. B 71, 184110 (2005)
[2] D. Lee et al., Aplied Physics Letter 98, 092903 (2011)

FM 11.23 Tue 18:00 P4

Reversible nanoscale patterning of WTe_2 with a scanning tunneling microscope — •Kevin Hauser[1,2], Danyang Liu[1], Berk Zengin[1], Jens Oppliger[1], Samuel Mañas-Valero[4], Catherine Witteveen[5], Fabian O. von Rohr[5], Jennifer E. Hoffman[2,3], and Fabian D. Natterer[1] — [1]Department of Physics, University of Zurich, Switzerland — [2]Department of Physics, Harvard University, Cambridge MA, USA — [3]School of Engineering & Applied Sciences, Harvard University, Cambridge MA, USA — [4]Instituto de Ciencia Molecular, Universitat de València, Spain — [5]Department of Quantum Matter Physics, University of Geneva, Switzerland

Manipulating the lattice structure of quantum materials that host ferroelectric or Weyl semimetal phases provides a route to control these states on nanometer length scales. Prior experiments on the type-II Weyl semimetal candidate WTe_2 have demonstrated ferroelectric switching on micrometer length scales and transient control of the predicted topological phase via ultrafast excitations. However, both approaches lack the ability to induce persistent, localized distortions on the nanometer scale. In this contribution, we use current pulses applied by a scanning tunneling microscope (STM) to write, move, and erase nanoscale lattice distortions on WTe_2. The resulting lattice distortions consist of picometer-scale in-plane and out-of-plane atomic displacements, accompanied by changes in the local density of states. The in-plane shifts are on the same order of magnitude as expected for ferroelectric switching. These results demonstrate local, reversible control of the lattice structure of WTe_2 on nanometer length scales.

FM 11.24 Tue 18:00 P4

Phase and microstructure evolution of SnO_x:Ta thin films as a function of the oxygen partial pressure during deposition — Cecilia Bauden[1], Lukas Prager[1], Frans Munnik[1], Fabian Ganss[1], Harish Parala[2], Anjana Devi[2], Carlos Romero-Muniz[3], Ramon Escobar-Galindo[3], and •Matthias Krause[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]IFW Dresden, Dresden, Germany — [3]Universidad de Sevilla, Sevilla, Spain

Recent research on SnO_2-based TCOs has focused on Ta-doped SnO_2 (TTO), since it surpasses In_2O_3:Sn and ZnO:Al in thermal stability under vacuum and in air [1, 2]. This work presents a Raman spectroscopy and XRD study on the phase and microstructure evolution of SnO_x:Ta thin films as a function of the oxygen partial pressure during thin film deposition by reactive DC magnetron sputtering. At low O_2 flow rates a phase structure comprising metallic β-Sn, SnO and Sn_3O_4 without incorporated Ta is found. Higher O_2 flow rates yield the formation of the rutile structure of SnO_2:Ta, where Ta replaces Sn as Ta_{Sn} and transfers free charge carriers into the Sn 5s* conduction band [3]. A resistivity minimum of 1.3 x 10^{-3} Ω cm, a maximum mobility 16 $cm^2\ (Vs)^{-1}$, and a distinct reflectivity edge in the NIR were found for the films with the best transport properties.

[1] F. Lungwitz et al., SolMat 196, 84-93 (2019); [2] M. Krause et al., J. Mat. Chem. A 11, 17686-17698 (2023); [3] M. Krause et al., J. Mat. Chem. A 13, 15128-15139 (2025).

FM 11.25 Tue 18:00 P4

Controlled synthesis of the magnetic topological insulator $MnSb_2Te_4$ with variable Curie temperature — •Laura Zeni Cunha[1], Laura T. Corredor[2,3], Anja U.B. Wolter[4], and Anna Isaeva[1,2,3] — [1]University of Amsterdam, The Netherlands — [2]TU Dortmund University, Germany — [3]Research Center Future Energy Materials and Systems, Germany — [4]Leibniz IFW Dresden, Germany

Magnetic topological materials $(MnX_2Te_4)(X_2Te_3)_n$ are promising candidates for spintronic and energy-efficient technologies.[1] $MnSb_2Te_4$ features tunable Mn content that enables optimization of the magnetic ground state and ordering temperature[2-4] - key requirements for potential applications. However, synthetic control over Mn stoichiometry remains to be fully harnessed. This work presents a controlled, rapid, and reproducible synthesis route to phase-pure $MnSb_2Te_4$ by using an optimized tellurium precursor. I investigate by powder XRD, EDX/SEM, and DC magnetization studies how varied synthetic parameters impact its structural and magnetic properties. I observe an increased stability range of ferrimagnetic $MnSb_2Te_4$ compared with Ref. [2], and demonstrate a clear correlation between synthesis conditions and the Tc, spanning more than 10 K across the samples. This insight into synthesis-structure-property relationship advance our goal of a topological ferromagnet with higher Tc, moving toward the quantum anomalous Hall effect at practical temperatures.

[1] Nat. Sci. Rev. 11 (2024), nwad282; [2] Phys. Rev. X 11 (2021), 021033; [3] Mater. Today Phys. 38 (2023), 101265; [4] Chem. Mater. 37 (2025), 1446-1456.

FM 11.26 Tue 18:00 P4

Simulation-based optimization of gain characteristics for 3D-nanoprinted microchannel plates — •Kamila Murat, Kristian Deneke, Robert Zierold, Stefanie Haugg, and Robert H. Blick — Universität Hamburg, Hamburg, Germany

Microchannel plates (MCPs) are essential components for signal amplification. However, accurately modeling the complex electron multiplication processes represents one of the most demanding challenges.

Direct laser writing (DLW) techniques enable enhanced design freedom that extends beyond conventional glass-drawn MCPs, allowing the fabrication of structures with diverse materials and complex geometries. Since experimentally iterating such printed structures is both time-consuming and costly, numerical methods become crucial for development.

However, existing theoretical descriptions of electron multiplication remain incomplete and probabilistic, which presents a significant challenge for accurate simulations. To address this, we employ a finite-element-based simulation framework in COMSOL Multiphysics to model the electrostatic fields and electron transport in a 480 μm-long, 12 μm-diameter MCP channel biased at 1000 V. Within this configuration we investigate how geometry, bias voltage, and incidence energy influence electron trajectories and the total gain. To model the underlying electron avalanche mechanism driven by secondary electron emission (SEE), different theoretical models are evaluated to analyze the material-dependent SEE parameters. The resulting workflow establishes a scalable basis for extensions of the model.

FM 11.27 Tue 18:00 P4

Polarons in $LiNb_{1-x}Ta_xO_3$ solid solutions on both sides of the Curie temperature — •Christa Fink-Bauer and Simone Sanna — Institute for Theoretical Physics, Justus-Liebig-University, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

Polaronic defects in LN, LT and their solid solutions $LiNb_{1-x}Ta_xO_3$ are important to understand their (electrical) conductivity. We do not only model these defects in the low-temperature ferroelectric phase, which is of great interest due to its spontaneous polarization leading to special properties as piezoelectricity, photoelasticity or nonlinear optical response, but also model the high-temprature paraelectric phase, which is stable above the Curie temperature and is of relevance for high-temperature applications. We calculate defect levels in the electronic band gap to extract activation energies for electronic transport. In addition, we calculate formation energies in pure LN and LT and their solid solutions, all from first principles using density-functional theory as implemented in VASP [1, 2]. [1] G. Kresse, J. Furthmüller, Computational Materials Science 6, 15 (1996). [2] G. Kresse, J. Furthmüller, Phys. Rev. B 54, 11169 (1996).

FM 11.28 Tue 18:00 P4

Local nanoscale probing of electron spins using NV centers in diamond — •Sergei Trofimov[1], Christos Thessalonikios[1], Victor Deinhart[2,3], Alexander Spyrantis[2], Lucas Tsunaki[1], Kseniia Volkova[1], Katja Höflich[2], and Boris Naydenov[1] — [1]Berlin Joint EPR Laboratory and Department Spins in Energy Conversion and Quantum Information Science (ASPIN), Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Leibniz-Institut für Höchstfrequenztechnik, Ferdinand-Braun-Institut (FBH), Berlin, Germany — [3]Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, Berlin, Germany

Substitutional nitrogen atoms in a diamond crystal (P1 centers) are crucial for creation of nitrogen-vacancy (NV) centers. However, P1's electron spin generates paramagnetic noise that degrades the NV's performance by shortening its coherence time. Bulk characterization methods of nitrogen concentration based on optical absorption or electron paramagnetic resonance often overlook local variations in the nitrogen content. In this work, we use a helium ion microscope to fabricate nanoscale NV center ensembles at predefined sites with a nano-scale resolution in a diamond crystal containing low concentrations of nitrogen. We then utilize these NV-based probes to measure the local P1 concentration on the level of 230 ppb using the double electron-electron resonance (DEER) technique. Moreover, by comparing the DEER spectra with numerical simulations, we determined the concentration of other unknown paramagnetic defects created during the ion implantation to be up to 15 ppb depending on the implantation dose.

FM 11.29 Tue 18:00 P4

Plug-and-play modification of a scanning electron microscope with a secondary electron yield detector — •Kristian Deneke[1], Stefanie Haugg[1], Isabel González Díaz-Palacio[2], Marc Wenskat[1,3], Wolfgang Hillert[2], Bent Andersen[1], Robert Zierold[1], and Robert Blick[1,3] — [1]Center for Hybrid Nanostructures, University of Hamburg, Germany — [2]Institute of Experimental Physics, University of Hamburg, Germany — [3]Deutsches Elektron-Synchrotron (DESY), Hamburg, Germany

Secondary electrons are already detected and used to achieve image contrast in a scanning electron microscope (SEM). However, measuring the secondary electron yield (SEY) requires a detector configuration that goes beyond the standard features of an SEM. The SEY is an important figure of merit for many different applications and research fields such as electron multipliers, vacuum cavities, and spacecrafts. Therefore, we present a plug-and-play configuration that allows an existing SEM to be modified with an SEY detector. This detector unit enables SEY measurements of conductive and insulating thin films in a pulsed operation mode. Furthermore, planar thin films can be examined not only at normal incidence, but also at an angle of inclination of the primary electrons, allowing for angular-dependent SEY characterization. Finally, the integration of our detector unit within an SEM enables the recording of a 2D SEY map, visualizing structural variations of patterned substrates. This detector setup could increase accessibility of SEY measurements and pave the way to improvements of applications and new measurement techniques.

FM 11.30 Tue 18:00 P4

A high-temperature optical spectroscopy study of congruent $LiTaO_3$ — •Ludmila Eisner[1], Angélique Hoffmann[2], Ani Manucharyan[2], Sebastian Inckemann[2], Yuriy Suhak[1], Steffen Ganschow[2], Holger Fritze[1], and Klaus.-D. Becker[3] — [1]Clausthal University of Technology, Germany — [2]Leibniz-Institut für Kristallzüchtung, Germany — [3]Technische Universität Braunschweig, Germany

Spectroscopic studies of congruent lithium tantalate (cLT) were performed to analyze the optical absorption edge under different thermal treatments in air and to relate its changes to band gap variations with temperature. At room temperature, the material exhibits an absorption edge near 4.45 eV. Thermal measurements, extending up to 900°C, show a systematic shift of about 0.138 eV toward lower photon energies per 100 K with increasing temperature. The treatments at reducing conditions (Ar/5% H_2) were found to induce significant changes in the spectra after cooling down to room temperature. These spectra show the formation of extended absorption tails down to photon energies of about 2.5 eV. This may suggest enhanced occupation or reconfiguration of intrinsic defect states, including polaronic states, vacancies, and antisite-related centers. These spectral changes largely evade observation under high-temperature in-situ conditions due to the redshift of the absorption edge. Comparison of spectra recorded after thermal cycling shows partial reversibility of these defect-related features. The present results provide a picture of how temperature and reduction-induced defect chemistry impact the optical response of cLT.

FM 11.31 Tue 18:00 P4

Analysing the laser-driven tetragonal-to-cubic phase-transition in ferroelectric $BaTiO_3$ using EXAFS spectroscopy as a local probe — •Janosch Tasto[1], Rajdwip Bhar[1], Simon Rauls[1], Marco Reinhard[2], Dimosthenis Sokaras[2], Uwe Bovensiepen[1], and Heiko Wende[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen — [2]SLAC National Accelerator Laboratory, Stanford University

This work aims to establish time-resolved Extended X-ray Absorption Fine Structure (tr-EXAFS) spectroscopy as a methodology for solids where the structural information of the EXAFS is combined with a pump-probe setup to study local dynamic lattice processes in the time domain.

As a proof of concept, we analyze the structural cubic-to-tetragonal phase-transition in the ferroelectric perovskite $BaTiO_3$. The coexistence of displacive and order-disorder phenomena accompanying this transition is a topic of debate in the literature on this extensively studied material.Difference-EXAFS scans at the Ti K-edge and the Ba L_3-edge between the pumped and unpumped state provide a direct way to investigate changes in lattice-structure and thermal-induced disorder in the vicinity of the absorbing atom. We correlate our spectroscopic findings with *ab initio* multiple-scattering calculations using the FEFF10 code to quantify structural dynamics.

We thank the Deutsche Forschungsgemeinschaft (in the framework of the Collaborative Research Center 1242) for financial support.

FM 11.32 Tue 18:00 P4

Correlation between grain size and dielectric properties in medium entropy titanate-based perovskite oxides — Amirhosein Paryab, •Doru Lupascu, and Vladimir Shvartsman — Institut für Materialwissenschaft Universität Duisburg-Essen Essen, Germany

High-entropy perovskite oxides have attracted significant attention as promising materials for energy storage applications. The configurational entropy is modulated by substituting different elements at a specific ionic site. If it is in the range of 0.7R-1.6R or above 1.6R, the oxides are called medium-entropy or high-entropy, respectively. We report a study of the influence of the synthesis method on the structure, dielectric, and ferroelectric properties of medium entropy titanate-based perovskite oxides (Ba0.34Sr0.33Ca0.33)TiO3 and (Ba0.25Sr0.25Ca0.25Pb0.25)TiO3. Compared to the solid state method, the sol-gel derived materials have a smaller grain size and higher lattice strain. This results in a more diffuse phase transition and a significant shift in the Curie temperature by 60 and 10 K in (Ba0.34Sr0.33Ca0.33)TiO3 and (Ba0.25Sr0.25Ca0.25Pb0.25)TiO3, respectively. Furthermore, fine grained samples were found to exhibit broader polarization hysteresis loops that could be ascribed to higher barriers to dipole switching and the pinning effect. The interplay of configuration entropy, microstructure, and functional behavior is analyzed.

FM 11.33 Tue 18:00 P4

Characterization and Fabrication of Silicon Wave Guides for the Study of Quantum Material Properties — •Sierra Randall Heinrich[1,2], Sebastian Zafra Koch[1,2], Florian Spickmann[1,2], Murat Sivis[1,2], Claus Ropers[1,2], and Hannes Böckmann[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]University of Göttingen, 4th Physical Institute, Göttingen, Germany

Placing quantum materials into optical cavities promises active control of material properties and functionality. Low-dimensional systems are particularly susceptible and exhibit electronic phases that can be switched by an external stimulus. However, the required extreme light-matter coupling is hampered by intrinsic cavity losses and poor overlap with optical modes. Here, we work towards the integration of a prototypic Peierls insulator at the surface of a silicon waveguide resonator. This project focuses on the creation of the resonator. A resonator couples the light into the sample by always totally internally reflecting it, thus generating the evanescent fields used in light matter coupling. To couple the light into the wafer, the angle of reflection has to be controllable. Here, we used diffraction gratings etched onto the surface with varying periods to achieve this. Next, we used Fabry-Pérot interference to maximize the effect of the evanescent fields. As a result, the resonance conditions of a 25 micrometer thick wafer were observed and accurately predicted for the first four resonance peaks. The two aspects of this project will be combined in future, with etched diffraction gratings on a thin wafer.

FM 11.34 Tue 18:00 P4

Understanding the formation of metal-semiconductor contacts in ferroelectric p-type oxides — •Ailu Sackey[1], Ruben Dragland[1], Egil Tokle[1], Zewu Yan[2,3], Edith Bourret[2], Jan Schultheiss[1], Mario Hentschel[4], and Dennis Meier[1,5] — [1]NTNU, Trondheim, Norway — [2]Lawrence Berkeley National Laboratory, Berkeley, CA, USA — [3]ETH Zurich, Zürich, Switzerland — [4]University of Stuttgart, Stuttgart, Germany — [5]University of Duisburg-Essen, Duisburg, Germany

Ferroelectric semiconductors exhibit highly tunable electronic responses, opening new pathways for nanoelectronics beyond Si-based approaches. Of particular interest are functional properties that arise at internal interfaces in ferroelectrics, such as domain walls or phase boundaries, which, when leveraged, can serve as ultra-small active elements or as extended 3D networks, requiring a thorough understanding of the contacts used for current injection and sensing.

Here we investigate metal-semiconductor contacts formed by deposited electrodes on the surface of the model p-type ferroelectric $ErMnO_3$. By cation doping and O_2 annealing, we methodically modify the charge carrier distribution and monitor the related changes. We find that donor doping promotes ohmic contact formation, whereas annealing in O_2-rich atmospheres leads to Schottky-like barriers. The results align with expected Fermi-level shifts and band-bending phenomena described by traditional semiconductor physics. Our findings offer fundamental guidance for controlling the contact formation in hexagonal manganites and related p-type ferroelectric semiconductors.

FM 11.35 Tue 18:00 P4

Energy Profile and Hopping Barriers for Small Electron Polarons at Ferroelectric Domain Walls in Bismuth Ferrite from First Principles — •Sabine Körbel — Friedrich Schiller University Jena, Germany

Evidence from first-principles calculations indicates that excess electrons in $BiFeO_3$ form small polarons with energy levels deep inside the electronic band gap. Hence, n-type electronic transport could occur by polaron hopping rather than by band-like transport. Here, using first-principles calculations, small electron polaron hopping in $BiFeO_3$ is investigated. Both bulk $BiFeO_3$ and a typical ferroelectric domain wall, the neutral 71° domain wall, are considered to account for experimental observations of electrical conductivity at domain walls in otherwise insulating ferroelectrics. The object of this study is to shed light on electron conduction in $BiFeO_3$ and the influence of pristine neutral ferroelectric domain walls. The computed energy barriers for small electron polaron hopping are near 0.2 eV, similar to other perovskite oxides, both in the bulk and within the neutral 71° domain wall. Trapping energies of small electron polarons at the three prevalent domain walls, the 71°, the 109°, and the 180° wall, are determined. The domain walls are two-dimensional traps for small electron polarons, with a trap

depth of about twice the thermal energy at room temperature. Based on these findings, the n-type mobility and the diffusion constant in $BiFeO_3$ are estimated, and experimental conductivity data for $BiFeO_3$ are discussed.

FM 11.36 Tue 18:00 P4

Smart DNA lithography as a tool for nanoelectronics — •Raufar Shameem[1], Charlotte Kielar[1], Christoph Hadlich[2], Borja Rodriguez-Barea[1], Ralf Seidel[2], and Artur Erbe[1] — [1]Institute of Ion Beam Physics and Materials Research, HZDR, Dresden, Germany — [2]Peter Debye Institute for Soft Matter Physics, University of Leipzig, Leipzig, Germany

Precise nanoscale patterning enables geometry-dependent functions across electrical, optical, and magnetic systems. DNA-templated hybrid lithography employs programmable molecular templates to define complex nanoscale shapes. Here, we use long DNA origami structures in a workflow integrating self-assembly, selective bottom-up oxide growth, and conventional top-down processing. The origami patterns form durable stencil masks on sapphire, guiding etching and metal deposition to create nanowire geometries beyond optical lithography. To generate these masks, DNA origami is assembled on sacrificial silicon, followed by controlled SiOx growth via chemical vapor deposition. Removing the DNA exposes nanowire-like and cavity-like oxide features that accurately reproduce the origami geometry and serve as robust patterning masks. AFM, SEM, and FIB cross sections verify shape transfer, growth behavior, and patterning resolution. This approach extends DNA-assisted lithography toward clean, versatile metal architectures for geometry-sensitive applications. It also improves integration with existing fabrication by providing stable masks, reliable shape transfer, and added flexibility in designing nanoscale features.

FM 11.37 Tue 18:00 P4

Theory-Guided Discovery of Ion-Exchanged Poly(heptazine Imide) Photocatalysts Using First-Principles Many-Body Perturbation Theory — •Zahra Hajiahmadi and Thomas D. Kühne — CASUS - Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf e.V. (HZDR), Untermarkt 20, D-02826 Görlitz, Germany

Poly(heptazine imides) (PHI) show strong promise in photocatalysis, but limited control over electronic properties continues to constrain their full potential. We modulated PHI's photocatalytic activity to overcome this limitation by incorporating mono-, di-, and trivalent metal cations into its framework. To elucidate the underlying mechanisms, we employed calculations based on many-body perturbation theory, a highly accurate approach for electronic structure calculations that provides improved accuracy in quasiparticle energy predictions compared to conventional density functional theory, particularly for band gaps and excitonic properties. Our analysis identifies several metal-doped PHI systems with electronic structures well suited for hydrogen and oxygen evolution, CO_2 reduction, and H_2O_2 production. Guided by these theoretical insights, we synthesized a subset of *M*-PHI materials (where *M* is either K, Na, Li, Ca, Mg, or Zn) predicted to enhance photocatalytic reactivity.

FM 11.38 Tue 18:00 P4

Soft X-ray Spectroscopy at the HESEB Beamline, SESAME — •Ahlam Farhan — SESAME, Allan, Jordan

The ID11-L Helmholtz-SESAME Soft X-ray Beamline (HESEB) represents a significant step forward in soft X-ray research infrastructure in the Middle East. Operating in the 70-2000 eV energy range, HESEB provides photon fluxes between 10-3404 Giga photons/s, with an energy resolution exceeding $E/\Delta E >$ 8000. The beamline delivers a focused spot size of 500*250μm and offers tunable circular polarisation, enabling precise investigations of the electronic and magnetic properties of a wide range of materials.

The X-ray absorption spectroscopy (XAS) end station is equipped with a motorised manipulator, magnetic sample holders, and a differential pumping system, allowing measurements under ambient conditions or in a helium atmosphere. This flexibility supports the study of vacuum-sensitive materials, including valuable cultural heritage samples.

Recent XAS and XMCD measurements demonstrate HESEB's excellent stability, high resolution, and precise polarisation control, establishing it as a versatile platform for soft X-ray spectroscopy and magnetic materials research at SESAME.

FM 12: German-French Focus Session: Materials Research in Polar Oxides – From Domain Engineering to Photonic and Electronic Devices I

chair: Simone Sanna (Justus-Liebig-Universität Gießen, DE)

The focus session is dedicated to bridge the gap between materials research in polar oxides and research fields that apply those materials, such as nonlinear and quantum optics, electronics or sensoring, spanning experimental studies and first-principles simulations.

Time: Wednesday 9:30–13:00 Location: BEY/0138

Invited Talk FM 12.1 Wed 9:30 BEY/0138

Shedding Light on Polar Topological Textures — •Salia Cherifi-Hertel — CNRS and University of Strasbourg, IPCMS

The study of topological polarization textures in ferroelectric materials represents a rapidly evolving frontier in ferroic research, with implications for solitonic information technologies and emergent phenomena in correlated oxides. Complex configurations, such as non-Ising and chiral domain walls, bubble domains, (anti)vortices, and polar (anti)skyrmions, highlight the diversity of polarization states in low-dimensional systems, where symmetry breaking, strain, and electrostatic boundary conditions produce novel functionalities. While piezoresponse force and transmission electron microscopies remain central to nanoscale characterization, optical methods are emerging as powerful, noninvasive alternatives. Second-harmonic generation (SHG) microscopy, in particular, provides intrinsic sensitivity to symmetry and polarization orientation, enabling three-dimensional mapping of polar architectures. This presentation will outline recent advances in SHG polarimetry combined with machine-learning-assisted analysis, enabling rapid, quantitative reconstruction of 3D polarization textures. This integrated approach offers a robust framework for probing polar topologies and uncovering the intricate coupling between structure, symmetry, and functionality in ferroic materials.

FM 12.2 Wed 10:00 BEY/0138

Origin and Evolution of Domain-Wall Conductivity in LiNbO3 — •Iuliia Kiseleva[1], Boris Koppitz[1], Matthias Roeper[1], Elke Beyreuther[1], Samuel Seddon[1], and Lukas Eng[1,2] — [1]Institute of Applied Physics, Technische Universität Dresden, Nöthnitzer Straße 61, Dresden, 01187, Germany — [2]ct.qmat: Dresden-Würzburg Cluster of Excellence - EXC 2147, TU Dresden

Ferroelectric domain walls, which effectively serve as two-dimensional interfaces, exhibit functionalities markedly distinct from those of the bulk, such as enhanced conductivity and strong coupling to external fields, making them promising for nanoelectronic applications. Among various systems, lithium niobate (LiNbO3) stands out due to its high Curie temperature, chemical stability, and thoroughly characterized bulk properties. Yet the microscopic origins and dynamic evolution of domain-wall conductivity remain insufficiently understood, largely due to limited in-situ, time-resolved characterization. Here, we combine in-situ second-harmonic-generation (SHG) microscopy with electrical transport measurements and complementary chemical analysis to investigate domain-wall behavior under controlled electric and mechanical loading. This multimodal approach enables real-time visualization of domain restructuring, correlation of conductivity changes with wall inclination, and the dynamics of defects. The results aim to advance the understanding of functional domain-wall states and the mechanism of electrical transport in ferroelectric 2D systems.

FM 12.3 Wed 10:15 BEY/0138

Persistent photoconductivity in reduced lithium niobate bidomain crystals — •Philipp Fahler-Muenzer, Marios Hadjimichael, Ana Sanchez-Fuentes, Richard Beanland, Eoin Moynihan, and Marin Alexe — University of Warwick, Coventry, United Kingdom

The uniaxial ferroelectric lithium niobate ($LiNbO_3$) can exhibit significantly enhanced domain wall (DW) conductivity, rendering it an interesting system for DW-based nanoelectronics. Specifically, head-to-head (h2h) DWs exhibit conductivities several orders of magnitude higher than that of the surrounding bulk. We create h2h DWs with a near-90° inclination angle by using the diffusion annealing technique, followed by chemical treatment to change the functional properties. The characterization of the structure and morphology is conducted by piezoresponse force microscopy and transmission electron microscopy. To characterize electronic transport, we use resistivity measurements under varying temperatures in dark or under UV light illumination, complemented by conductive atomic force microscopy. Our findings indicate only transient conductivity at the DWs, but substantial differences in photoconductivity between monodomain and bidomain crystals, with persistent photoconductivity in crystals with DWs. Furthermore, we report a drastic drop in domain wall photoconductivity upon heating above 80°C, which can be explained by the emptying of charge carrier traps in the DW as the system gains higher thermal energy.

FM 12.4 Wed 10:30 BEY/0138

Photocurrent-based recognition in time-series tasks using reservoir computing — •Yan-Meng Chong[1], Atreya Majumdar[2], Ingvild Hansen[1], Karin Everschor-Sitte[2], and Dennis Meier[1,2,3] — [1]Department of Materials Science and Engineering, Norwegian University of Science and Technology (NTNU), Trondheim, Norway — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [3]Research Center Future Energy Materials and Systems, Research Alliance Ruhr, Bochum, Germany.

In reservoir computing, input data are mapped into higher dimensional space, translating non-linear problems into linearly solvable ones. In general, any physical system that possesses non-linearity, complexity, short-term memory, and reproducibility can serve as reservoir. Here, we investigate the ferroelectric semiconductor $ErMnO_3$ as a potential candidate material for reservoir computing. We show that the system displays pronounced non-linear changes in photocurrent under varying light intensity. The response can be tuned by changing the metal-semiconductor contacts (Schottky- or Ohmic-like behavior) used for readout, determining the timescale on which the photocurrent vanishes after illumination. This relaxation behavior in the OFF state gives fading memory. We perform training on variations in the output (photocurrent), which allows for recognition in time-series tasks. Interestingly, ferroelectric domain walls can also be used as reservoirs with characteristic photocurrent signals, giving new opportunities to down-scale or enhance the complexity of physical reservoirs.

Coffee break

FM 12.5 Wed 11:00 BEY/0138

Properties of Charged Interfaces in Uniaxial Ferroelectrics — •Conor McCluskey, Kristina Holsgrove, Andrew Rogers, James Dalzell, Ronan Lynch, Raymond McQuaid, Tchavdar Todorov, and Marty Gregg — Queen's University Belfast, United Kingdom

When the polarisations of neighbouring ferroelectric domains abut, a bound charge develops at the interface. Often, these charged domain walls show enhanced electrical conductivity, which is typically taken as a sign that the polar divergence is fully screened by the mobile transport carriers. Transport measurements, however, suggest the carrier densities associated with domain wall conductivity lie well below that expected for a fully screened ferroelectric bound charge. In fact, some charged domain walls lack enhanced conductivity entirely. In these cases, polar rotation occurs to fully avoid the development of bound charge, leading to topological patterns in the polarisation field. Here, we discuss the interfaces formed between thermally bonded lithium niobate single crystals generated with intentional head-to-head character. We show that the interfaces formed uniquely host both of these properties: enhanced conductivity, and a striking array of polarisation vortices. Furthermore, since this interface is formed by thermal bonding of two crystalline structures, there is freedom to introduce relative lattice twists between the two parent crystals, which is unavailable at regular domain walls within a single parent crystal. We will discuss the interplay of strain and electrostatics at these unique interfaces in the context of their emergent functionality.

FM 12.6 Wed 11:15 BEY/0138

Polar Discontinuities, Emergent Conductivity, and Critical Twist-Angle-Dependent Behaviour at Wafer-Bonded Ferroelectric Interfaces — Andrew Rodgers[1], Kristina Holsgrove[1], Conor McClusky[1], Samuel Seddon[2], Marty Gregg[1], and •Lukas M. Eng[2,3] — [1]Centre for Quantum Materials and Technologies, School of Mathematics and Physics, Queen's University Belfast, UK — [2]Institut für Angewandte Physik (IAP)- Nöthnitzer Str. 61, 01187 Dresden — [3]ct.qmat: Dresden-Würzburg Cluster of Excellence*EXC 2147, TU Dresden, Germany

Probing novel properties, arising from twisted interfaces, has traditionally relied on the stacking of exfoliated 2D materials and the spontaneous formation of van der Waals (vdW) bonds. So far, investigations involving intimate covalent or ionic bonds have not been a focus. Yet, we show here that an established technique, involving thermocompressional wafer bonding, works well for creating twisted non-vdW interfaces. We have successfully bonded z-cut lithium niobate single crystals to create ferroelectric oxide interfaces with strong polar discontinuities and have mapped the associated emergent interfacial conductivity. In some instances, a dramatic change in microstructure occurs, involving local dipolar switching. A twist-induced collapse in the capability of the system to effectively screen interfacial bound charge is implied. Importantly, this only occurs around specific moiré twist angles with sparse coincident lattices and associated short-range aperiodicity. In quasicrystals, aperiodicity is known to induce pseudo-bandgaps and we suspect a similar phenomenon here.

FM 12.7 Wed 11:30 BEY/0138

Machine learned potential for ferroelectric heterostructure BaTiO3/SrTiO3 — •Lan-Tien Hsu[1], Jonathan Schmidt[2], Aaron Iten[2], Nicola Spaldin[2], and Anna Grünebohm[1] — [1]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Faculty of Physics and Astronomy, and Center for Interface-Dominated High Performance Materials (ZGH), Ruhr-University Bochum, Germany — [2]Department of Materials, ETH Zürich, Zürich, CH-8093, Switzerland

Ferroelectric heterostructures offer a platform to realize topological patterns with functionalities relevant to future electronic devices.[1] While short-range machine-learned interatomic potentials can capture ferroelectric instabilities in pure materials, long-range dipole interactions remain essential for heterostructures, where depolarizing field plays a role.[2] We address this challenge by combining MACE message-passing networks with a latent Ewald-summation scheme[3] capable of learning long-range interactions and inferring Born effective charges without explicit training on response properties. The model predicts transition temperature and spontaneous polarization of $BaTiO_3$ in close agreement with experiments. It further captures the multidomain formed in heterostructures, consistent with coarse-grained effective-Hamiltonian results, and generalizes well to untrained configurations, including those containing oxygen vacancies.

[1] Das *et al*, Nature **568**, 368-372 (2019)
[2] Yu *et al*, Phys. Rev. B **112**, 104324 (2025)
[3] Zhong *et al*, 10.48550/arXiv.2504.05169

FM 12.8 Wed 11:45 BEY/0138

From Stacking Faults to Field-Stabilized Polarity: Connecting RP Phases and the MFP Phase in $SrTiO_3$ — •Christian Ludt[1,2], Hartmut Stöcker[1,2], Matthias Zschornak[1,2,3], and Dirk C. Meyer[1,2] — [1]TU Bergakademie Freiberg, 09599 Freiberg, Germany — [2]Zentrum für Effiziente Hochtemperatur-Stoffwandlung, 09599 Freiberg, Germany — [3]Hochschule für Technik und Wirtschaft Dresden, 01069 Dresden, Germany

Polar functionalities in perovskites often arise from a subtle interplay between lattice distortions, defect chemistry, and stacking faults. In this work, particular attention is given to the migration-induced field-stabilized polar (MFP) phase in $SrTiO_3$, a recently identified polar state that arises from field-driven oxygen mobility and picometer-scale cation displacements. To provide a structural framework for understanding and enhancing this phenomenon, the electronic properties of Ruddlesden-Popper-type (RP) stacking faults in $SrO(SrTiO_3)_n$ are analyzed using density functional theory. These faults introduce symmetry breaking, modified lattice environments and characteristic changes in the electronic structure that closely resemble the local conditions required to form the MFP phase. By combining insights from RP-layered configurations with the field- and defect-driven mechanisms underlying MFP formation, a unified perspective emerges in which stacking faults act as natural templates that support, amplify, or localize MFP-like polar distortions. This connection highlights new pathways for engineering polar responses and optoelectronic functionalities in complex perovskite oxides.

Coffee Break

FM 12.9 Wed 12:15 BEY/0138

Integration of imprint-free and low coercivity ferroelectric $BaTiO_3$ thin films on silicon — Jingtian Zhao[1,2], Majid Ahmadi[1,2], Beatriz Noheda[1,2], and •Martin F. Sarott[1,2] — [1]Zernike Institute for Advanced Materials, University of Groningen, The Netherlands — [2]Groningen Cognitive Systems and Materials Center (CogniGron), University of Groningen, The Netherlands

Highly-crystalline ferroelectric oxides integrated on Si hold great promise for energy-efficient memory and logic technologies. Exploiting epitaxial strain engineering in these materials is, however, severely hampered on Si, where the large structural mismatch often results in an inferior interfacial quality and causes a degradation of the ferroelectric switching characteristics. In this work, we present the growth of single-crystalline $BaTiO_3$ thin films on Si, exhibiting imprint-free switching, low coercivity, high remanent polarization, and no fatigue for over 10^{10} switching cycles. We accomplish this via the insertion of a $SrSn_{1-x}Ti_xO_3$ layer on $SrTiO_3$-buffered Si. This layer serves as a pseudo substrate that alleviates the *thermal strain* that the Si substrates imposes on the $BaTiO_3$ layer, while simultaneously providing moderate compressive strain that stabilizes a pure out-of-plane polarization. Thus, our work paves the way toward the fabrication of Si-compatible, low-power-consuming ferroelectric devices for non-volatile memory applications.

FM 12.10 Wed 12:30 BEY/0138

Polarity and polarons in WO_3 through epitaxial shear strain — •Ewout van der Veer[1], Martin Sarott[1,2], Jack Eckstein[3,5], Stijn Feringa[1], Dennis van der Veen[1], Johanna van Gent González[1], Majid Ahmadi[1,2], Horatio Cox[1,2], Ellen Kiens[4], Gertjan Koster[4], Bart Kooi[1,2], Michael Carpenter[3], Ekhard Salje[3], and Beatriz Noheda[1,2] — [1]ZIAM, Uni. of Groningen, Netherlands (E. vd V. now: Fac. of Phys., UDE, Duisburg, Germany and RC FEMS, Bochum, Germany) — [2]CogniGron, Uni. of Groningen, Netherlands — [3]Dept. of Earth Sci., Uni. of Cambridge, UK — [4]MESA+ Inst., Uni. of Twente, Netherlands — [5]Center for Nano. Mater. Sci., ORNL, USA

Tungsten oxides have been investigated for gas sensing, catalytic and electrochromic capabilities. Epitaxial thin films of WO_3 on (110)-oriented $YAlO_3$

even exhibit piezoelectricity and conductivity at monoclinic twin walls due to local strain gradients. We grew epitaxial films of WO_3 on (001)$YAlO_3$ by pulsed laser deposition and reveal a previously unreported polar phase by imposing epitaxial shear strain, stabilizing a triclinic structure up to large film thicknesses and elevated temperatures. The films have periodic in-plane domains with needle bifurcations and enhanced conductivity at domain walls. STEM shows that these walls exhibit a reduction of a structural distortion, evidence for recently predicted anti-distortive polarons. Our films are structurally and functionally different from known bulk phases and previous epitaxial films due to subtle epitaxial interactions. They are candidates for oxide electronics, neuromorphic computing and catalysis.

FM 12.11 Wed 12:45 BEY/0138

Inducing Strain Gradients in Transition Metal Oxides using Ferroelastic Domain Patterns — •Freya Watson[1], Aditya Singh[1], Katarzyna Sopinska[1], Daniel Chaney[2], Marin Alexe[1], and Marios Hadjimichael[1] — [1]University of Warwick, Coventry, United Kingdom — [2]ESRF, avenue des Martyrs, 38043 Grenoble Cedex 9, France

Strain engineering is a powerful tool for accessing new and versatile properties of materials. The use of ferroelectric domain patterns instead of conventional substrates further allows for the modification of the properties of these materials using electric fields. $PbTiO_3$ is a ferroelectric and ferroelastic perovskite which forms a periodic in-plane and out-of-plane domain structure when deposited on (110)-$DyScO_3$ substrates, caused by lattice mismatch. In this work, we explore inducing strain gradients in metallic perovskite thin films grown on this $PbTiO_3$ domain structure. Using this approach we are able to effectively couple strain between heterostructure interfaces and produce large anisotropy in electronic transport and material properties, which are found to be tuneable by altering $PbTiO_3$ layer thickness, and thus domain period. The effects of this strain engineering are demonstrated by scanning probe techniques, microscopy imaging and 4-probe resistivity measurements.

FM 13: Topical Session: Dislocations in Functional Materials I (joint session MM/FM)

Time: Wednesday 10:15–11:30 Location: SCH/A251

See MM 23 for details of this session.

FM 14: Focus Session: Materials Research in Polar Oxides – From Domain Engineering to Photonic and Electronic Devices II

chair: Conor McCluskey (Queen's University Belfast, UK)

The focus session is dedicated to bridge the gap between materials research in polar oxides and research fields that apply those materials, such as nonlinear and quantum optics, electronics or sensoring, spanning experimental studies and first-principles simulations.

Time: Wednesday 15:00–16:00 Location: BEY/0138

FM 14.1 Wed 15:00 BEY/0138

Probing ferroelastic domain properties of lanthanum aluminate via spontaneous Raman scattering — •Robin Buschbeck[1], Susanne C. Kehr[1], Lukas M. Eng[1,2], and Samuel D. Seddon[1] — [1]TU Dresden, Institute of Applied Physics, Nöthnitzer Strasse 61, 01187 Dresden, Germany — [2]ct.qmat: Dresden-Würzburg Cluster of Excellence EXC 2147, TU Dresden, 01062 Dresden, Germany

Lanthanum aluminate ($LaAlO_3$, LAO) is a rhombohedrally distorted oxide perovskite, exhibiting ferroelastic twinning at room temperature. Frequently employed as a thin film substrate [1], it is often overlooked [2] for being optically uniaxial and thus birefringent. The effect of the ferroelastic twins sees an in-plane rotation of this optical axis, with regions of opposing optical axes coexisting (delineated by twin walls).

Here, we present a detailed experimental analysis of LAO(100) using spontaneous Raman scattering (SR). SR is a widely employed technique for obtaining spectral information from a broad range of materials [3]. Using SR, we demonstrate several spatially resolved non-trivial, three-dimensional intrinsic properties of LAO. Special attention is given to the different LAO(100) domains and their behaviour under various SR measurement conditions, including polarization-dependent and spatially resolved in-plane or depth-dependent measurements.

[1] R. W. Simon et al., Springer, Boston, MA (1989)
[2] S. Kustov, et al., Applied Physics Letters 112, 042902 (2018)
[3] A. Orlando et al., Chemosensors 9, 262 (2021)

FM 14.2 Wed 15:15 BEY/0138

Strain Driven Ferroelastic Switching and Barkhausen Type Behavior in $LaAlO_3$ — •Vladyslav Kovtunovych, Matthias Roeper, Lukas M. Eng, and Samuel D. Seddon — Institut für Angewandte Physik (IAP)- Nöthnitzer Str. 61, 01187 Dresden

Lanthanum aluminate ($LaAlO_3$; LAO) is an oxide perovskite widely used in nano-electronics, and frequently employed as a thin-film substrate therein due to its convienient lattice match to many multiferroic and/or ferroelectric materials. Although oftentimes overlooked, LAO is an improper ferroelastic, posessing crystallographic domains delineated by twin walls, responding to the global application to strain akin to ferromagnetic or ferroelectric materials to magnetic or electric fields respectively. This study focuses on twin wall motion, which was induced and recorded using a commercial Razorbill strain cell with a high-resolution capacitive sensor. Measurements of $LaAlO_3$ under increasing uniaxial compression, revealed the expected jerky domain wall motion indicative of Barkhausen noise, the stochastic stepped reordering of local ordering parameters common among all ferroic materials. This scale invariant physics acts as a power law governing all length scales, from avalanches on mountains down to the nanoscale. Complementary XRD measurements of the expected Bragg peak splitting are correlated with polarised light microscopy imaging all as a function of lattice strain, to observe this effect in a whole new light.

FM 14.3 Wed 15:30 BEY/0138

Single crystal growth of stoichiometric lithium tantalate — •Sebastian Inckemann, Roberts Blukis, Angélique Hoffmann, Matthias Bickermann, and Steffen Ganschow — Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, 12489 Berlin, Germany

A material isomorphous to the intensively investigated lithium niobate (LiNbO3, LN) that has the same inherent non-stoichiometry is lithium tantalate (LiTaO3, LT). Despite similar characteristics to LN, the properties of LT are significantly less studied, even though there are notable differences that favor the use of LT in certain applications. Of special interest is the investigation of stoichiometric LT (sLT) compared to congruent LT (cLT), as the lithium deficiency in cLT causes a high concentration of defects (Kim et al., 2001). Literature describes multiple methods to achieve stoichiometric LN single crystals, exemplary via the double crucible method. However, the growth method reporting a crystal composition closest to the stoichiometric ratio is the growth via the flux method (Polgár et al., 2002). Due to the similarities between LN and LT an analogous approach is the most promising, with the use of K_2O as a solvent showing the best results in the case of LN (Polgár et al., 1997). To ensure an efficient single crystal growth in this system, knowledge about the Li_2O-K_2O-Ta_2O_5 phase diagram is vital (Mühlberg et al., 2008). As there is no literature regarding this phase diagram, this presentation will present our current progress by combining DTA, PXRD and SEM measurements. Furthermore, results regarding the single crystal sLT growth attempts will be presented.

FM 14.4 Wed 15:45 BEY/0138

Poling and acoustic characterization of near-stoichiometric $Li(Nb,Ta)O_3$ crystals — •Éva Tichy-Rács[1], Stepan Hurskyy[1], Steffen Ganschow[2], Fatima El Azzouzi[1], Holger Fritze[1], and Yuri Suhak[1] — [1]Clausthal University of Technology, Goslar, Germany — [2]Leibniz Institut für Kristallzüchtung, Berlin, Germany

$Li(Nb,Ta)O_3$ solid solutions bridge the high Curie temperature of $LiNbO_3$ and the thermal stability of $LiTaO_3$, while maintaining a strong piezoelectric performance, making them attractive for high-temperature sensing and actuation. The

intrinsic properties of $LiNbO_3$, $LiTaO_3$ and, consequently, their $Li(Nb,Ta)O_3$ solid solutions are well known to be highly sensitive to lithium stoichiometry. In the present work the acoustic properties of near-stoichiometric $LiNb_{1-x}Ta_xO_3$ (x=0; 0.45; 1) single crystals are investigated as a function of temperature and time by resonant piezoelectric spectroscopy. The near-stoichiometric compositions were obtained by the vapor transport equilibration (VTE). Subsequently, the samples were electrically poled to ensure a single-domain state. The study shows that acoustic losses in nsLT remain in the range of 10^{-4}–10^{-3} up to 620 °C, i.e., within the ferroelectric phase, and increase monotonically with temperature, though only weakly, with an activation energy of about 0.05 eV. In contrast, nsLN and nsLNT45 exhibit a pronounced loss increase above 600 °C, attributed to the conductivity-related relaxation mechanism. Under constant operation at 600 °C for 350 h, all samples demonstrate excellent long-term stability, with resonance frequency deviations not exceeding ± 100 ppm of the initial value.

FM 15: Nanoscale Probing of Functional Properties

chair: Jiali He (Norwegian University of Science and Technology, Norway)

Time: Wednesday 15:00–15:45 Location: BEY/0E40

FM 15.1 Wed 15:00 BEY/0E40

Nanoscale Phonon Dynamics Studied In-Situ by Laser Stimulated Vibrational Electron Energy-Gain Spectroscopy — •Mairi McCauley[1,2], Joel Martis[3], Ondrej Krivanek[3], Ben Plotkin-Swing[3], Tolga Wagner[1,2], Hüseyin Çelik[1,4], Grigory Kornilov[1], Katrina Coogan[1,2], Meng Zhao[1,2], Andreas Mittelberger[3], Matthias Meffert[5], Luca Piazza[5], Tracy Lovejoy[3], Guillaume Radtke[6], Christoph Koch[1,2], and Benedikt Haas[1,2] — [1]Department of Physics, Humboldt-Universität zu Berlin, Berlin, Germany — [2]Center for the Science of Materials Berlin, Humboldt-Universität zu Berlin, Berlin, Germany — [3]Bruker AXS LLC, Kirkland, WA, USA — [4]Institute for Physics and Astronomy, Technische Universität Berlin, Berlin, Germany — [5]DECTRIS AG, Baden-Daettwil, Switzerland — [6]Sorbonne Université, CNRS UMR 7590, MNHN, IMPMC, Paris, France

Advances in instrumentation allow to directly probe phonon dispersions at the nanoscale using electron energy gain and loss spectroscopy (EEGS/EELS) within a scanning transmission electron microscope (STEM). By integrating a laser injection system, we enable the investigation of stimulated phonons at the spatial resolution determined by the electron beam. A synchronised laser-detector configuration enables nanosecond-scale time-resolved measurements. The thermal conductivity of amorphous carbon and silicon nitride was investigated by local time-resolved temperature measurements and is compared to numerical simulations. Ongoing work applies the system to study phonon transport through defects and interfaces at atomic resolution.

FM 15.2 Wed 15:15 BEY/0E40

Photoluminescence Spectroscopy of Platinum (II) and Palladium (II) Dimers in Organic Molecular Single Crystals Under Pressure — Paul Steeger[1], Tobias Theiss[2], Dominik Schwab[3], Ivan Maisuls[2], •Vedhanth Senthiappan Vellaiappan Uthayasurian[1], Robert Schmidt[1], Ilya Kupenko[4], Carmen Sanchez Valle[4], Steffen Michaelis de Vasconcellos[1], Nikos L. Doltsinis[3], Cristian A. Strassert[2], and Rudolf Bratschitsch[1] — [1]Institute of Physics, University of Münster — [2]Institut für Anorganische und Analytische Chemie, University of Münster — [3]Institute of Solid State Theory, University of Münster — [4]Institute of Mineralogy, University of Münster

Cyclometalated transition-metal complexes are promising for applications ranging from bioimaging to light-emitting diodes. We investigate two tailored biscyclometalated Pd(II) and Pt(II) complexes, which feature ligands that promote head-to-tail dimer formation to enable interactions between their metal centers [1]. We prepare molecular single crystals and apply hydrostatic pressure with a diamond anvil cell in the GPa range [2]. The photoluminescence shows a prominent redshift under pressure. Density functional theory calculations link this effect to a reduced metal-metal distance. Importantly, the observed mechanochromism is reversible, which holds the promise for pressure sensing and optical storage applications. References: [1] T. Theiss et al., J. Am. Chem. Soc. 145, 3937 (2023), [2] P. Steeger et al., Nano Lett. 25, 2628 (2025)

FM 15.3 Wed 15:30 BEY/0E40

A novel Approach to parametrize a ferroelectric Phase-Field Model from atomistic Simulation Data — •Frank Wendler[1], Dilshod Durdiev[2], Xuejian Wang[1], Hikaru Azuma[3], Takahiro Tsuzuki[3], Tomohiro Ogawa[3], Ryo Kobayashi[3], Masayuki Uraganase[4], Shuji Ogata[3], and Michael Zaiser[1] — [1]Institute of Materials Simulation, FAU Erlangen-Nürnberg, Dr.-Mack-Str. 77, 90762 Fürth, Germany — [2]Division Mechanics of Functional Materials, TU Darmstadt, Germany — [3]Physical Science and Engineering Department, Nagoya Institute of Technology, Japan — [4]RIKEN Center for Biosystems Dynamics Research, Japan

Based on molecular dynamics simulations using a core-shell potential for polarization switching in ferroelectric BaTiO3 (BTO) with and without vacancy defects, a parametrization framework for phase-field simulations is established. Crucial material properties such as elastic and piezoelectric tensor components, kinetic coefficients, as well as domain wall characteristics are extracted from the MD results to adjust the anisotropic gradient energy. The 6th order Landau polynomial coefficients are derived from statistical analysis of polarization switching data, including the activation parameters for BTO that govern domain nucleation. The proposed energy landscape favours polarization switching in two subsequent 90° steps over 180° switching, which was observed experimentally and in recent MD simulations. The method is important for phase-field simulations of domain nucleation and domain wall motion in presence of point defects carrying mono- or dipolar electric fields as well as elastic strain fields.

FM 16: Topical Session: Dislocations in Functional Materials II (joint session MM/FM)

Time: Wednesday 15:45–17:15 Location: SCH/A251

See MM 27 for details of this session.

FM 17: Highlighted Talk: Piled higher, probed deeper: X-ray insights into ferroelectric devices (Martina Müller)

Chair: Anna Grühnebohm (Ruhr-Universität Bochum), Jan Schultheiß (NTNU Trondheim)

Time: Thursday 9:30–10:00 Location: BEY/0138

Invited Talk FM 17.1 Thu 9:30 BEY/0138

Piled higher, probed deeper: X-ray insights into ferroelectric devices — •Martina Müller — Fachbereich Physik, Universität Konstanz

In ferroelectrics, the nothing is mighty: The key to shaping the ferroelectric functionalities of oxide/nitride materials and devices lies in the tunability of their oxygen/nitrogen sublattice, particularly their defect structure. While dopants and vacancies are a key aspect of emerging ferroelectricity in HfO_2 and AlScN, their detection is much more subtle than that of atomic properties. This is because the experimental observation of e.g. oxygen vacancies means the detection of something absent. This requires access to indirect signatures, which often are of very low intensity and located within a device structure - a combination of experimental conditions that are challenging to meet in practice.

This talk presents recent advances in the expertise required to detect defects and dopants related ferroelectric functionality in HfO_2 and AlScN using synchrotron radiation. Bulk-sensitive hard X-ray photoelectron spectroscopy (HAXPES) enables the non-destructive depth profiling of heterostructures, revealing spectroscopic fingerprints also in subtle core-level signatures. Performing HAXPES 'in operando' is a powerful tool for determining the band alignment and chemical state of interfaces under operating conditions of real-world ferroelectric devices.

FM 18: German-French Focus Session: (Anti)ferroic states – ferroelectrics, ferroelastics and antiferroelectrics II

chair: Elzbieta Gradauskaite (CNRS/Thales, FR)

This focus session explores recent advances in understanding and control of (anti)ferroic states. Emphasis will be placed on theoretical modelling, advanced characterization techniques, and the engineering of emergent properties for use in nano-electronic devices. The session aims to bridge fundamental research with emerging device-relevant functionalities, bringing together experimental, and theoretical perspectives on ferroic materials.

Time: Thursday 10:15–12:45 Location: BEY/0138

Invited Talk FM 18.1 Thu 10:15 BEY/0138

Stabilizing antiferroelectricity in PbZrO3 thin films using epitaxial tensile strain — •Vincent Garcia — Laboratoire Albert Fert, CNRS, Thales, Univ. Paris-Saclay, France

The antiferroelectric nature of lead zirconate, the historical and most studied antiferroelectric material, has recently been challenged. Progress in atomic-level characterization using aberration-corrected scanning transmission electron microscopy (STEM) has revealed the complex nature of polar textures in PbZrO3. In single crystals, ferrielectric phases have been detected, while in PbZrO3 epitaxial films, thickness reduction engenders competition among antiferroelectric, ferrielectric and ferroelectric phases. All studies so far on PbZrO3 films have utilized commercially-available oxide single crystals with large compressive lattice mismatch, causing the films to undergo strain relaxation within a few nanometres. Interestingly, first principles calculations have predicted that tensile strain can stabilize antiferroelectricity down to the nanometre scale. Here we use tensile strain imposed by artificial substrates of LaLuO3 to stabilize a pure antiferroelectric phase in epitaxial ultrathin films of PbZrO3. Sharp double hysteresis loops of polarization vs electric field in these PbZrO3-based capacitors show zero remanent polarization, and atomic scale mapping of polar displacements using STEM reveals the characteristic antipolar pattern of the Pbam phase in film thicknesses down to 9 nanometres. These results highlight the critical role of coherent epitaxial strain in the phase stability of PbZrO3.

Invited Talk FM 18.2 Thu 10:45 BEY/0138

Strain effects in free-standing membranes of antiferroelectric Lead Zirconate — •Umair Saeed[1,2], Huazhang Zhang[3,4], David Pesquera[1], Philippe Ghosez[3], Nini Pryds[5], Jose Santiso[1], Felip Sandiumenge[6], and Gustau Catalan[1,7] — [1]ICN2, Catalonia — [2]UAB, Spain — [3]ULiège, Belgium — [4]WUT, China — [5]DTU, Denmark — [6]ICMAB, Catalonia — [7]ICREA, Catalonia

Antiferroelectrics like PbZrO3 (PZO) exhibit reversible switching between antiferroelectric and ferroelectric phases. However, complex energy landscape of PZO and few lattice matching substrates render strain engineering challenging. In this context, free-standing membranes provide a unique opportunity for strain tuning due to their flexibility.

We studied PZO membrane capacitors under homogeneous in-plane strain applied via bending, observing that the hysteresis decreases under in-plane compression and increases under tension. The results suggest that the changes in the switching behavior originate from the modification of energy barriers between the phases under the influence of strain rather than the energies of the phases. Molecular dynamic simulations show that this response depends on crystallographic directions of strain and electric field.

In wrinkled stand-alone PZO membranes, on the other hand, high strain gradients induce flexoelectric effects, leading to non-canonical antiferroelectric-like ordering under tensile and ferroelectric phases under compressive strain, highlighting strain as a tool to control PZO functionalities.

FM 18.3 Thu 11:15 BEY/0138

Strain induced ferroelastic twin-domain dynamics in lanthanum aluminate — •Matthias Roeper[1], Robin Buschbeck[1], Jakob Wetzel[1], Lukas M. Eng[1,2], and Samuel D. Seddon[1] — [1]Institute of Applied Physics, TU Dresden, Nöthnitzer Strasse 61, 01187 Dresden, Germany — [2]ct.qmat: Dresden-Würzburg Cluster of Excellence - EXC 2147, TU Dresden, 01062 Dresden, Germany

Over the last decades scientific attention of the oxide perovskite lanthanum aluminate ($LaAlO_3$) has turned (due to the absence of ferroelectric contributions) from originally only an active interfacial substrate material into a model system of ferroelastic twin domain walls. Our new results explore ferroelastic twin-domain dynamics induced by the controlled application of uniaxial strain in single crystalline samples. The domains are spacially resolved by Atomic Force Microscopy and μ-Raman Spectroscopy as a function of applied strain, as well as structural analysis by X-ray diffraction. All experimental investigations are complemented by density functional perturbation theory calculations.

FM 18.4 Thu 11:30 BEY/0138

MD data-driven physics-informed neural network for multi-scale modelling of ferroelectric: parameter identification and field reconstruction — •Xuejian Wang[1], Frank Wendler[1], Hikaru Auzuma[2], and Shuji Ogata[2] — [1]Institute of Materials Simulation, Department of Materials Science and Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg, Fürth, Germany — [2]Graduate School of Engineering, Nagoya Institute of Technology, Nagoya, Japan

A persistent challenge in multiscale ferroelectric modeling is connecting atomistic information with continuum phase-field descriptions. Here, we develop a PINN framework driven by MD polarization data. The loss function combines supervised fitting of MD-derived polarization fields with physics-based residuals of the steady-state phase-field PDEs. Minimizing the total loss enables the network to reconstruct polarization, strain, stress, and electric field distributions, while simultaneously identifying key phase-field parameters, including characteristic energy and length scales, gradient anisotropy, and Landau coefficients. Using these PINN-identified parameters in COMSOL reproduces ferroelectric domain structures and their electromechanical responses with high fidelity. This approach provides an efficient route to establishing atomistic-to-continuum links and inferring physical properties directly from polarization configurations.

FM 18.5 Thu 11:45 BEY/0138

Evidence of ferroelectricity in epitaxially strained tungsten trioxide thin films — •Nives Strkalj[1,2], Zhuotong Sun[1], Ming Xiao[1], Ziyi Yuan[1], Xuan T. Nguyen[1], Simon M. Fairclough[1], Caterina Ducati[1], Giuliana Di Martino[1], and Judith L. MacManus-Driscoll[1] — [1]University of Cambridge, UK — [2]Institute of Physics, Zagreb, Croatia

Ferroelectric films offer a promising path to faster, more energy-efficient CMOS technologies. Here, we report the deposition of epitaxial tungsten trioxide films at temperatures below 400°C using atmospheric pressure spatial chemical vapour deposition. In these films, epitaxial strain imposed by the substrate promotes the formation of the low-temperature polar phase at room temperatures, evidenced by x-ray diffraction, scanning transmission electron microscopy, piezoresponse force measurements, and Raman spectroscopy. Exploring ferroelectricity in ultrathin tungsten trioxide films could provide a new platform for polarization-controlled electronic and optical applications.

FM 18.6 Thu 12:00 BEY/0138

Investigating metallicity in layered Carpy-Galy ferroelectrics through topotactic transformation. — •Lilia Huynh[1], Marko Kuvezdic[1], Dongxin Zhang[1], Annouk Goossens[1], Luis Moreno[1], Alexandre Gloter[2], Lucia Iglesias[1], Manuel Bibes[1], and Elzbieta Gradauskaite[1] — [1]Laboratoire Albert Fert, Palaiseau, France — [2]Laboratoire de Physique du Solide, Orsay, France

Combining seemingly incompatible properties within a single material can yield unconventional functionalities. For instance, polar metals host inversion-symmetry breaking displacements despite finite metallicity. However, they remain scarce, as conventional ferroelectricity usually relies on orbital rehybridization and gets suppressed by free charge carriers. Here, we report the epitaxial stabilization of the layered Carpy-Galy ferroelectric $Sr_2Nb_2O_7$ ($A_nB_nO_{3n+2}$, $n = 4$), which exhibits a geometric in-plane polarization driven by collective octahedral rotations. These films can be successfully transformed into the metallic perovskite $SrNbO_3$ through a topotactic interfacial reduction mediated by an Al overlayer, which drives oxygen-vacancy migration and electron doping. This redox-engineering route enables fine, continuous and even reversible tuning of oxygen stoichiometry, allowing us to stabilize intermediate $Sr_2Nb_2O_{7-x}$ phases, as confirmed by XRD, XPS, STEM, and transport measurements. In contrast to bottom-up synthesis of polar metals, this top-down strategy provides fine control of metallicity in a geometric ferroelectric host and opens avenues for exploring charge- and spin-transport phenomena in polar metals.

FM 18.7 Thu 12:15 BEY/0138

Dynamical tuning of the depletion region at a single ferroelectric domain wall — •Jiali He[1], Ruben Dragland[1], Jan Schultheiss[1], Zewu Yan[2,3], Edith Bourret[3], and Dennis Meier[4] — [1]NTNU, Norway — [2]ETH Zurich, Switzerland — [3]LBNL, USA — [4]University of Duisburg-Essen, Germany

Ferroelectric domain walls (DWs) are promising building blocks for future nanoelectronics, combining ultra-small feature size with emergent device-relevant behaviors. Most studies so far focused on bulk crystals and thin films, where the measured response reflects convoluted contributions from, e.g., the hidden subsurface wall structures and the networks they form. The intrinsic behavior of individual DWs thus often remains unclear. In my talk, I will present the extraction of a single insulating ferroelectric DW, situated in a 1-μm-thick $ErMnO_3$ lamella, mounted on a conductive back electrode. This configuration enables a well-defined top-bottom current path using an AFM tip as movable top electrode. Consistent with previous measurements on single crystals, we observe that the initially thin insulating wall (~200 nm electronic width) transforms under applied bias into a narrow conductive core surrounded by a broad asymmetric depletion region, leading to a fivefold increase in apparent wall width. Systematic bias variation demonstrates a highly tunable electronic wall width, manifesting as voltage-controlled expansion and contraction of the depletion region. The results corroborate that functional DW properties known from crystals are transferable to nano-structured device-relevant systems, revealing new possibilities for electronic signal control.

FM 18.8 Thu 12:30 BEY/0138

Hybrid antiferroelectric-ferroelectric-ferroelastic domain walls in non-collinear antipolar oxides — •Ivan N. Ushakov[1], Mats Topstad[1], Muhammad Z. Khalid[1], Niyorjyoti Sharma[2], Christoph Grams[3], Ursula Ludacka[1], Jiali He[1], Kasper Hunnestad[1], Mohsen Sadeqi-Moqadam[1], Julia Glaum[1], Sverre M. Selbach[1], Joachim Hemberger[3], Petra Becker[3], Ladislav Bohatý[3], Amit Kumar[2], Jorge Íñiguez-González[4,5], Antonius T.J. van Helvoort[1], and Dennis Meier[1,6] — [1]NTNU, Trondheim — [2]QUB, Belfast — [3]University of Cologne — [4]LIST, Luxembourg — [5]University of Luxembourg — [6]University of Duisburg-Essen

Antiferroelectrics are emerging as advanced functional materials and are fertile ground for unusual electric effects. Here, we demonstrate how antiferroelectricity induces noncollinearity in dipolar order and establish it as an additional degree of freedom, unlocking physical nanoscale properties that are symmetry-forbidden in classical antiferroelectrics. We show that antiferroelectrically driven noncollinear order of electric dipole moments in $K_3[Nb_3O_6|(BO_3)_2]$ leads to a coexistence of antiferroelectric and ferroelectric behaviors. Besides the double-hysteresis loop observed in antiferroelectrics, a pronounced piezoresponse and electrically switchable hybrid domains are observed, forming atomically sharp and micrometer long charged domain walls with inseparably entangled antiferroelectric and ferroelectric properties. Hybrid antiferroelectric-ferroelectric responses are expected in a wide range of noncollinear systems, giving a new dimension to the research on antiferroelectrics and multifunctional oxides in general.

FM 19: Advanced Microscopy and Tomography for Functional Materials

chair: Manuel Zahn (University of Augsburg)

Time: Thursday 10:15–12:45 Location: BEY/0E40

FM 19.1 Thu 10:15 BEY/0E40

Electron Beam-Induced Currents as a Quantitative Probe for Nanoscale Semiconductor Devices — •Sebastian Schneider[1], Sebastian Beckert[1], René Hammer[2], Markus König[3], Grigore Moldovan[2], Darius Pohl[1], and Bernd Rellinghaus[1] — [1]Dresden Center for Nanoanalysis (DCN), TU Dresden, Dresden, Germany — [2]Point Electronic GmbH, Halle (Saale), Germany — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Electron beam-induced current (EBIC) mapping in the scanning transmission electron microscope (STEM) enables the direct visualization of charge carrier transport with nanometer resolution. We present a comparative STEM-EBIC study on silicon photodiode lamellae prepared by gallium and xenon focused ion beam milling. The EBIC mapping reveals the p-n junction and allows for the extraction of the effective electron and hole diffusion lengths as a function of local thickness. These values are up to three orders of magnitude smaller than bulk EBIC results, highlighting strong surface recombination and preparation-induced artifacts. Complementary I-V measurements show significant deviations from the expected diode-like behavior, which we attribute to high resistive contacts at the metal-semiconductor interfaces. Our findings emphasize the critical role of sample preparation for quantitative EBIC analysis.

Financial support by the DFG through TRR 404, project no. 528378584, is gratefully acknowledged.

FM 19.2 Thu 10:30 BEY/0E40

X-ray Stress Tensor Tomography — •Peter Modregger[1,2], Ahmar Khaliq[1,2], and Felix Wittwer[1,2] — [1]Physics Department, University of Siegen — [2]Center for X-ray and Nano science, CXNS, DESY, Hamburg

The possibility for tomographic reconstrution of strain and stress tensor present in poly-crystalline samples has been discussed for nearly two decades. We will demonstrate the successful retrieval of all 6 strain/stress tensor components in martensitic steel samples from experimental data acquired at the ID11 beamline of the ESRF. Compared to established techniques this novel approach for the depth-resolved determination of stress states offers the tantalizing advantages of a simple experimental setup, isotropic gauge volumes and faster scans. In our presentation, we will discuss the possible adverse effects of detector parallax and crystallographic texture. Further, we will provide specific experimental requirements such as the required photon flux or the available scattering angles. With these in mind, we have achieved a strain sensitivity of 10^{-4} and a stress sensitivity of 20 MPa.

FM 19.3 Thu 10:45 BEY/0E40

Developing a resuable optical fiber-based sensing system for in-situ X-ray radiaiton monitoring — Ali Karatutlu[1,2], Esra Kendir Tekgül[2], Zehra Gizem Mutlay[1], Andriy Budnyk[1], Gianluca Iori[3,4], Philipp Hans[5], Fareeha Hameed[5], and •Bülend Ortaç[1] — [1]Bilkent University, Institute of Materials Science Nanotechnology and National Nanotechnology Research Center (UNAM), Ankara, 06800 Turkey — [2]Sivas University of Science and Technology, Department of Engineering Basic Sciences, Sivas, 58100 Turkey — [3]Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland — [4]GratXray, Villigen, Switzerland — [5]Synchrotron-light for Experimental Science and Applications in the Middle East (SESAME), Allan, 19252, Jordan

Specialty optical fibers doped with rare-earths such as Yb, and Tm are utilized for various applications from medical to high-power beam delivery for materials processing. Nevertheless, radiation-induced defects can occur due to irradiation, causing a degradation of beam quality. In this study, we utilize this type of degradation, referred to as radiation-induced attenuation, as an X-ray sensing and the conditions in the in-situ recovery of color centers. The experiments were conducted at hard X-ray beamline at BEATS, SESAME, using different monochromatic beams such as 10 keV and 20 keV, suggesting the origin of color centers playing role in the RIA and the sensing and recovery behavior that are related to the optical and morphological effects of the X-ray irradiation.

FM 19.4 Thu 11:00 BEY/0E40

Multiscale characterization of porous carbon fibers — •Markus Löffler[1], Mohsen Sadeghi Bogar[2,3], Paul Bertram[3,4], Jan Wolf[2,3], Darius Pohl[1], Thomas Behnisch[2,3], Iris Kruppke[3,4], Chokri Cherif[3,4], Maik Gude[2,3], and Bernd Rellinghaus[1] — [1]Dresden Center for Nanoanalysis (DCN), cfaed, TUD Dresden University of Technology (TUD), Dresden, Germany — [2]Institute of Lightweight Engineering and Polymer Technology (ILK), TUD, Dresden, Germany — [3]Research Center Carbon Fibers Saxony, TUD, Dresden, Germany — [4]Institute of Textile Machinery and High Performance Material Technology (ITM), TUD, Dresden, Germany

Porous carbon fibers (PCF) are valued for structural energy storage because they combine low density, high thermal and electrical conductivity, low thermal expansion, strong mechanical properties, and a large specific surface area. Key pore features - volume, shape, and connectivity - determine their suitability for use as electrodes in batteries, supercapacitors, and as structural materials. A hierarchical pore structure with sizes from 2 nm to over 50 nm is desirable. These PCFs are made by wet-spinning polyacrylonitrile (PAN) with nanocellulose as a pore-forming additive, followed by electron beam irradiation, stabilization, and carbonization. To understand how processing affects pore development, fibers are analyzed at various stages and scales using submicro-XCT, FIB, SEM, and TEM. All fibers show a low density of large pores, while precursor and irradiated fibers also have a high density of nanoscale pores.

FM 19.5 Thu 11:15 BEY/0E40

Tomographic Electron Holography reveals 3D-Potential Variations from Surface Segregation in p-n doped InGaAs Nanowires — •Kai-Luis Jakob[1], Laura Niermann[1], Tore Niermann[1], Frederik Otto[1], Rahel Specht[1], Daniel Wolf[2], Esmaielpour Hamidreza[3], Gregor Koblmüller[1], and Michael Lehmann[1] — [1]TU Berlin — [2]IFW Dresden — [3]TU München

Mapping the three-dimensional electrostatic potential distribution at the nanoscale is crucial for tuning the electrical properties of semiconductor nanostructures, such as InGaAs nanowires utilized in optoelectronics. Off-axis electron holography enables measurement of the projected electrostatic potential

with nanoscale spatial resolution; however, the 3D information typically remains inaccessible. In this work, we combine electron holography with tomography to reconstruct 3D potentials, thereby investigating subtle effects such as surface segregation, Fermi-level pinning, and damages induced by Focused Ion Beam preparation. Here, we focus on MBE-grown InGaAs nanowires featuring an axial p-n junction. A tilt series of holograms is acquired over a wide tilt range in a FEI Titan 80-300 TEM. Projected electrostatic potentials are reconstructed individually and aligned for tomographic reconstruction. This approach allows us to access the electrostatic potential and resolve both axial and radial changes from the wire core to its surface. We observed a largely constant potential step across the axial p-n junction of 0.5 V, however, near-surface regions exhibited deviations from it. At the surface of the n-doped segment, we found a thin p-type layer, likely attributable to known surface segregation.

Coffee break

FM 19.6 Thu 11:45 BEY/0E40

Advanced Polymer-Tungsten Nanocomposites for Radiation Shielding and X-ray Computed Tomography Applications — Taylan BAŞKAN[1], Saliha MUTLU[2,3], Bülend ORTAÇ[3], Ali KARATUTLU[3,4], Sevil SAVAŞKAN YILMAZ[2,3], and •Ahmet Hakan YILMAZ[1] — [1]Karadeniz Technical University Physics Department, Trabzon, 61080, Türkiye — [2]Karadeniz Technical University Chemistry Department, Trabzon, 61080, Türkiye — [3]National Nanotechnology Research Center (UNAM) and Institute of Materials Science Nanotechnology, Bilkent University, Ankara, 06800, Türkiye — [4]Sivas University of Science and Technology, Department of Engineering Basic Sciences, Sivas, 58100 Turkey

The growing trend of ionizing radiation in biomedicine and industry has intensified the need for efficient and reliable radiation shielding materials. In our current work, we incorporated W nanoparticles and WO3 nanoparticles with varying proportions in the PMSQ polymer to synthesize dual-functional nanocomposites with simultaneous gamma ray shielding and contrast enhancement in computed tomography imaging. This study will present the three-dimensional micro-evolutions of biodegraded polymer-metal/polymer-metal oxide composite materials using synchrotron-based X-ray computed tomography methods upon post γ-radiolysis exposure from 0.5 kGy to 5 kGy. The synchrotron-based XCT available at BEATs in SESAME demonstrates the internal structural defects and morphology non-destructively in the vicinity of resolved micro-scales with 650 nm resolution.

FM 19.7 Thu 12:00 BEY/0E40

Defects in Materials: Limitations of the Trapping Model - the Influence of Corrupt Components in Positron Lifetime Spectra - cured by a New Spectrometer? — Torsten Staab, •Dominik Boras, and Danny Petschke — LCTM / IFB, Department of Chemistry, University of Wuerzburg, Roentgenring 11, D-97070 Wuerzburg, Germany

Positron lifetime spectroscopy is able to extract densities for defects (e.g. vacancies or dislocations) from the measured spectroscopic data by applying the so-called trapping model, which describes the decomposition of lifetime spectra into two or more components (lifetimes and intensities). Since the procedure of fitting several exponential decays folded by a mimicked instrumental resolution function (IRF) is a so-called ill-posed problem, the goodness of the fit relies heavily on the quality of the recorded data. By our digital twin of a positron lifetime spectrometer we could clearly see the strong influence of back scattered and corrupted coincidences on recorded spectra. Unfortunately, even by physically filtering digitised pulses, those events cannot be removed. One way to reduce their effect are changes in the geometry (90° instead of 180°) of the detector set-up leading to heavy losses in efficiency (about 90%). However, this leads to much more realistic bulk positron lifetimes of light materials (Mg, Al, Si) in accordance with calculations, and enables correct decompositions by the trapping model. We present here a new fully digitised spectrometer with an IRF described by one singe Gaussian and a FWHM of 128ps together with 22-Na sources without positronium having a single lifetime component.

FM 19.8 Thu 12:15 BEY/0E40

Characterising electron vortex beams inside crystalline materials via vorticity — •Christian Bick, Dorothee Hüser, and Tobias Klein — Physikalisch-Technische Bundesanstalt, Braunschweig, Germany

Convergent electron beams with an orbital angular momentum (OAM), also known as electron vortex beams or twisted electrons, have been investigated for multiple applications in material science. Recently, first measurements of vortex electron magnetic circular dichroism (EMCD) in the electron microscope have been reported.

We present a simulation-based study on vortex beam behaviour inside crystalline material utilising vorticity as a local property to characterise the beam. This quantity, which is widely used in fluid mechanics, can be understood as a local measure of OAM . We relate it to commonly used integrated quantities like the total OAM and channelling strength in order to further the understanding of the beams behaviour inside of model crystals and discuss possible measurements.

FM 19.9 Thu 12:30 BEY/0E40

Toward Atomic-scale Imaging of Resistive Switching Mechanisms in Prussian Blue Memristors — •Mohammed Fayis Kalady[1], Johannes Schultz[1], Michael Pohlitz[2], Falk Röder[1], Darius Pohl[3], Daniel Wolf[1], and Axel Lubk[1,4] — [1]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [2]Faculty of Physical Engineering/Computer Sciences, University of Applied Sciences, Zwickau, Germany — [3]DCN, TU Dresden, Germany — [4]IFMP, TU Dresden, Germany

Prussian blue and its analogues are promising materials for memristive devices based on resistive switching. To obtain a microscopic understanding of the structural and chemical processes responsible for switching, we employed a detailed high-resolution transmission electron microscopy (HRTEM), scanning transmission electron microscopy combined with electron energy loss and energy dispersive x-ray spectrum imaging (STEM-EELS and STEM-EDX) studies on pristine films and on films previously subjected to electrical biasing. The pristine film exhibits a homogeneous distribution of K, Fe, C, N, and O, whereas the electrically biased regions display clear nanoscale modifications, including local changes in elemental distribution and a phase transition from Prussian blue to Prussian white. The electrical measurements on the bulk reveal transitions between low-resistance and high-resistance states, demonstrating bipolar switching behavior across multiple cycles. These results provide the first steps toward in-situ TEM biasing experiments aimed at directly resolving elemental migration pathways and phase evolution under applied voltages.

FM 20: Excursion and Network-Event at Infineon Dresden AG (joint session FM/HL)

We are organizing an Excursion and Network-Event to Infineon Dresden AG.
Only for registered and selected participants.
Please register until latest February 12th here:
https://www.icams.de/news-events/events/registration-infineon/?api=561b8d7cfcb678e9f0938830d78cf979

Time: Thursday 13:30–17:00 Location: Infineon

Only for registered and selected participants.

FM 21: Members Assembly

We will elect our spokespersons, plan the programme for the coming years, and award the poster prize. This is also your opportunity to suggest topics for focus sessions, symposia, and plenary speakers for the next DPG conference!

chairs: Jan Schultheiß (NTNU, NO), Anna Grünebohm (Ruhr University Bochum, DE), FM spokespersons

Time: Thursday 18:00–18:45 Location: BEY/0138

All members of the Functional Materials Division are invited to participate.

FM 22: Focus Session: Materials Discovery III – New materials and functionalities by general principles

chairs: Hiroki Taniguchi (Nagoya University, JP), Akitoshi Nakano (Nagoya University, JP)

Discovering new functional materials is crucial to advance today's technologies, ranging from caloric cooling via catalysis to next-generation energy conversion and storage, such as thermoelectric, ferroelectric, and ionic conductor materials. New materials also form the basis for potential applications in quantum information technologies. This session provides a platform to highlight functional materials discoveries and how they come about. Notably, systematic searches with high-throughput synthesis approaches, as well as predictions from materials informatics, have helped to go beyond serendipitous discoveries in recent years. However, intuition guided by general principles remains an important factor. In this session, we particularly welcome contributions that showcase the discovery of new functional materials with original approaches. Diverse material systems - from well-established to emerging and niche classes across condensed-matter and materials physics - will be featured. Bringing together diverse discoveries in a single session will help delineate general principles and inspire future work.

Time: Friday 9:30–12:45 Location: BEY/0138

Invited Talk FM 22.1 Fri 9:30 BEY/0138

Topological thermoelectrics for solid state cooling — •Yu Pan[1] and Claudia Felser[2] — [1]Chongqing University, Chongqing, China — [2]Max Planck Institute for Chemical Physics of Solids

Thermoelectric effects enable the direct conversion between thermal energy and electrical energy, and has broad application potential in areas such as thermoelectric power generation, solid-state cooling, and precise temperature control. Classic thermoelectric materials mainly focus on heavily doped narrow bandgap semiconductor materials, whose thermoelectric performance is limited above room temperature (> 300 K). So far, further enhancement of thermoelectric performance at low temperatures (<300 K) faces significant challenges, severely restricting the application of thermoelectric materials in low-temperature solid-state cooling. In recent years, the surge of topological quantum materials has triggered many novel thermoelectric transport behaviors, especially the significantly enhanced low-temperature thermoelectric performance under magnetic fields, providing new opportunities to greatly improve low-temperature thermoelectric performance. For example, their linear-dispersion energy band structures and ultrahigh mobility significantly enhance the magneto-Seebeck effect and Nernst effect. On the other hand, topological quantum materials with broken symmetry can exhibit an anomalous Nernst thermoelectric potential far higher than that of conventional ferromagnets due to the presence of nonzero Berry curvature, laying a scientific foundation for thermoelectric applications of the anomalous Nernst effect under low or even zero magnetic fields.

FM 22.2 Fri 10:00 BEY/0138

Topological quantum materials for high performance heterogenous catalysis — •Xia Wang and Claudia Felser — Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany

The electronic structure of a catalyst plays a pivotal role in governing its performance1. Topological quantum materials, known for their symmetry-protected electronic states, offer a unique platform to bridge solid-state topology and heterogeneous catalysis. When combined with chirality, topological quantum materials give rise to novel material systems exhibiting distinct chiral phenomena, opening new avenues for the development of next-generation chiral catalysts. Situated at the interface of condensed matter physics and chemistry, the emerging field of topological catalysis exploits the exotic quantum properties of topological quantum materials to not only enhance catalytic activity and selectivity but also to enable fundamental studies of reaction mechanisms. Our recent experimental and theoretical work demonstrates a direct link between spin-orbit coupling and the kinetics of oxygen electrocatalysis, including both the oxygen reduction and evolution reactions. Furthermore, we show that external stimuli such as magnetic fields can effectively tune catalytic performance by modifying the topological features of the electronic structure. Together, these insights establish topological quantum materials as a compelling framework for designing high-performance, field-tunable catalysts, with far-reaching implications for asymmetric synthesis to probing the origins of life.

FM 22.3 Fri 10:15 BEY/0138

Ta2PdSe6: A guide towards high performance thermoelectric semimetals — •Akitoshi Nakano — Nagoya University, Nagoya, Japan

We have recently discovered that a transition-metal chalcogenide Ta2PdSe6 exhibits an extraordinary thermoelectric property despite its semimetal character. Ta2PdSe6 crystallizes in a layered structure, each layer of which consists of quasi-one-dimensional chains formed by prismatic TaSe6 and square-planner PdSe4. The thermoelectric property measured along this direction is highly exotic; an ultra-high conductivity (σ) above 10^6 Ω^-1cm^-1 is compatible with a substantial thermopower (S) of 40 μVK^-1 at 20K. As a result, the power factor (= S^2σ) reaches above 2000 μWcmK^-2, which is top level among bulk thermoelectric materials thus far.

Furthermore, we have found that the thermal conductivity of Ta2PdSe6 is relatively small (~ 100 Wm^-1K^-1) for such a good electrical conductor associated with a serious violation of the Wiedemann-Franz law. As a result, the thermoelectric figure of merit Z (= S^2$\sigma\kappa$^-1) of Ta2PdSe6 at 14 K reaches as high as 3*10^-3 (K^-1), which is comparable to Bi2Te3 at 300 K.

In the presentation, we will discuss the origin of the anomalous transport properties of Ta2PdSe6 from the viewpoint of the carrier dynamics.

FM 22.4 Fri 10:30 BEY/0138

Symmetry-Driven Transitions Between Flat Bands and Dirac Cones in Bilayer Kagome Lattices — •Taylan Gorkan — Bilkent University-UNAM

Flat bands (FBs) and Dirac cones represent two distinctive features of topological electronic systems, yet a unified mechanism enabling transitions between them has remained elusive to date. Here, we demonstrate a symmetry-governed and tunable transition from flat bands to Dirac cones in AB-stacked bilayer kagome lattices. This transition is mediated by the interplay between destructive quantum interference (DQI), C3 rotational symmetry, and spatial inversion symmetry. Strong interlayer coupling enhances DQI and stabilizes compact localized states that produce FBs, while weaker coupling allows C3 and inversion symmetries to dominate, giving rise to robust Dirac nodal points. Using a minimal tight-binding model, we map the continuous evolution of topological states-including type-II and type-III Dirac cones, spin-1 Dirac nodes, and partial flat bands-as a function of interlayer coupling. We further demonstrate this transition mechanism by examining an AB-stacked bilayer derived from the experimentally synthesized Nb3TeCl7 structure. In particular, first-principles calculations on bilayer Nb3TeCl7 reveal that vertical strain/pressure modulates interlayer interactions, enabling the entire FB-Dirac cones transition sequence. These findings establish a realistic novel pathway for gaining further insights into flat-band physics and engineering tunable topological phases in two-dimensional materials.

FM 22.5 Fri 10:45 BEY/0138

Emergent High Conductivity Transport Channel in $Bi_{12}Rh_3Ag_6I_9$ Single-Crystalline Multilayer Heterostructure — •Nicolas Perez[1], Eduardo Carrillo-Aravena[2], Christian Niclaas Saggau[1], Kornelius Nielsch[1], and Michael Ruck[2] — [1]Leibniz Institute for Solid State and Materials Research Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany — [2]Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, 01062 Dresden, Germany

$Bi_{14}Rh_3I_9$-type weak 3D topological insulators (TIs) can be seen as nano-periodic multilayer heterostructures of 2D TIs spaced by topologically trivial insulators. The newest member $Bi_{12}Rh_3Ag_6I_9$ exhibits 2D cationic conductivity in the silver iodide spacer, which allows to electrochemically adjust the Fermi level, and has the widest band gap so far in this family of compounds, 286 meV. It shows strongly increasing diamagnetism at low temperatures in a field perpendicular to the layers. Magnetoresistance measurements in macroscopic crystals reveal confinement and oscillatory behaviour, which coincides with a drastic drop in resistivity both parallel and across the layers. The observation of such an effect in a crystalline multilayer structure is compatible with the theoretically predicted formation of a collective [1+1]-dimensional sheath state involving all lateral crystal faces and probably arising from tunneling between the protected edge states of the numerous closely spaced 2D TI layers. A macroscopic system of some 10^5 coupled spin channels appears promising for applications in spintronics and quantum computation.

FM 22.6 Fri 11:00 BEY/0138

Simulating the Schrödinger equation in anti-Hermitian electrical circuits — •Ivan Scolan[1], Ronny Thomale[2], Jasper Van Wezel[3], Viktor Könye[3], Ali Moghaddam[4], Jeroen Van Den Brink[1], and Joseph Dufouleur[1] — [1]Leibniz Institute for Solid State and Materials Research Dresden — [2]Institute for Theoretical Physics and Astrophysics, University of Würzburg — [3]Institute for Theoretical Physics Amsterdam — [4]Faculty of Engineering and Natural Sciences, Tampere Finland

In recent years, a number of condensed matter lattice models have been realized using classical electric circuits, exploring topological phases hitherto inaccessible experimentally. In these previous works, the Hamiltonian of a system was implemented in a topo-electronic circuit, thus possessing the same spectrum as any equivalent condensed matter system, but the dynamics of the electronic circuit remained distinct from the quantum dynamics given by the Schrödinger equation. Here we propose a new way to realize electronic circuits that are equivalent to solid-state lattices based on anti-hermitian circuits the dynamic of which perfectly follows the Schrödinger dynamics.

Intrinsic symmetries of these circuits allow the experimental measurement of all eigenstates. Using this framework, we apply it to a 1D atomic chain with position-dependent hopping terms and experimentally retrieve the theoretical results presented in Mertens et al. (2022), Morice et al. (2021). Finally, we show how our method can be used to develop novel electronics which can be used for concrete applications and also for solving fundamental physics problems.

Coffee Break

FM 22.7 Fri 11:30 BEY/0138

Photo-dielectric synaptic plasticity in Zn-substituted $BaAl_2O_4$ — •Hiroki Taniguchi — Department of Physics, Nagoya University, Nagoya 464-8602, Japan

Optical control of material properties is pivotal for advancing the evolution from conventional electronics to next-generation photoelectronics. Although a variety of photo-induced phenomena, including the photovoltaic effect and photoconduction, have been well established as key mechanisms for photoelectronic devices, the optical manipulation of dielectric responses has remained comparatively unexplored.

Here, I demonstrate a photo-dielectric effect in partially Zn-substituted $BaAl_2O_4$, in which the dielectric permittivity increases under below-bandgap photo-irradiation without inducing photoconduction. First-principles calculations indicate that Zn substitution creates a unique defect complex. Upon photo-irradiation, photo-generated electron*hole pairs form a local dipole around this defect complex, producing an additional polarization contribution and consequently enhancing the dielectric permittivity. Furthermore, transient permittivity measurements under sequential pulsed optical excitation reveal synaptic-plasticity-like responses in Zn:$BaAl_2O_4$, highlighting its potential for neuromorphic device applications.

FM 22.8 Fri 11:45 BEY/0138

Triclinic distortion in titanite-type oxides CaSnGeO5 and SrSnGeO5 — •Taro Kuwano[1], Hiroko Yokota[1], Manabu Hagiwara[2], Toshiya Uohashi[3], Akitoshi Nakano[3], and Hiroki Taniguchi[3] — [1]4259 Nagatsuta-cho, Midori-ku, Yokohama, Kanagawa, 226-8501 Japan — [2]3-14-1 Hiyoshi, Kohoku-ku, Yokohama, Kanagawa, 223-8522 Japan — [3]Furo-cho, Chikusa-ku, Nagoya, Aichi, 464-8602 Japan

Titanite-family oxides have been emerging as a novel vein of antiferroelectric materials owing to their unique pseudo-one-dimensional structure hosting "antipolar arrangement of polar chains." In this study, we focus on another characteristic feature of the titanite-type structure: ferroelastic phase transition associated with triclinic distortion. We will propose one couple of representatives, SrSnGeO5 and CaSnGeO5, which exhibit the phase transition at about 150 and 600 K, repectively. In comparison with the cases of SrZrGeO5 and CaZrGeO5, the origin of the triclinc distortion will be discussed.

FM 22.9 Fri 12:00 BEY/0138

Interplay between Lattice Dynamics and Free Electrons in Polar Metals: A Chemical-Bonding Perspective — •Hiroto Kikuchi[1], Suguru Yoshida[1], Hiroshi Takatsu[1], Kantaro Murayama[1], Peter Lemmens[2], and Hiroshi Kageyama[1] — [1]Department of Energy and Hydrocarbon Chemistry, Graduate School of Engineering, Kyoto University, Nishikyo-ku, Kyoto 615-8510, Japan — [2]Institute for Condensed Matter Physics, Technische Universitat Braunschweig; Braunschweig 38106, Germany

Polar-nonpolar (P-NP) transitions in metals such as $LiOsO_3$ show that polar order can coexist with metallicity, defining "polar metals" as a new class of quantum materials. However, the microscopic mechanism remains under debate, with competing scenarios invoking electron-phonon coupling and coordination bonding.

We recently found that metallic $LiReO_3$, isostructural with $LiOsO_3$ and adopting the $LiNbO_3$-type structure, undergoes a P-NP structural transition at T_s = 170 K. Unlike the second-order transition in $LiOsO_3$, $LiReO_3$ shows thermal hysteresis and strong lattice softening, indicating enhanced fluctuations between polar and nonpolar phases.

We investigated Raman scattering across T_s, combined with phonon calculations and crystal orbital Hamilton population (COHP) analysis, and reveals strongly redshifted LiO_6-related optical phonons in $LiReO_3$ compared with $LiOsO_3$. These results, supported by computed force constants and bond strengths, provide a unified picture of phonon softening and polar stability in metallic $LiReO_3$.

FM 22.10 Fri 12:15 BEY/0138

NaSICON with Mg and Ca as charge carriers — •Katharina Helmbrecht and Axel Gross — Institute of Theoretical Chemistry, Ulm University, 89069 Ulm, Germany

While the Mo_6S_8 chevrel phase is frequently used as cathode material in Mg–ion batteries, theoretical studies on this material are comparatively scarce. Mo_6S_8 as a cathode material for mono– and multivalent–ion batteries is an interesting candidate. Furthermore, magnesium and calcium both show much promise a charge carriers for a suitable battery system of the future.

In this work we study the behavior of mono– and multi–valent charge carriers (Li, Na, K, Mg, Ca, Zn, Al) at the low vacancy limit of intercalation and its influence on stability and kinetics of Mo_6S_8 intercalation compounds to reach fundamental understanding of the material and its properties.

Upon varying the charge carriers in the Chevrel phase at the upper vacancy limit in a previous study [1], their diffusion barriers were observed to scale linearly with the ion size, almost independent of the charge of the considered ions. This indicates a rather unique and geometry dominated diffusion mechanism in the chevrel phase and raises the question whether this trend persists at the lower vacancy limit.

[1] K. Helmbrecht, H. Euchner, A. Groß, Batteries Supercaps **5**, e202200002 (2022).

FM 22.11 Fri 12:30 BEY/0138

High pressure crystallography: from mineral physics to material sciences — •Leonid Dubrovinsky — BGI, Bayreuth University, Bayreuth, Germany

Modern science and technology rely on the fundamental knowledge of matter that is provided by crystallographic studies. About a decade ago, our group pioneered an approach to the SCXRD data collection and analysis for the products of chemical reactions in laser heated DACs. Since then we have designed and built new instrumentation to enable sophisticated in situ experiments in house and on synchrotron radiation facilities. Our efforts have pushed the range of static pressures achievable in a DAC up to 1 TPa and enabled single-crystal X-ray diffraction experiments at such extreme conditions. Structural studies at simultaneous high pressures of over ~200 GPa and temperatures of several thousand degrees have also become possible. This has led to remarkable findings in solid state physics, mineral physics, and chemistry at extreme conditions.We illustrate application of new methodology for simultaneous high-pressure and high-temperature single crystal diffraction studies using examples of investigations of chemical and phase relations in the halides, nitrides, and carbonates.

FM 23: Focus Session: (Anti)ferroic states – Magnetic and magnetoelectric III (joint session FM/MA)

chair: Morgan Trassin (ETH Zurich, CH)

This focus session explores recent advances in understanding and control of (anti)ferroic states. Emphasis will be placed on theoretical modelling, advanced characterization techniques, and the engineering of emergent properties for use in nano-electronic devices. The session aims to bridge fundamental research with emerging device-relevant functionalities, bringing together experimental, and theoretical perspectives on ferroic materials.

Time: Friday 9:30–11:30 Location: BEY/0E40

Invited Talk FM 23.1 Fri 9:30 BEY/0E40

Mapping topological textures in compensated magnets with X-rays — •Claire Donnelly — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Extending spin systems to three dimensions promise significant opportunities for applications, for example providing higher density devices and new functionalities associated with complex topology and greater degrees of freedom. Until now, however, insight into three dimensional spin systems has mainly been limited to ferromagnetic and ferrimagnetic systems through X-ray magnetic tomography [1], where a variety of topological textures [1,2], as well as 3D dynamics [3,4], have been observed. In this talk I will describe our recent work mapping topological textures in compensated systems. I will first describe the development of X-ray linear orientation tomography [5], which we have harnessed to map three-dimensional orientation fields - both crystallographic [5], and antiferromagnetic - at the nanoscale. Second, I will present our recent mapping of topological textures in altermagnets [6], harnessing both X-ray circular and linear magnetic dichroism. These insights into the formation of topological textures in compensated magnets not only paves the way for enhanced understanding of these systems, but also towards the next generation of technological devices.

[1] C. Donnelly et al., Nature 547, 328 (2017). [2] C. Donnelly et al., Nat. Phys. 17, 316 (2021) [3] C. Donnelly et al., Nature Nanotechnology 15, 356 (2020). [4] S. Finizio et al., Nano Letters (2022) [5] A. Apseros et al., Nature 636, 354 (2024) [6] R. Yamamoto et al., Phys. Rev. Appl. 24, 034037 (2025)

FM 23.2 Fri 10:00 BEY/0E40

Exploring Magnetoelectric Effects in 1T-$FeCl_2$/bilayer-GaSe Multiferroic Heterostructures — •Fahmida Fakhera[1], Oliver J. Conquest[1], Carla Verdi[1,2], and Catherine Stampfl[1] — [1]School of Physics, The University of Sydney, NSW 2006, Australia — [2]School of Mathematics and Physics, The University of Queensland, QLD 4072, Australia.

Multiferroic materials exhibit multiple ferroic orders simultaneously, including ferromagnetism and ferroelectricity [1]. A recent study [2] on sliding ferroelectricity in bilayer GaSe adds a novel dimension, making it useful as a ferroelectric (FE) sublayer in multiferroic heterostructures. We employ first-principles density functional theory (DFT) to investigate the interlayer and intralayer sliding mechanisms of FE GaSe. Moreover, this study investigates the structural and electronic properties, energy band alignments, magnetic anisotropy, binding energies, electric dipole moments, and interfacial charge transfer of different stackings of 1T-$FeCl_2$/bilayer GaSe. For all stackings, the magnetic anisotropy energies indicate an in-plane easy axis of magnetization in both upward and downward polarization directions. The contact interfaces form Ohmic contacts, enabling sufficient charge transfer between the layers. As the first study on sliding-induced FE and ferromagnetic interfaces, this work offers new insights into the design and understanding of multiferroic materials for the future.

[1] X. Feng, J. Liu, X. Ma, and M. Zhao, Physical Chemistry Chemical Physics 22, 7489 (2020). [2] F. Fakhera, O.J. Conquest, C. Verdi, and C. Stampfl, Physical Review Materials 9, 054402 (2025).

FM 23.3 Fri 10:15 BEY/0E40

Nonlinear phononic slidetronics — •Pooja Rani and Dominik Juraschek — Eindhoven University of Technology, Eindhoven, Netherlands

We investigate ultrafast switching of ferroelectricity in bilayer hexagonal boron nitride using nonlinearly driven phonons. Conventional coherent phonon excitation mechanisms such as infrared absorption, Raman-based techniques, and terahertz sum-frequency excitation produce too small a shear-mode amplitude to overcome the barrier between stacking orders. Using first-principles calculations and phenomenological modeling, we demonstrate instead that strong excitation of high-frequency intralayer phonons dynamically tilts the interlayer potential, enabling efficient and deterministic switching at experimentally accessible pulse strengths. Our results establish nonlinear phononic slidetronics as a powerful method for ultrafast, energy-efficient control of stacking order and related electronic phases in van der Waals materials, with potential for future all-optical ferroelectric memory devices.

Coffee break

FM 23.4 Fri 10:45 BEY/0E40

Resolving the chemical depth profile of ultrathin EuO films by grazing incidence HAXPES measurements — •Katharina Wehrstein[1], Umut Parlak[1], Pia Düring[1], Oliver Rehm[1], Andrei Gloskovskii[2], Christoph Schlueter[2], and Martina Müller[1] — [1]FB Physik, Uni Konstanz — [2]DESY

Magnetic proximity effects enable control of magnetic order in ferromagnetic insulators without altering their intrinsic properties. Europium oxide (EuO) thin films coupled with heavy metals (HM) are promising systems for spintronic applications, in which spin-polarized states are induced, altered or converted via interface coupling. These systems require a sharp interface between the metal and the EuO layer, as well as stoichiometric EuO. As ferromagnetic Eu(II)O is metastable and tends to oxidize to paramagnetic $Eu(III)_2O_3$, investigating the depth-resolved chemical and thus magnetic nature of an EuO layer is mandatory to observe and eventually tune magnetic proximity effects.

Ultrathin EuO films (2-15 nm) were prepared by molecular beam epitaxy on $Pt/SrTiO_3$ and $W/SrTiO_3$ substrates. Grazing incidence hard X-ray photoelectron spectroscopy (GIXPES) enables high X-ray intensity at the sample surface due to reflection of the X-ray beam on the heavy metal layer, leading to the formation of X-ray standing waves. By changing the incidence angle of the X-ray beam, spectra with modulated depth-sensitivity were recorded, revealing variations in the Eu^{3+} content at different depths of the ultrathin EuO layer. This yields a chemical depth profile and thus a magnetic profile that provides insight into the magnetic behavior of the EuO/HM system.

FM 23.5 Fri 11:00 BEY/0E40

Optical manipulation of multiferroic phases in $BiFeO_3$ thin films — •Bixin Yan[1], Lauren J. Riddiford[1,2], Ales Hrabec[1,2], Annika Mechnich[3], Christian L. Degen[3], Manfred Fiebig[1], and Morgan Trassin[1] — [1]Department of Materials, ETH Zurich, Switzerland — [2]PSI Center for Neutron and Muon Sciences, PSI, Switzerland — [3]Department of Physics, ETH Zurich, Switzerland

Employing light as a means of actively tuning material properties unlocks the potential for non-invasive, remote, and macroscopic control over technology-relevant functionalities. In our work, we demonstrate optical control over multiferroic phases in prototypical magnetoelectric $BiFeO_3$ (BFO) thin films, utilizing above-bandgap UV light illumination. Taking advantage of the enhanced response at the strain-driven morphotropic phase boundary, we show that by modifying the electrostatic boundary conditions with photoinduced charge carriers, the rhombohedral-like (R-like) phase of BFO can be selectively suppressed within the tetragonal-like (T-like) phase BFO matrix. Furthermore, the electronic origin of such an optical response permits a pronounced polarization-dependent R-to-T-phase conversion. Finally, using scanning nitrogen-vacancy magnetometry, we correlate optically induced ferroelectric phase conversion with a change from uncompensated magnetic ordering to G-type antiferromagnetic ordering. Our work thus presents a novel approach to writing multiferroic states, which is key to magnetoelectric oxide electronics.

FM 23.6 Fri 11:15 BEY/0E40

Time resolved X-ray diffraction study of polarization reversal in uniaxial ferroelectric $BaMgF_4$ single crystals — •Nathan Leubner[1,4], Sara Polo-Filisan[2], Gaetano Bonetti[2], Hiroki Tanaka[2], Matthias Zschornak[3], Dirk C. Meyer[1], Carsten Richter[2], and Semën Gorfman[4] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg — [2]Leibniz-Institut für Kristallzüchtung, Berlin — [3]Fakultät Maschinenbau, HTW Dresden — [4]Department of Materials Science and Engineering, Tel Aviv University, Israel

$BaMgF_4$ (BMF) is a uniaxial ferroelectric material crystallizing in the orthorhombic space group $Cmc2_1$ and being a compelling candidate for frequency conversion in far ultraviolet regime. In this work, we present time-resolved X-ray diffraction (XRD) studies of single-crystalline BMF under applied electric fields, enabling direct observation of atomic-scale structural changes during domain switching. Complementary dielectric measurements provide insights into the kinetics of domain wall motion. The XRD data reveal the electric-field dependence of strain, allowing for the determination of the components of the piezoelectric tensor of BMF. Furthermore, by exploiting the resonant Friedel pair contrast between oppositely polarized domains, we achieve a direct determination of the crystal structure of each domain. This approach eliminates the need for conventional correction factors (e.g., absorption, extinction), offering a robust and accurate alternative to traditional structure refinement methods. Our findings advance the fundamental understanding of ferroelectric switching in BMF.

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Overview of Invited Talks and Sessions

(Lecture halls POT/0006, POT/0051, POT/0081, and POT/0251; Poster P1)

Invited Talks

HL 2.1	Mon	9:30–10:00	POT/0051	**Intrinsically stretchable polymers and devices for biosensing applications** — •Ulrike Kraft
HL 2.2	Mon	10:00–10:30	POT/0051	**Complexity in Organic Mixed Ionic Electronic Conductors and its Application in Neuromorphic Computing** — •Hans Kleemann
HL 2.3	Mon	10:30–11:00	POT/0051	**Organic Neuromorphic Interfaces for Biohybrid Systems: Material and Structural Biomimicry of Synaptic Plasticity** — •Francesca Santoro
HL 2.4	Mon	11:15–11:45	POT/0051	**Fully-organic flexible detectors for real-time dose monitoring during radio/proton therapy** — •Beatrice Fraboni
HL 2.5	Mon	11:45–12:15	POT/0051	**Organic LEDs and photodetectors for light-based diagnostics and therapy** — •Caroline Murawski, Rabiul Islam, Siddhartha Saggar, Jens P. Weber
HL 4.1	Mon	9:30–10:00	POT/0251	**X-ray nanodiffraction studies of lead-halide perovskite supercrystals** — Jonas Hiller, Robert Thalwitzer, Ata Bozkurt, Matheus Ferreira, Richard Hodak, Fabian Strauss, Elke Nadler, Gerard Hinsley, Bihan Wang, Kuan Hoon Ngoi, Witold Rudzinski, Ekaterina Kneschaurek, Wojciech Roseker, Michael Sprung, Dmitry Lapkin, Dmitry Baranov, Frank Schreiber, Ivan Vartanyants, Marcus Scheele, •Ivan Zaluzhnyy
HL 11.1	Mon	15:00–15:30	POT/0251	**Quantum Repeater Hardware made from Silicon Carbide** — •Jörg Wrachtrup
HL 11.2	Mon	15:30–16:00	POT/0251	**Diamond based quantum sensing for drug testing** — •Romana Schirhagl
HL 11.3	Mon	16:00–16:30	POT/0251	**The oxygen-related ST1 centre in diamond: a room temperature coherently controllable electron spin** — •Sebastien Pezzagna
HL 11.4	Mon	16:45–17:15	POT/0251	**Silicon quantum emitters emitting in the optical telecommunication range for scalable quantum photonic circuits** — •Yonder Berencén
HL 11.5	Mon	17:15–17:45	POT/0251	**Advances in materials processing for quantum sensing** — •Adam Gali
HL 16.1	Tue	9:30–10:00	POT/0081	**Tailoring the performance of WSe_2 quantum emitters via cavity quantum electrodynamics and coherent driving** — •Ivan Solovev
HL 16.2	Tue	10:00–10:30	POT/0081	**Deterministic single-photon emitters in 2D materials** — •Ursula Wurstbauer
HL 16.3	Tue	10:30–11:00	POT/0081	**Resolving atomic and electronic structure of point defects in MoS_2 by first-principles calculations and scanning tunneling microscopy** — •Hannu-Pekka Komsa
HL 16.4	Tue	11:15–11:45	POT/0081	**Polarization dynamics of isolated defects in hexagonal boron nitride** — Serkan Paçal, Çağlar Samaner, Furkan Ağlarci, Ömer S. Tapşin, •Serkan Ateş
HL 16.5	Tue	11:45–12:15	POT/0081	**Defect-driven quantum emission in 2D materials** — •Magdalena Grzeszczyk
HL 25.1	Wed	9:30–10:00	POT/0251	**Quantum dots for single-electron current sources** — •Johannes C. Bayer, Thomas Gerster, Dario Maradan, Niels Ubbelohde, Klaus Pierz, Hans W. Schumacher, Frank Hohls
HL 25.2	Wed	10:00–10:30	POT/0251	**Optical readout of reconfigurable in-plane magnetic domains in CrSBr** — •Aleksandra Łopion, Pierre-Maurice Piel, Manuel Terbeck, Jan-Hendrik Larusch, Jakob Henz, Marie-Christin Heissenbüttel, Thorsten Deilmann, Michael Rohlfing, Zdenek Sofer, Ursula Wurstbauer
HL 25.3	Wed	10:30–11:00	POT/0251	**Ferroelectric switching in Mn-doped epitaxial $BaTiO_3$ films and superlattices on silicon** — •Alfredo Blázquez Martínez, Valentin Väinö Hevelke, Ibukun Olaniyan, Minh-Anh Luong, Ines Häusler, Sven Wiesner, Christoph T. Koch, Dong-Jik Kim, Catherine Dubourdieu

HL 25.4	Wed	11:15–11:45	POT/0251	**Tunability of quantized Hall plateaus** — •Serkan Sirt, Vladimir Umansky, Stefan Ludwig
HL 25.5	Wed	11:45–12:15	POT/0251	**How to achieve high gain in organic photodetectors?** — •Johannes Benduhn
HL 30.1	Wed	15:00–15:30	POT/0081	**Dual proximity engineering of spin-orbit and magnetic effects in graphene heterostructures** — •Christoph Kastl
HL 42.1	Thu	11:15–11:45	POT/0006	**Transition Metal Nitride Semiconductors for Photoelectrochemical Energy Conversion** — •Verena Streibel, Laura I. Wagner, Elise Sirotti, David A. Egger, Ian D. Sharp
HL 46.3	Thu	15:30–16:00	POT/0051	**Antisymmetric vibrations in the excited state dynamics of quadrupolar dyes** — Somayeh Souri, Katrin Winte, Daniel Lünemann, Daniel Timmer, Elena Mena-Osteritz, Sergei Tretiak, Christoph Lienau, •Antonietta De Sio
HL 49.1	Thu	16:15–16:45	POT/0081	**Phonon-mediated nonlinearity and defects in hexagonal boron nitride** — •Nahid Talebi
HL 53.1	Fri	9:30–10:00	POT/0051	**Organic semiconductors: Opening new perspectives in sustainable electronics** — •Karl Leo

Invited Talks of the joint Symposium SKM Dissertation Prize 2026 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	HSZ/0002	**Stochastic-Calculus Approach to Non-equilibrium Statistical Physics** — •Cai Dieball
SYSD 1.2	Mon	10:00–10:30	HSZ/0002	**Nonuniform magnetic spin textures for sensing, storage and computing applications** — •Sabri Koraltan
SYSD 1.3	Mon	10:30–11:00	HSZ/0002	**Anomalous Quantum Oscillations beyond Onsager's Fermi Surface Paradigm** — •Valentin Leeb
SYSD 1.4	Mon	11:00–11:30	HSZ/0002	**Coherent Control Schemes for Semiconductor Quantum Systems** — •Eva Schöll
SYSD 1.5	Mon	11:30–12:00	HSZ/0002	**On stochastic thermodynamics under incomplete information: Thermodynamic inference from Markovian events** — •Jann van der Meer

Invited Talks of the joint Symposium Designing Quantum Materials with Light: From Floquet to Cavity Engineering (SYFC)

See SYFC for the full program of the symposium.

SYFC 1.1	Mon	9:30–10:00	HSZ/AUDI	**Subcycle videography of strong-field controlled band structures** — •Rupert Huber, Manuel Meierhofer, Ulrich Höfer
SYFC 1.2	Mon	10:00–10:30	HSZ/AUDI	**Engineering Quantum Materials through Structured Cavity Vacuum Fluctuations** — •Angel Rubio
SYFC 1.3	Mon	10:30–11:00	HSZ/AUDI	**Floquet engineering of quantum materials: from semiconductors to semimetals** — •Shuyun Zhou
SYFC 1.4	Mon	11:15–11:45	HSZ/AUDI	**(Quantum) Light Control of Materials** — •Dante Kennes
SYFC 1.5	Mon	11:45–12:15	HSZ/AUDI	**Lightwave-driven electrons in a Floquet topological insulator** — Daniel Lesko, Tobias Weitz, Weizhe Li, Selina Nöcker, Celina Hüttner, Tamara Pröbster, Simon Wittigschlager, Christian Heide, Ofer Neufeld, •Peter Hommelhoff

Invited Talks of the joint Symposium Interacting Degrees of Freedom in Ultrathin Quantum Films (SYQF)

See SYQF for the full program of the symposium.

SYQF 1.1	Fri	9:30–10:00	HSZ/AUDI	**Exciton dressing by extreme nonlinear magnons in a layered semiconductor** — •Geoffrey M. Diederich
SYQF 1.2	Fri	10:00–10:30	HSZ/AUDI	**A tale of demons and decay in two-dimensional (alter)magnets** — •Alexander Mook
SYQF 1.3	Fri	10:30–11:00	HSZ/AUDI	**Magnetism, light and matter - Role of excitons in two-dimensional magnets** — •Florian Dirnberger
SYQF 1.4	Fri	11:15–11:45	HSZ/AUDI	**Advantages and challanges of resonance Raman scattering with infrared excitation energy** — •Leonetta Baldassarre
SYQF 1.5	Fri	11:45–12:15	HSZ/AUDI	**Shining light on 2D antiferromagnets** — •Dmytro Afanasiev

Sessions

HL 1.1–1.12	Mon	9:30–12:45	POT/0006	**Optical Properties I**
HL 2.1–2.7	Mon	9:30–12:45	POT/0051	**Focus Session: Biocompatible Organic Semiconductors for Artificial Intelligence**
HL 3.1–3.12	Mon	9:30–12:45	POT/0081	**2D Materials I – Excitonic properties**
HL 4.1–4.8	Mon	9:30–12:00	POT/0251	**Perovskite and Photovoltaics: Synthesis and Performance**
HL 5.1–5.7	Mon	10:30–12:30	TRE/MATH	**2D Materials: Electronic structure, excitations, etc. I (joint session O/HL/TT)**
HL 6.1–6.7	Mon	15:00–18:15	HSZ/0003	**Focus Session: Tunable Correlations in van der Waals Quantum Materials I (joint session TT/DS/HL)**
HL 7.1–7.11	Mon	15:00–17:45	HSZ/0204	**2D Materials beyond graphene: Growth, structure and substrate interaction (joint session O/HL/TT)**
HL 8.1–8.12	Mon	15:00–18:15	POT/0006	**Ultra-fast Phenomena I**
HL 9.1–9.6	Mon	15:00–16:30	POT/0051	**Oxide Semiconductors: Growth and Fabrication**
HL 10.1–10.6	Mon	15:00–16:30	POT/0081	**2D Materials II – Electronic and transport properties (joint session HL/TT)**
HL 11.1–11.7	Mon	15:00–18:15	POT/0251	**Focus Session: Quantum Emitters in 3D Semiconductors**
HL 12.1–12.7	Mon	16:45–18:30	POT/0051	**Heterostructures, Interfaces and Surfaces: Photonics**
HL 13.1–13.7	Mon	16:45–18:30	POT/0081	**2D Materials III – Interlayer excitons**
HL 14.1–14.4	Tue	9:30–10:45	HSZ/0105	**Focus Session: Tunable Correlations in van der Waals Quantum Materials II (joint session TT/DS/HL)**
HL 15.1–15.9	Tue	9:30–12:00	POT/0006	**Organic Semiconductors: Optics and Photonics**
HL 16.1–16.7	Tue	9:30–12:45	POT/0081	**Focus Session: Quantum Emitters in 2D Semiconductors**
HL 17.1–17.10	Tue	9:30–12:15	POT/0251	**Quantum Dots and Wires: Rings, Wires and Transport**
HL 18.1–18.10	Tue	10:00–12:45	POT/0051	**Nanomechanical systems (joint session HL/TT)**
HL 19.1–19.7	Tue	10:30–12:30	HSZ/0201	**Graphene: Growth, structure and substrate interaction (joint session O/HL)**
HL 20.1–20.66	Tue	18:00–20:00	P1	**Poster I**
HL 21.1–21.4	Wed	9:30–10:30	HSZ/0101	**Focus Session: Quantum Sensing with Solid State Spin defects II (joint session TT/HL/MA)**
HL 22.1–22.6	Wed	9:30–11:00	POT/0006	**Biocompatible Organic Semiconductors**
HL 23.1–23.10	Wed	9:30–12:15	POT/0051	**Transport Properties**
HL 24.1–24.12	Wed	9:30–12:45	POT/0081	**2D Materials IV – Emerging materials and properties**
HL 25.1–25.5	Wed	9:30–12:15	POT/0251	**Focus Session: Young Semiconductor Forum**
HL 26.1–26.56	Wed	9:30–11:30	P1	**Poster II**
HL 27.1–27.8	Wed	10:30–12:30	TRE/MATH	**2D Materials: Electronic structure, excitations, etc. II (joint session O/HL/TT)**
HL 28.1–28.11	Wed	15:00–17:45	HSZ/0401	**Topology and symmetry protected materials & Topological insulators (joint session O/HL/TT)**
HL 29.1–29.5	Wed	15:00–16:15	POT/0006	**Quantum Transport and Quantum Hall effects (joint session HL/TT)**
HL 30.1–30.7	Wed	15:00–17:15	POT/0081	**2D Materials V – Magnetic, spintronic, and topological properties (joint session HL/TT)**
HL 31.1–31.5	Wed	15:00–16:15	POT/0251	**Materials and Devices for Quantum Technology I**
HL 32.1–32.9	Wed	15:00–17:30	REC/C213	**2D Materials 2 (joint session DS/HL)**
HL 33.1–33.5	Wed	16:30–17:45	POT/0006	**Nitrides I – Growth and fabrication**
HL 34.1–34.5	Wed	16:30–17:45	POT/0051	**Quantum Dots and Wires: Telecom Wavelength**
HL 35.1–35.9	Wed	16:30–19:00	POT/0251	**Optical Properties II**
HL 36.1–36.4	Wed	17:30–18:30	POT/0081	**2D Materials VI – Optoelectronic properties**
HL 37.1–37.6	Thu	9:30–11:00	POT/0006	**Nitrides II – Designed properties and LED**
HL 38.1–38.12	Thu	9:30–12:45	POT/0051	**Materials and Devices for Quantum Technology II**
HL 39.1–39.11	Thu	9:30–12:30	POT/0081	**2D semiconductors VII – CrSBr and related heterostructures**
HL 40.1–40.11	Thu	9:30–12:30	POT/0251	**Oxide Semiconductors: Transport and Spectroscopy**
HL 41.1–41.7	Thu	11:00–12:45	HSZ/0101	**Quantum Dots and Point Contacts (joint session TT/HL)**
HL 42.1–42.5	Thu	11:15–12:45	POT/0006	**Nitrides III – Emerging thin films and electrochemistry**
HL 43	Thu	13:30–17:00	Infineon	**Excursion and Network-Event at Infineon Dresden AG (joint session FM/HL)**
HL 44.1–44.11	Thu	15:00–17:45	HSZ/0204	**2D Materials: Electronic structure, excitations, etc. III (joint session O/HL/TT)**
HL 45.1–45.8	Thu	15:00–17:15	POT/0006	**Perovskite and Photovoltaics: Spectroscopy**
HL 46.1–46.7	Thu	15:00–17:15	POT/0051	**Ultra-fast Phenomena II**
HL 47.1–47.4	Thu	15:00–16:00	POT/0081	**2D Materials VIII – Quantum emitters and defects**
HL 48.1–48.8	Thu	15:00–17:15	POT/0251	**Heterostructures, Interfaces and Surfaces: Fabrication and Structure**

HL 49.1–49.4	Thu	16:15–17:30	POT/0081	**Quantum Emitters in 2D Semiconductors**
HL 50	Thu	17:45–19:15	POT/0051	**Members' Assembly**
HL 51.1–51.12	Fri	9:30–12:30	HSZ/0401	**2D Materials: Stacking and heterostructures (joint session O/HL/TT)**
HL 52.1–52.5	Fri	9:30–10:45	POT/0006	**THz and MIR Physics in Semiconductors**
HL 53.1–53.6	Fri	9:30–11:15	POT/0051	**Organic Semiconductors: Carrier Dynamics**
HL 54.1–54.12	Fri	9:30–12:45	POT/0081	**2D Materials IX – Photonic properties and devices**
HL 55.1–55.11	Fri	9:30–12:30	POT/0251	**Quantum Dots and Wires: (Single) Photonics**
HL 56.1–56.5	Fri	11:15–12:30	POT/0006	**Quantum Emitters in 3D Semiconductors**
HL 57.1–57.5	Fri	11:30–12:45	POT/0051	**Nitrides IV – Optical properties**

Members' Assembly of the Semiconductor Physics Division

Thu 17:45–19:15 POT/0051

Sessions

– Invited, Topical, Contributed Talks, and Posters –

HL 1: Optical Properties I

Time: Monday 9:30–12:45 Location: POT/0006

HL 1.1 Mon 9:30 POT/0006

Critical-Point Analysis of Ta_3N_5 Light Absorbers from Room-Temperature Photo-Modulated Spectroscopy — •Matthias Quintern[1,2], Johannes Dittloff[1,2], Lukas Wolz[1], Gabriel Grötzner[1,2], Johanna Eichhorn[1], and Ian D. Sharp[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Department of Physics, 85748 Garching, Germany — [2]Technical University of Munich, Walter Schottky Institute, 85748 Garching, Germany

Tantalum nitride (Ta_3N_5) thin films are promising photoanode materials for solar water splitting. However, the fundamental nature of the Ta_3N_5 bandgap remains under debate. To overcome the limitations of conventional Tauc-plot analysis, we built a new combined photoreflectance (PR) and phototransmittance (PT) setup. Our measurements indicate a direct fundamental bandgap of 2.1 eV, but also reveal higher-energy critical points. Furthermore, we find that the PR and PT spectra closely match temperature-corrected transient absorption spectra. The overall differences in the transmission spectra are minor, suggesting that the samples share a similar bulk electronic structure. At the same time, the more surface-sensitive PR signals exhibit greater variations and even additional sub-gap features in some samples. By performing measurements using different pump wavelengths and power densities, as well as employing a phase analysis, we assign individual features of PR spectra to a surface layer. This has implications for out-of-plane charge transport properties and interfacial energies, both of which are crucial parameters for photoelectrochemical performance.

HL 1.2 Mon 9:45 POT/0006

OptiMate3B: Three-body-information-based prediction of optical spectra for semiconductors and insulators — •Malte Grunert, Max Grossmann, and Erich Runge — Institute of Physics and Institute of Micro- and Nanotechnologies, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Optical spectra of semiconductors and insulators are essential both for many technologically important applications as well as for the understanding of materials. However, their computation via adequate ab initio techniques remains prohibitively expensive for either large-scale studies or many realistic systems. Recently however, machine learning techniques have emerged as promising alternative. We present OptiMate-3B, a line graph attention network capable of predicting the optical spectra of semiconductors and insulators under both the independent particle approximation and the random phase approximation - i.e. incorporating local-field effects - within milliseconds. OptiMate-3B incorporates three-body information to capture angular information in crystalline materials, further enhancing its predictive accuracy. Having been trained on tens of thousands of high-fidelity first-principles spectra, the model generalizes across a broad chemical and structural space. Its open and user-friendly interface facilitates direct integration into high-throughput materials workflows, providing an efficient surrogate for ab initio optical spectroscopy.

HL 1.3 Mon 10:00 POT/0006

Intensity-dependent excitonic second- and third-harmonic generation enhanced by static electric fields — Ruixin Zuo[1], •Matthias Reichelt[1], Cong Ngo[1], Xiaohong Song[2], Weifeng Yang[2,3], and Torsten Meier[1] — [1]Department of Physics and Center for Optoelectronics and Photonics Paderborn (CeOPP), Paderborn University, Warburger Straße 100, D-33098 Paderborn, Germany — [2]School of Physics and Optoelectronic Engineering, Hainan University, Haikou 570288, China — [3]Center for Theoretical Physics, Hainan University, Haikou 570288, China

The many-body Coulomb interaction plays a decisive role in the ultrafast photoinduced carrier dynamics governing semiconductor high-harmonic generation, see, e.g., [1,2]. Moreover, static electric fields were shown to surprisingly enhance excitonic second- and third-harmonic generation [3]. Here, we study this enhancement for material models corresponding to transition-metal dichalcogenides and study the dependencies on several parameters.

[1] A. Trautmann, R. Zuo, G. Wang, W.-R. Hannes, S. Yang, L. H. Thong, C. Ngo, J. T. Steiner, M. Ciappina, M. Reichelt, H. T. Duc, X. Song, W. Yang, and T. Meier, Proc. SPIE **11999**, 1199909 (2022).

[2] J. Hader, J. Neuhaus, J. V. Moloney, and S. W. Koch, Opt. Lett. **48**, 2094 (2023).

[3] R. Zuo, M. Reichelt, C. Ngo, X. Song, W. Yang, and T. Meier, arXiv:2511.05112.

HL 1.4 Mon 10:15 POT/0006

Thin Films of Size-Selected Cu_2ZnSnS_4 and Cu_2NiSnS_4 Nanocrystals: Structural and Optical Properties — •Oleksandra Ivakhno-Tsehelnyk[1], Serhiy Kondratenko[2], Volodymyr Dzhagan[3], and Dietrich R.T. Zahn[1] — [1]Semiconductor Physics & Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology. — [2]Taras Shevchenko National University of Kyiv, 01601 Kyiv, Ukraine. — [3]Lashkaryov Institute of Semiconductor Physics, NAS of Ukraine, 03038 Kyiv, Ukraine.

An investigation was conducted into thin films of Cu_2NiSnS_4 (CNTS) and Cu_2ZnSnS_4 (CZTS) nanocrystals (NCs) in the context of their promising use for photovoltaics (PV). Colloidal NC ensembles were obtained by "green" colloidal synthesis and directly subjected to size-selective centrifugation, yielding fractions of different sizes. This approach provides a relatively non-toxic and scalable method of producing light-absorbing NC materials. The thin films were prepared by spin-coating the NC fractions onto various substrates. A range of analytical techniques were employed to investigate their properties, encompassing Raman spectroscopy, atomic force microscopy (AFM), X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), and spectroscopic ellipsometry. These techniques enabled the investigation of the relationship between the crystal structure, composition, morphology, and optical properties with the size of CZTS and CNTS nanocrystals.

HL 1.5 Mon 10:30 POT/0006

Simulations of the nonlinear optical dynamics of quantum dot ensembles in a microcavity — •Mohit Kumar[1,2], Hendrik Rose[2], and Torsten Meier[1,2] — [1]Department of Physics and Center for Optoelectronics and Photonics Paderborn (CeOPP), Paderborn University, Warburger Strasse 100, D-33098 Paderborn, Germany — [2]Institute for Photonic Quantum Systems (PhoQS), Paderborn University, Warburger Strasse 100, D-33098 Paderborn, Germany

Recently, it has been demonstrated that photon echoes emitted from ensembles of inhomogeneously-broadened quantum dots can be controlled in several ways by suitably designed light pulses [1,2]. The strong coupling of a single two-level system to the mode of a microcavity results in a complex nonlinear optical dynamics [3]. Here, we present numerical simulations of the coherent dynamics of quantum dots ensembles, described as two-level systems, inside a single-mode microcavity. The coupling to the field mode results in a complex dynamics which is studied numerically as function of the relevant system parameters and for different excitation conditions.

[1] A. N. Kosarev, H. Rose, S. V. Poltavtsev, M. Reichelt, C. Schneider, M. Kamp, S. Höfling, M. Bayer, T. Meier, and I. A. Akimov, Comm. Physics **3**, 228 (2020).

[2] S. Grisard, A. V. Trifonov, H. Rose, R. Reichhardt, M. Reichelt, C. Schneider, M. Kamp, S. Höfling, M. Bayer, T. Meier, and I. A. Akimov, ACS Photonics **10**, 3161 (2023).

[3] M. Koch, J. Shah, and T. Meier, Phys. Rev. B **57**, R2049(R) (1998).

HL 1.6 Mon 10:45 POT/0006

Optical Limiting Induced by Excited-State Absorption in Thiophene Oligomers — •Mustapha Driouech, Michele Guerrini, and Caterina Cocchi — Friedrich-Schiller Universität Jena, Institute for Condensed Matter Theory and Optics, 07743 Jena, Germany

Optical limiting (OL) is a nonlinear effect that reduces light transmission at high intensities, providing protection for sensitive optical devices and human eyes. Non-perturbative ab initio methods have proven to be powerful predictive tools for OL [1]. In this work, we investigate the optical absorption spectra of a set of thiophene oligomers under the influence of a broadband, instantaneous electric field [2]. At sufficiently high intensities, absorption peaks that are absent in the linear response emerge below the absorption onset in the linear regime. To elucidate the optical nonlinearities involved, we perform pump-probe simulations and analyze the population dynamics, revealing that these emergent features originate from excited-state absorption in the near-infrared to visible region. Further analysis, taking into account both molecular length and applied laser intensity, demonstrates how these factors influence the nonlinear response. Our results show that this fully ab initio approach can accurately capture and unravel the fundamental processes driving optical nonlinearities in thiophene oligomers.

[1] C. Cocchi, et al., Phys. Rev. Lett. 112, 198303 (2014).

[2] M. Driouech, et al., J. Phys. Chem. Lett 16, 11867 (2025).

15 min. break

HL 1.7 Mon 11:15 POT/0006

Polarization-resolved Raman measurements on optically anisotropic crystals — •Susanne Moritz, Lukas Trefflich, Ron Hildebrandt, Marius Grundmann, and Chris Sturm — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Germany

Raman spectroscopy provides a powerful, non-destructive way to probe lattice vibrations, crystal symmetry, and electron-phonon interactions. For years, optically anisotropic materials have been gaining importance in solid-state physics research. These materials are investigated by measuring the Raman intensity in two configurations, namely cross-polarized and parallel polarization. However, due to their low symmetry, this is not sufficient in order to extract the properties of the Raman tensor and extensive polarization-resolved Raman measurements are required for a precise determination, particularly of the Raman tensor [1,2,3]. Here, we present an efficient measurement scheme in order to determine the Raman tensor of optically anisotropic materials with high precision. Special care must be taken regarding the influence of the used polarizing optics, such as half-wave plates, as well as the impact of the non-idealities of all optical elements included in the setup, such as mirrors or beam splitters. For this purpose, we also show a procedure for calibrating these elements.

[1] C. Kranert et al., Phys. Rev. Lett. **116**, 127401 (2016)
[2] C. Kranert et al., Sci. Rep. **6**, 35964 (2016)
[3] R. Hildebrandt et al., Appl. Phys. Lett. **119**, 121109 (2021)

HL 1.8 Mon 11:30 POT/0006

Quadrupole Transitions in Molecules from Real-Time Time-Dependent Density Function Theory — •Anvar Khujakulov[1], Michele Michele Guerrini[1], Carlo Andrea Rozzi[1], and Caterina Cocchi[2] — [1]Institute for Condensed Matter Theory and Optics, 07743 Jena, Germany — [2]Istituto Nanoscienze - 41125 Modena, Italy

The breakdown of the dipole approximation in tightly focused or short-wavelength laser fields is driven by spatial electric field variations, leading to significant beyond-dipole effects including quadrupole transitions and a nonlinear optical response [1]. We extend the Yabana-Bertsch implementation of real-time time-dependent density functional theory to include quadrupole transitions in the absorption cross-sections and apply the developed approach to atoms and small molecules. Our results reveal absorption peaks appearing above the linear absorption onset, a clear signature of quadrupole transitions. Critically, for molecules with appropriate symmetry, the quadrupole contribution to the absorption cross-section is maximized when a specific molecular axis aligns with the electric field gradient, analogous to the dipole case. By systematically rotating the molecular axis relative to the laser polarization vector, we calculate the orientation-dependent absorption cross-section and differentiate the contributions from dipole and quadrupole transitions. We quantitatively demonstrate that quadrupole transition is not a minor effect but a significant contributor to absorption spectra beyond the dipole approximation.

[1] C. Cocchi, et al., Phys. Rev. Lett. 112, 198303 (2014).

HL 1.9 Mon 11:45 POT/0006

Phase-matched electron-photon interactions enabled by 3D printed helical waveguides — •Masoud Taleb[1], Mohsen Samadi[2], and Nahid Talebi[1] — [1]Institute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Department of Electrical and Information Engineering, Kiel University, 24143 Kiel, Germany

We demonstrate a new phase-matching mechanism between free electrons and guided optical modes using 3D-printed helical waveguides. The structure consists of a polymer micro-fiber coated with a thin gold layer, fabricated by two-photon polymerization. When an electron beam propagates parallel to the helix axis, the helical geometry extends the optical path and enables sequential, phase-synchronous coupling to a plasmonic hybrid mode. This interaction unifies elements of Smith-Purcell and Cherenkov emission and yields a strong, highly directional visible-light output. Cathodoluminescence measurements reveal a dominant emission near 2.1-2.2 eV, collimated along the electron trajectory and exhibiting circular polarization dictated by the helix handedness. The observed photon yield (~0.02 photons per electron for an 11-turn helix) exceeds that of planar electron-driven photon sources by more than two orders of magnitude. These results introduce helical micro-waveguides as an efficient platform for directional, polarization-controlled electron-photon interactions.

HL 1.10 Mon 12:00 POT/0006

Quantum-engineered CaAlSiN3 via terbium substitution: coupling spin, optical, and lattice responses in a rare-earth nitride host — •Sikander Azam and Jan Minar — University of West Bohemia New Technologies - Research Centre Univerzitní 8 301 00 Plzeň Czech Republic

Rare-earth nitrides attract interest because they link optical activity, magnetism, and mechanical stability. CaAlSiN3 is a robust wide-gap host, but the microscopic role of terbium substitution is not well established. We study pristine and Tb-doped CaAlSiN3 (8.5 and 17 percent) using spin-polarized density functional theory within GGA+U and spin-orbit coupling in WIEN2k. Tb narrows the bandgap and introduces 4f-derived mid-gap states that enhance visible-range absorption. The densities of states show hybridization between Tb 4f levels and the surrounding network. The optical response shows higher absorption, a larger refractive index, and shifts in dielectric features that follow these electronic changes. Simulated Tb L*-edge X-ray absorption spectra display white-line shifts and peak broadening with increasing Tb content, consistent with the modified unoccupied 4f states. Tb carries a strong local moment, raising the total moment to about 11.8 μB at higher doping. All compositions remain mechanically stable, and bulk and shear moduli increase moderately. The piezoelectric response also strengthens, with d33 and e33 roughly doubling compared to the undoped host. These results show that Tb substitution tunes the electronic, magnetic, optical, and mechanical behaviour of CaAlSiN*, supporting its potential in photonic and spin-related applications.

HL 1.11 Mon 12:15 POT/0006

Accurate computation of Berry connection purely limited by basis set completeness — Martin Thümmler[1], •Alexander Croy[1], Thomas Lettau[2], Ulf Peschel[2,3], and Stefanie Gräfe[1,3,4] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena — [2]Institute of Condensed Matter Theory and Optics, Friedrich Schiller University Jena — [3]Abbe School of Photonics, Friedrich Schiller University Jena — [4]Fraunhofer Institute for Applied Optics and Precision Engeneering Jena

Wannierization provides a reliable framework for interpolating operator matrix elements in the Brillouin zone. This Fourier-type interpolation of the matrix elements of **k**-local operators, e.g., the Hamiltonian, is well understood. However, the Berry connection is computed from the overlap matrices of the cell periodic parts of the Bloch functions with different **k** and hence non-local. So far, all proposed interpolation schemes do not account for the matrix structure of the overlap matrices, but treat the matrix elements as independent when computing the Berry connection. In this work, we propose a consistent interpolation scheme based on the matrix logarithm. Its accuracy is only limited by the basis set incompleteness of the considered bands in the ab-initio calculation. The quality of the new interpolation scheme is demonstrated by an improved agreement between the velocity and momentum operator over the full Brillouin zone. As an application, we demonstrate how this refinement impacts the predicted linear and non-linear optical properties of semiconductors.

HL 1.12 Mon 12:30 POT/0006

Focused Ion Beam (FIB) patterned Microcavities for Topological Lasers — •Lorenz Löffler[1,4], Dominik Horneber[1,4], Jakob Lindenthal[2,4], Johannes Düreth[1,4], Markas Sudzius[2,4], Monika Emmerling[1], Martin Kamp[3], Simon Betzold[1,4], Johannes Benduhn[2,4], Sven Höfling[1,4], Karl Leo[2,4], and Sebastian Klembt[1,4] — [1]University of Würzburg, Physikalisches Institut, Lehrstuhl für Technische Physik — [2]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP), and Institute of Applied Physics, Technische Universität Dresden — [3]University of Würzburg, Physikalisches Institut and Wilhelm-Conrad-Röntgen-Research Center for Complex Material Systems — [4]Würzburg-Dresden Cluster of Excellence ct.qmat

Topological lasers can be realized by coupling individual photonic resonators in topologically non-trivial lattice geometries. Optical microcavities have been found to be a promising platform for studying topological laser interfaces with long-range coherence. The fabrication of such structures typically involves etching of the microcavity and through the emitter layer. In our work, we create the photonic potential by FIB milling of a glass substrate prior to depositing dielectric Bragg reflectors. This technique allows the potential to be engineered while keeping the emitter layer intact. Here, the emitter is either semiconductor quantum wells or the organic semiconductor Alq_3 doped with DCM dye. By exploring modified lattice geometries that enhance the interface-to-bulk ratio as well as temperature-dependent studies, we aim for the next step towards practical topological lasers.

HL 2: Focus Session: Biocompatible Organic Semiconductors for Artificial Intelligence

This Focus Session deals with electronic components that interface with biological systems and offer diverse possibilities in research and applications, e.g., in healthcare. Carbon-based organic semiconductors are particularly well-suited to this interface: They enable electronic devices with a broad spectrum of electronic and optoelectronic functions that are biocompatible and often even resorbable by the body. Furthermore, they are particularly well-suited for neuromorphic functions that enable local data analysis computing towards artificial and neurohybrid intelligence. Turning this vision into practice requires extensive interdisciplinary research on semiconductor materials, components, and electronic systems. This Focus Session aims to provide an overview of the current state of the art including new organic materials, devices and core applications in bioelectronic interfaces.

Organized by Karl Leo

Time: Monday 9:30–12:45 Location: POT/0051

Invited Talk HL 2.1 Mon 9:30 POT/0051

Intrinsically stretchable polymers and devices for biosensing applications — •Ulrike Kraft — Organic Bioelectronics Research Group, MPI for Polymer Research, Mainz, Germany

Organic electrochemical transistors (OECTs) currently attract vast interest for biosensing applications due to their, intrinsic signal amplification and low operating voltages, enabling sensing in close contact to the human body and in aqueous environments with liquid analytes. Furthermore, the low elastic modulus of polymers can be tailored to match that of soft biological tissues, drawing increasing interest towards soft and stretchable health-monitoring devices.

The first part of the talk will focus on our work on biosensors based on planar OECTs that are functionalized with antibodies for e.g. the detection of the SARS-CoV-2 spike protein or with aptamers for the detection of e.g. cytokines, which are proteins crucial for immune regulation and inflammatory responses.

In the second part, I will summarize our efforts on stretchable electronics including a fast and reliable transfer-printing method for the deposition of conductive polymer films (e.g. PEDOT:PSS) onto stretchable, biodegradable substrates Taking advantage of this method and infusing the substrates with small-molecule plasticizers that also diffuse into the conductive films, improves the electrical performance as well as the mechanical properties. Lastly, this platform is employed for studying the effect of strain on the figures-of-merit of intrinsically stretchable OECTs.

Invited Talk HL 2.2 Mon 10:00 POT/0051

Complexity in Organic Mixed Ionic Electronic Conductors and its Application in Neuromorphic Computing — •Hans Kleemann — Technische Universität Dresden, Dresden, Germany

Complexity is decisive property enabling systems to work at the edge of chaos, which is necessary for resource-efficient computing and the design of intelligent machines. The complex behavior of a system originates from the nonlinear properties of all its components, resulting in a plethora of different signatures such as multi-state stability, stochastic oscillations, etc. These nonlinear properties and their couplings need to be understood and modeled to develop intelligent & energy-efficient computers.

Organic mixed ionic-electronic conductors (OMIECs) based on conjugated polymers open up a fascinating field of research where the ionic-electronic coupling, in combination with correlation effects at high charge carrier densities enables the implementation of various paradigms of neuromorphic computing. In this contribution, I will discuss the various signatures of nonlinearity and complexity that have been observed in OMIECs in recent years and review the current understanding of these effects. Furthermore, I will discuss how phenomena such as hysteresis and bistability can be employed to design fundamental elements of asynchronous computing, such as spiking neurons or C-elements, providing the foundation for the efficient implementation of approaches of stochastic computing in hardware. Finally, I will present a technology platform that allows us to integrate such devices in all-printed, complementary circuits operating above 1kHz.

Invited Talk HL 2.3 Mon 10:30 POT/0051

Organic Neuromorphic Interfaces for Biohybrid Systems: Material and Structural Biomimicry of Synaptic Plasticity — •Francesca Santoro — Forschngszentrum Jülich

Organic neuromorphic interfaces offer a promising route toward biohybrid systems that emulate neural function. We present PEDOT:PSS-based organic electrochemical transistors that exploit mixed ionic*electronic conduction and biocompatibility to reproduce key mechanisms of synaptic plasticity. Through the integration of bio-gels and azopolymer-functionalized conjugated polymers, neural activity is modulated by chemical and optical stimuli, enabling short- and long-term plasticity and interactions with neurotransmitters such as dopamine and glutamate. Beyond planar devices, 2.5D and 3D microfabricated organic semiconductor architectures fabricated by two-photon lithography or electrodeposition mimic neuronal morphology and promote cell adhesion and connectivity. The mechanical compliance of these materials supports stable interfacing with soft tissues, underscoring the role of material and structural biomimicry in next-generation organic biohybrid neuromorphic platforms.

15 min. break

Invited Talk HL 2.4 Mon 11:15 POT/0051

Fully-organic flexible detectors for real-time dose monitoring during radio/proton therapy — •Beatrice Fraboni — Department of Physics and Astronomy , University of Bologna, Italy

The development of detectors for high energy ionizing radiation is a long-lasting research topic not only for fundamental applications but also for medical applications in radio and hadron therapy. Innovative sensors are needed, able to provide, in-situ and in real-time, an accurate recording and mapping of the dose delivered during a treatment plan. Organic small molecules and polymers are promising active layers for advanced dosimetry purposes, as their mechanical features allow the development of devices able to adapt to complex contoured surfaces with outstanding portability (low power operation) and lightweight. They also provide the unique possibility to develop human-tissue-equivalent dosimeters, thanks to their density and composition. The physical process of radiation detection for organic thin- film based detectors will be discussed in two different configurations: 1) the direct one, based on a simple planar device with an organic thin film as active conversion layer, and 2) the indirect one, based on a polysiloxane-based scintillating layer effectively coupled to an organic phototransistor (OPT). A new kinetic model has been developed to describe the organic dosimeter response mechanism under photon/proton irradiation and to provide further insight into the physical processes controlling its response.

I.Fratelli et al Science Advances 11, 7633 (2025) S. Calvi et al., NPJ Flexible Electronics 7,5 (2023)

Invited Talk HL 2.5 Mon 11:45 POT/0051

Organic LEDs and photodetectors for light-based diagnostics and therapy — •Caroline Murawski[1,2], Rabiul Islam[1,2], Siddhartha Saggar[1,2], and Jens P. Weber[1,2] — [1]Institute of Solid-State Electronics, TUD Dresden University of Technology, 01062 Dresden, Germany — [2]Kurt Schwabe Institute for Sensor Technologies, 04736 Waldheim, Germany

Light-based biomedical sensing and therapy enables highly precise, timely and contactless interventions and range from neuronal stimulation via optogenetics over sensing cellular activity by functional fluorescence to monitoring health signals using wearable devices. Organic semiconductors are ideally suited building blocks due to their tunability of material properties, mechanical flexibility and ability for patterning to microscopic shapes. Here, I will present the development of organic LEDs (OLEDs) and photodiodes (OPDs) as light sources and sensors for biomedical applications. The OLEDs are tailored towards high power output and application-specific angular and spectral emission properties. Devices are fabricated on flexible substrates, patterned to sub-mm scale, and applied in optogenetics and fluorescence imaging. Furthermore, I will show flexible OPDs used for photoplethysmography at ambient light conditions and under water.

HL 2.6 Mon 12:15 POT/0051

Reservoir computing with mixed ionic-electronic conductors — •Richard Kantelberg, Hans Kleemann, and Karl Leo — Institut für Angewandte Physik, TU Dresden

Reservoir computing (RC) is a promising paradigm for machine learning that utilizes dynamic systems, termed as reservoirs, to process and analyze complex temporal data. Organic mixed ionic electronic conductors (OMIECs) have emerged as a novel class of materials with intriguing properties, such as their ability to exhibit both electronic and ionic conductivity, as well as their biocompatibility, flexibility, and low power consumption[1]. These features make OMIECs particularly suitable for the development of unconventional computing architectures in the field of bioelectronics[2]. We present recent findings interlinking electronic conductivity, system nonlinearity and reservoir size with the

neuromorphic functionality and RC performance of self-organized and structured OMIEC reservoirs. This study includes novel insights into the differences and similarities of p-type, n-type and ambipolar semiconductors in terms of operation speed and energy consumption. The recent progress in reservoir computing using organic mixed ionic electronic provides valuable knowledge for the targeted development OMIEC reservoirs.

References 1.*Paulsen, B. D., Tybrandt, K., Stavrinidou, E. & Rivnay, J. Organic mixed ionic*electronic conductors. Nat. Mater. 19, 13*26 (2020). 2.*van de Burgt, Y., Melianas, A., Keene, S. T., Malliaras, G. & Salleo, A. Organic electronics for neuromorphic computing. Nat. Electron. 1, 386*397 (2018).

HL 2.7 Mon 12:30 POT/0051

Redundant information in physical reservoir computing — •Andreas Hofacker, Richard Kantelberg, Hans Kleemann, and Karl Leo — Dresden Integrated Center for Applied Physics and Photonic Materials (DC-IAPP), TU Dresden, Dresden, Germany

Maximizing the processing power of a physical reservoir given its physical constraints is crucial for practical applications, but remains an open problem. As a basis for such an optimization, a quantity measuring reservoir capability is needed. To address this need, we propose the use of independent component analysis for assessing information content in reservoir outputs. We present evaluations of organic mixed ionic-electronic conductor based physical and simulated reservoirs and show that task-specific performance is linked to information redundancy in the output channels. By leveraging this insight, sparser reservoir readout can be realised without loss of performance.

HL 3: 2D Materials I – Excitonic properties

Time: Monday 9:30–12:45 Location: POT/0081

HL 3.1 Mon 9:30 POT/0081

Exciton-Electron Complexes in Multilayer Transition-Metal Dichalcogenides — •Florian Hirsch[1], Alexandra Hübler[1], Jonas von Milczewski[2], and Richard Schmidt[1] — [1]Institute for Theoretical Physics, Heidelberg University, Philosophenweg 16, 69120 Heidelberg, Germany — [2]Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

Understanding few-body correlations in van der Waals heterostructures is essential for uncovering emergent electronic phases in layered quantum materials. We report recent progress in identifying exciton-electron-electron bound states in multilayer transition-metal dichalcogenides (TMDs). Starting from the two-body problem, we employ complementary theoretical approaches to characterize bound states and systematically extend this framework to the four-body regime. Within an effective-mass model, we solve the resulting few-body Hamiltonians using exact diagonalization, enabling efficient exploration of material and geometric parameters. This allows us to map out regimes in which such exciton-electron complexes become bound. Our results provide a versatile framework for investigating exciton-mediated correlations in complex multilayer TMD structures and related systems, including platforms where exciton-induced electron pairing or superconductivity may emerge.

HL 3.2 Mon 9:45 POT/0081

Intra- and Interlayer Excitons in TMDC bilayers under external influence — •Jan-Hauke Graalmann and Michael Rohlfing — University of Münster, Institute of Solid State Theory, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany

External influences lead to several changes in the optical spectrum of TMDC bilayers obtained by solving the Bethe-Salpeter. We discuss both the effect of applied pressure and that of an electric field [1,2].

To get the deformation induced by applied pressure, we use Hooke's law. In this case, our investigations show an effective shift of the intralayer A exciton whose direction depends on the stress conditions and we observe a similar behavior for the interlayer exciton, while the shift rate is smaller for the latter. Our results for the 2H-MoS_2 bilayer compare very well with available room-temperature measurements for the interlayer exciton.

An electric field applied perpendicular to the 2H-$MoSe_2$ bilayer does not lead to a deformation, but instead to a Stark shift of the excitons. To explain that, we focus on the lifting of the degeneracy in the band structure by breaking the symmetry of the potential.

[1] P. Steeger, J. Graalmann et al., nano Lett., 23, (2023)
[2] J. Jasiński et al., Nat Commun 16, 1382, (2025)

HL 3.3 Mon 10:00 POT/0081

Optical probing of the gate-tunable electronic band structure of bilayer graphene using a WSe_2 sensor layer — •Jonas Blum[1], David Tebbe[1], Takashi Taniguchi[2], Kenji Watanabe[2], Lutz Waldecker[1], Christoph Stampfer[1,3], and Bernd Beschoten[1] — [1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, Aachen, Germany — [2]National Institute for Materials Science, Namiki, Tsukuba, Japan — [3]PGI-9, Forschungszentrum Jülich, Jülich, Germany

Rydberg excitons in transition-metal dichalcogenide monolayers are highly sensitive to their dielectric environment. Previous work has shown that reflection-contrast spectroscopy provides a non-invasive optical probe of their binding energies, enabling the detection of subtle variations in the charge-carrier density n in adjacent layers of van der Waals (vdW) heterostructures. Here, we apply this technique to a fully hBN-encapsulated WSe_2/bilayer-graphene (BLG) device with graphite top and bottom gates and compare the optical response with transport measurements. By applying a displacement field D, we open a band gap in BLG. As the Fermi level is tuned from the valence band across the band gap into the conduction band, we capture changes in n through shifts in the 2s exciton binding energy. These measurements further allow us to resolve the layer population of BLG upon sign reversal of D. We also demonstrate optical quantum Hall measurements, enabling extraction of gate lever arms optically. Unlike transport measurements, this optical technique offers highly local, spatially-resolved access to the electronic band structure of BLG.

HL 3.4 Mon 10:15 POT/0081

Anisotropic Excitonic Response in $MoSe_2$-WSe_2 Lateral Heterostructures — •Miguel Morales Cocera[1,2], Franz Fischer[1,2], Carl Emil Mørch Nielsen[1], and Gabriel Bester[1] — [1]University of Hamburg, Institute of Physical Chemistry, 22761 Hamburg, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg, Germany

We investigate lateral heterostructures of transition-metal dichalcogenide monolayers, in particular $MoSe_2$-WSe_2. In these systems, the one-dimensional (1D) interface together with the type-II band alignment enables the emergence of 1D exciton physics within a two-dimensional monolayer material, with the "interlayer" excitons retaining near monolayer-level brightness. Motivated by the recent experimental observation of these spatially indirect excitons [1], we calculate the exciton and trion fine structure using ab initio many-body screened configuration interaction [2]. We find that the lowest bright exciton state is non-degenerate due to the loss of symmetry induced by the 1D interface. Moreover, the many-body dipoles of these two excitons lie along different in-plane polarization axes, leading to an anisotropic optical response that may be useful for optoelectronic applications.

[1] R. Rosati, et al., Nat. Commun. 14, 2438 (2023)
[2] Mørch Nielsen, C.E., Fischer, F. & Bester, G. npj 2D Mater. Appl. 9, 11 (2025)

HL 3.5 Mon 10:30 POT/0081

Substrate interaction on local exciton/trion ratio in mono- to few-layer WS2 — •Appanna Parvangada[1,2], Dmitrii Sychev[1], and Ilka Hermes[1] — [1]Leibniz Institute of Polymer Research Dresden e.V., Dresden, Germany — [2]Institute of Applied Physics, Dresden University of Technology, Dresden, Germany

Two-dimensional Tungsten Disulfide (WS2) possesses distinctive optoelectronic properties such as high photoluminescence yield, a tunable band gap, large exciton binding, quantum confinement, strong-light matter interaction. The combination with low dimensionality makes them a favorable candidate for a variety of lightweight and flexible optoelectronic devices such as photodetectors, solar cells and LEDs.

However, large-scale industrial implementation of optoelectronic 2D materials is often impeded by their high spatial heterogeneity, caused by nanoscale variations in layer thickness, substrates interactions and local strain. Thus, standard optical characterization methods like Photoluminescence (PL) and Raman spectroscopy, which commonly provide such information, can lack the spatial resolution to resolve these variations. Here, electrical atomic force microscopy (AFM) methods with in-situ illumination at different wavelengths deliver nanoscale information on the impact of layer thickness, changes in substrates interactions and local strain onto the material's optoelectronic response.

In our study, we demonstrate the capability of photo-Kelvin probe force microscopy (pKPFM) to capture local photo-potential in mono- and few-layer WS2 and correlate PL spectroscopy. Furthermore, we investigate the impact of substrates on the local charge carriers.

HL 3.6 Mon 10:45 POT/0081

Signatures of efficient intervalley scattering by acoustic phonons in WSe2 monolayers — •Hendrik Lambers[1], Daniel Groll[2], Daniel Wigger[2], Nihit Saigal[1], Lara Blinov[1], Tilmann Kuhn[2], Alexander W. Holleitner[3], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster — [2]Institute of Solid State Theory, University of Münster — [3]Walter Schottky Institute, Technical University of Munich

When group VI TMDC are thinned down to the monolayer limit, their bandgap transfers from indirect to direct. While their strong exciton dominated light-matter coupling can be easily investigated by optical spectroscopy, exciton-phonon coupling is often inaccessible, even though it is important for exciton thermalization and intervalley scattering. We employ resonant Raman scattering at cryogenic temperatures to study the exciton phonon coupling in WSe_2 monolayers. In resonance with the WSe_2 exciton, we observe rich Raman spectra. Here, we focus on the resonance profiles of the degenerated A_1'/E' mode, that exhibits two asymmetric resonance peaks that cannot be described by a first order Raman scattering process. A higher-order Raman scattering process including simultaneous generation and annihilation of acoustic M-point phonons describes the experimental resonance profile well. Our results indicate a strong electron phonon coupling and efficient intervalley scattering between the nearly degenerate direct and indirect exciton transitions in WSe_2. The findings are relevant to understand unusual bright emission in WSe_2 monolayers despite spin-forbidden lowest interband transition.

15 min. break

HL 3.7 Mon 11:15 POT/0081

Transport of exciton complexes in the presence of Fermi sea of free carriers in monolayer semiconductors — •Minushree Rout[1], Koloman Wagner[1,2], Jonas Ziegler[1,2], Raul Perea-Causin[3], Samuel Brem[4], Ermin Malic[4], and Alexey Chernikov[1] — [1]Institute of Applied Physics, Technische Universität Dresden, Germany — [2]Department of Physics, University of Regensburg, Germany — [3]Department of Physics, Stockholm University, Sweden — [4]Department of Physics, Philipps-Universität Marburg, Germany

Exciton-carrier interactions in doped monolayer semiconductors present an interesting and technologically relevant scenario in solid-state physics. Among the consequences is the formation of trions-three particle system formed when excitons bind with free charge carriers. Here, we aim to explore how trion-phonon and exciton-carrier interactions influence excitonic quasiparticle diffusion using transient microscopy. Theoretical results predict that trions have reduced mobility at low carrier densities due to strong phonon coupling and increased mass. At higher densities, effective trion diffusion should increase significantly due to the Fermi pressure effect. Previous experimental studies revealed that exciton diffusion shows a non-monotonic dependence on carrier density, transitioning from elastic scattering regime to the formation of bound quasiparticle states like trions and fermi-polarons. This work aims to uncover the fundamental mechanisms governing the transport of light-emitting quasiparticles in the presence Fermi-bose mixtures in 2D semiconductors and experimentally test the prediction of the Fermi-pressure effect.

HL 3.8 Mon 11:30 POT/0081

Investigation of dynamics and character of excitons in WSe_2 and $MoSe_2$ multilayers — •Anna Weindl[1], Matthias Brem[1], Jennifer Lehner[1], Kenji Watanabe[2], Takashi Taniguchi[3], and Christian Schüller[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93053 Regensburg — [2]Research Center for Functional Materials, National Institute for Materials Science, Tsukuba Ibaraki 305-0044, Japan — [3]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Tsukuba Ibaraki 305-0044, Japan

We report about our time-resolved Faraday ellipticity (TRFE) experiments on multilayers of the transition metal dichalcogenide WSe_2 and $MoSe_2$. In a continuation of our recent work by Raiber et al. [1], we aim to investigate the nature of the pseudospin oscillations that appear in the TRFE signal when we apply an in-plane magnetic field to our multilayer samples. Now we try to characterize and manipulate these oscillations by playing with different experimental parameters. Varying the angle of the magnetic field, adding an electric field or investigating the layer dependence are examples for our toolbox of parameters to gain further insights into the dynamics of the multilayers. The current results, for example on the resonance behavior of the oscillations and the layer-dependent starting point of the oscillations, will be presented.

[1] S. Raiber *et al.*, Ultrafast pseudospin quantum beats in multilayer WSe_2 and $MoSe_2$, Nat. Commun. 13, 4997 (2022).

HL 3.9 Mon 11:45 POT/0081

In-situ mapping of pressure-induced exciton traps in suspended MoS2 monolayers using Fabry-Perot interference — •Niklas Walter[1,3], Leonard Geilen[1,3], Lukas Schleicher[2,3], Alexander Musta[1,3], Anne Rodriguez[3], Benedict Brouwer[1,3], Eva Weig[2,3], and Alexander Holleitner[1,3] — [1]Walter Schottky Institute, TU Munich, Germany — [2]Chair of Nano and Quantum Sensors, TU Munich, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany

We demonstrate the in-situ readout of the spatial profile of suspended MoS2 monolayers hosted on substrates with nanostructured holes. As the profiles are spatially bent, the suspended MoS2 monolayers act as exciton traps with a tunable luminescence intensity and energy. The tunability is realized by controlling the environmental pressure on the monolayers, which allows one to control hundreds of suspended MoS2 monolayers on a single substrate. The in-situ readout is based on Fabry-Perot interferences and a model of the corresponding reflectance contrast maps of the investigated monolayers.

HL 3.10 Mon 12:00 POT/0081

Coherent two-dimensional electronic spectroscopy integrated with confocal microscopy for probing 2D materials — •Trideep Kawde, Pavel Trofimov, Matteo Russo, Anton Trenczek, and Hélène Seiler — Freie Universität Berlin, 14195, Berlin, Germany

Two-dimensional electronic spectroscopy is a powerful tool for probing ultrafast processes in van der Waals materials and heterostructures. As these structures are typically only 10x100 μm in size and highly heterogeneous, the challenge of ultrafast studies on such materials is to balance requirements in spatial and angular resolutions - often requiring highly dispersive microscope objectives - with temporal resolution. We present a coherent 2D electronic spectroscopy setup integrated with a confocal back focal plane imaging setup, featuring high magnification, spatial and angle resolution, while maintaining a time resolution of ~15 femtosecond. We demonstrate this approach on an exfoliated WSe_2 monolayer. The data reveal <100 femtosecond homogeneous linewidth broadening of the A exciton lineshape, indicating rapid exciton-energy fluctuations. These measurements provide insight into dephasing mechanisms such as excitation-induced dephasing, which sets fundamental limits to coherent control and quantum-optical applications.

HL 3.11 Mon 12:15 POT/0081

Acousto-optic characterization of van der Waals systems — •Felix Ehring, Benjamin Mayer, Hubert Krenner, Ursula Wurstbauer, and Emeline Nysten — Institute of Physics, University of Münster, Germany

With wavelengths in the micrometer range at GHz frequencies, surface acoustic waves (SAWs) are a versatile tool for radio frequency control and probing of charge carrier dynamics in novel semiconductor nanostructures. They are generated on a piezoelectric chip and routed over long distances to couple either mechanically or electrically to many solid-state nanosystems [1]. In our experiments, we fabricated hybrid lithium niobate SAW-devices in which different mechanically exfoliated transition metal dichalcogenide (TMDC) 2D materials were transferred. We investigated the influence of SAW-induced dynamic electric and strain fields on the photoluminescence (PL) of various TMDCs and their heterostructures. By combining optical and acoustic measurements, we were able to gain insights on the charge carrier dynamics and their resulting impact on exciton recombination and lifetime [2].

[1] Per Delsing et al 2019, J. Phys. D: Appl. Phys. 52 353001 [2] Emeline Nysten et al 2024, Adv Mater 36 e2402799

HL 3.12 Mon 12:30 POT/0081

Dark exciton activation in WSe_2 monolayer by tip-enhanced photoluminescence spectroscopy — Adlen Smiri, Fenda Rizky Pratama, and •Takeshi Nakanishi — MathAM-OIL AIST, Sendai, Japan

Dark excitons in 2D transition metal dichalcogenide semiconductors are characterized by long lifetimes, making them highly attractive candidates for quantum computing and optoelectronics.The purpose of this paper is to theoretically address the interactions between local electromagnetic fields and dark excitonic states, and show that the strong out-of-plane near field from a metallic tip enhances radiative recombination of spin-forbidden dark excitons by providing additional in-plane momentum to overcome momentum mismatch [1]. Using ab initio calculations, a Wannier-Mott exciton model, and a numerical solution of the Laplace equation, we model the tip-enhanced near-field and its interaction with excitons via first-order time-dependent perturbation theory. Focusing on WSe_2 monolayers, we demonstrate that the activation of dark excitons is attributed to the strong z-component of the near field induced by the tip. We also analyze substrate screening effects on excitonic properties and lifetimes. Our results offer a theoretical framework for controlled activation of dark excitons toward quantum and nanophotonic applications.

[1] Adlen Smiri, F. R. Pratama and Takeshi Nakanish, npj 2D Materials and Applications 9, 88 (2025)

HL 4: Perovskite and Photovoltaics: Synthesis and Performance

Time: Monday 9:30–12:00 Location: POT/0251

Invited Talk HL 4.1 Mon 9:30 POT/0251

X-ray nanodiffraction studies of lead-halide perovskite supercrystals — Jonas Hiller[1], Robert Thalwitzer[1], Ata Bozkurt[1], Matheus Ferreira[2], Richard Hodak[1], Fabian Strauss[1], Elke Nadler[1], Gerard Hinsley[3], Bihan Wang[3], Kuan Hoon Ngoi[3], Witold Rudzinski[4], Ekaterina Kneschaurek[1], Wojciech Roseker[3], Michael Sprung[3], Dmitry Lapkin[1], Dmitry Baranov[2], Frank Schreiber[1], Ivan Vartanyants[3], Marcus Scheele[1], and •Ivan Zaluzhnyy[1] — [1]University of Tübingen — [2]Lund University — [3]Deutsches Elektronen-Synchrotron DESY — [4]University of Krakow

We synthesize mechanically robust supercrystals built from cubic lead halide perovskite nanocrystals by a two-layer phase diffusion self-assembly with acetonitrile as the antisolvent. This method yields highly faceted thick supercrystals, which are robust enough to be picked up and relocated by microgrippers. We employed X-ray nanodiffraction together with high-resolution scanning electron microscopy and atomic force microscopy to reveal the structure of $CsPbBr_3$, $CsPbBr_2Cl$, and $CsPbCl_3$ supercrystals and explain their unusual mechanical robustness. We show that the removal of organic ligands from perovskite nanocrystals results in a size gradient of the nanocrystals within the supercrystals.

Hiller et al., ACS Nano **19** (2025) 26117

HL 4.2 Mon 10:00 POT/0251

Impact of Antisolvents on Halide Perovskite Nanocrystal Synthesis — •Tim Julius Hashagen, Leo Luber, and Alexander Skyrme Urban — Nanospectroscopy Group, Nano-Institute Munich, Department of Physics, Ludwig-Maximilians-Universität München, Königinstraße 10, 80539 Munich, Germany

Lead halide perovskite nanocrystals (NCs) offer highly tunable optical properties and high photoluminescence efficiencies, making them promising for optoelectronic and photocatalytic applications. Their synthesis, however, is extremely sensitive to the choice of antisolvent, which governs nucleation and growth kinetics and thereby the structural and optical quality of the resulting NCs. [1] In this work, we systematically investigate how structural and chemical variations among antisolvents affect the formation of CsPbBr2 NCs. By tuning precursor compositions and antisolvent identities, we identify clear trends in crystallization behavior and photoluminescence characteristics. These experimental results are combined with a Gaussian Process regression model that encodes antisolvent geometry to predict NC emission wavelengths.[2] The model performs accurately for well-represented antisolvent classes but still faces challenges when extrapolating to sparsely sampled or previously unseen antisolvents. Our combined experimental and data-driven approach highlights the decisive role of antisolvent molecular structure in NC synthesis and demonstrates a pathway toward predictive control over perovskite nanocrystal properties.

[1]K. Frank et al., Nat. Commun. 2024, 15, 8952.
[2]N. A. Henke et al., Adv. Mater. 2025, e09472.

HL 4.3 Mon 10:15 POT/0251

Tuning Lead Halide Perovskite Nanocrystal Properties via Controllable Synthesis and Machine-Learning Insights — •Maximilian Dörfler, Leo Luber, and Alexander Urban — Nanospectroscopy Group, Nano-Institute Munich, Department of Physics, Ludwig-Maximilians-Universität München, Königinstraße 10, 80539 Munich, Germany

Halide perovskite nanocrystals (NCs) combine high photoluminescence efficiency with tunable emission, but achieving narrow linewidths requires tightly controlled, highly monodisperse synthesis. In this work, we perform in situ observations of CsPbBr3 NC formation under ambient conditions and systematically evaluate how synthesis parameters shape their optical response. By analyzing the evolving photoluminescence spectra, we assess how reaction time, dilution, and precursor-to-antisolvent ratios jointly influence crystal growth and resultant morphology. The in situ approach allows us to track nanocrystal growth pathways and provides the opportunity for real-time steering of the synthesis. Particular emphasis is placed on understanding the conditions under which the NCs adopt 2D versus 3D morphologies. In future work, we will employ machine-learning tools - specifically Bayesian optimization - to efficiently navigate the sparsely sampled synthesis parameter space. This data-driven strategy aims to identify regions that yield high quantum efficiencies and narrow linewidths, enabling rapid discovery of conditions that favor predominantly monodisperse nanocrystals or nanoplatelets with minimal experimental iteration.

HL 4.4 Mon 10:30 POT/0251

Scalable Perovskite-Silicon Tandem Photovoltaics by Hybrid 2-Step Inkjet Printing — •Theresa Kuechle[1], Raphael Pesch[1,2], Jinzhao Li[1,2], and Ulrich W. Paetzold[1,2] — [1]Light Technology Institute, KIT, Germany — [2]Institute of Microstructure Technology, KIT, Germany

In recent years, the power conversion efficiency (PCE) of perovskite-silicon tandem photovoltaics has improved significantly on a lab scale. For photovoltaics industry, fully scalable processes are required to ensure homogeneous thin-film formation while maintaining conformity to the bottom cell.

Here, we show a hybrid two-step process for the perovskite thin film fabrication whereby inorganic components are evaporated, followed by inkjet printing of organic components. Our approach addresses scalability challenges and highlights the suitability of inkjet printing with a green solvent for the fabrication of large textured tandem solar cells. We show that optimizing the stoichiometry is necessary and can be achieved by fine-tuning the dots per inch in the second step. Through inkjet printing parameter optimization, we achieve wide-band gap single-junction perovskite solar cells with close to 20 % PCE. Additionally, we successfully fabricate large-textured (3 to 5 μm pyramid size) tandem solar cells with an active area of 1 cm^2, achieving a single-JV-scan PCE of 27.4 %. These results underscore the potential of this hybrid fabrication process to overcome upscaling hurdles and advance the development of highly efficient tandem solar cells for industrial applications.

HL 4.5 Mon 10:45 POT/0251

A Materials Perspective on Sequential Inorganic Scaffold Deposition for Hybrid-Processed Perovskite Thin Films — •Ronja Pappenberger[1,2], Julian Petry[1,2], Alexander Welle[3,4], Tonghan Zhao[1], Alexander Diercks[2], Raphael Pesch[1,2], Paul Fassl[1,2], and Ulrich W. Paetzold[1,2] — [1]Institute of Microstructure Technology, KIT, Germany — [2]Light Technology Institute, KIT, Germany — [3]Institute of Functional Interfaces, KIT, Germany — [4]Karlsruhe Nano Micro Facility, KIT, Germany

As perovskite solar cells (PSCs) advance toward industrial-scale production, fabrication processes must combine high-throughput with simple integration. In this regard, the hybrid two-step deposition route has emerged as a promising method, allowing for conformal coatings on micron-scale textures, a critical feature for perovskite/silicon tandem photovoltaics. This work presents a fully sequential route, wherein the inorganic materials CsCl and PbI_2 are deposited separately, simplifying industrial implementation compared to co-deposition. Microstructural analysis shows that sequential deposition promotes vertical PbI_2 growth with a secondary tilted orientation, unlike the horizontal orientation from co-deposition. Elemental distribution reveals high diffusivity for Cs, formamidinium, and I, yielding a homogeneous distribution in the perovskite absorber, while Pb and Cl remain largely scaffold-bound. PSCs with a 1.69 eV bandgap achieve efficiencies of 19.3% (co-deposition) and 18.7% (sequential), highlighting fully sequential hybrid deposition as a promising route toward industrial PSC production.

15 min. break

HL 4.6 Mon 11:15 POT/0251

How stable are mixed-metal chalcohalides? — •Pascal Henkel[1], Jarno Laakso[1], Jingrui Li[2], and Patrick Rinke[1,3] — [1]Department of Applied Physics, Aalto University, Espoo, Finland — [2]Xi'an Jiaotong University, Xi'an, China — [3]Technical University of Munich, Garching, Germany

Perovskite-inspired quaternary mixed-metal chalcohalides (MMCHs, $M(II)_2M(III)Ch_2X_3$) are an emerging materials class for photovoltaics,[1,2] capable of delivering high conversion efficiencies.[3] Yet, their thermodynamic stability remains largely unexplored.

We assess the thermodynamic stability of 54 MMCH compounds by modelling their phase diagrams using DFT, *pymatgen* tools from Materials Project[4] and the Alexandria Materials Database.[5] All studied MMCHs lie above the convex hull, independent of their space group ($Cmcm$, $Cmc2_1$, $P2_1/c$). Accounting for computational uncertainty (mostly from the applied exchange-correlation functional) moves a considerable fraction of MMCHs close to or below the hull. The MMCH decomposition paths follow five reactions, with $4\,M(II)_2M(III)Ch_2X_3 \leftrightarrow 2\,M(III)_2Ch_3 + 6\,M(II)X_2 + 2\,M(II)Ch$ occurring most frequently. Experiments show that compounds close to the convex hull can be synthesized, whereas compounds far from the hull decompose following the predicted reactions. Overall, our results show that MMCHs are synthesizable, but fabrication conditions need further optimisation.

[1] *Chem. Mater.* **35**, 7761-7769 (2023), [2] *Phys. Rev. Materials* **9**, 115405 (2025), [3] *Mater. Horiz.* **8**, 2709 (2021). [4] *Chem. Mater.* **20**, 1798-1807 (2008). [5] https://alexandria.icams.rub.de/.

HL 4.7 Mon 11:30 POT/0251

minimizing ionic losses in DMSO-free tin-based perovskite solar cells — •Paria Forozi Sowmeeh[1], Shengnan Zuo[2], Chiara Frasca[2], Biruk Alebachew Seid[1], Sercan Ozen[1], Wentao Liu[2], Mahmoud Hussein Aldamasy[2], Yuan Zhang[3], Fengshuo Zu[2,3], Norbert Koch[2,3], Martin Stolterfoht[4], Antonio Abate[2], Artem Musiienko[2], and Felix Lang[1] — [1]Institute of Physics and Astronomy University of Potsdam, Potsdam-Golm, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [3]Department of Physics, Humboldt University of Berlin, Berlin,

Germany — [4]Electronic Engineering Department, The Chinese University of Hong Kong, Hong Kong SAR, China

The presence of mobile ions and the potential toxicity of Pb-based perovskite solar cells remain two major drawbacks for their commercialization despite their exceptional optoelectronic properties. On the other hand, Sn-based perovskites, which are believed to exhibit smaller ion-induced instabilities, have been revealed as eco-friendly perovskite counterparts, though thorough investigations are still missing. Herein, we investigate the nature of mobile ions, quantify the ionic loss within Sn-based perovskite solar cells and compare with those of Pb-based and mixed PbSn devices. We report minimal ionic losses and over 10-fold lower ion densities in DMSO-free processed Sn samples compared to Pb-based perovskites. The Sn-based devices also exhibit the lowest associated ionic losses with sustained device stability upon illumination. This study paves the way for development of innovative, stable thin film solar cells with suppressed ion migration.

HL 4.8 Mon 11:45 POT/0251

Beyond 1D: How Edge Effects Impact Ion Densities and Stability in Perovskite Solar Cells — •Jarla Thiesbrummel[1,2], Francisco Peña-Camargo[2], Bruno Ehrler[3], Dilara Abdel[4], Patricio Farrell[4], and Felix Lang[1] — [1]University of Potsdam, Potsdam, Germany — [2]Helmholtz-Zentrum zu Berlin, Berlin, Germany — [3]AMOLF, Amsterdam, Germany — [4]Weierstrass Institut, Berlin, Germany

Understanding how mobile ions redistribute within metal halide perovskites is essential for interpreting device stability and quantitative ion-density measurements. While most studies focus on ion transport along the device stack, lateral ion motion and edge effects remain relatively unexplored, despite their strong relevance, especially in small-area, lab-scale photovoltaic devices. In this work, we investigate side collection of ions at device edges and its consequences for both apparent ion densities and long-term material stability, using a combination of 2D drift-diffusion simulations and experiments.

HL 5: 2D Materials: Electronic structure, excitations, etc. I (joint session O/HL/TT)

Time: Monday 10:30–12:30 Location: TRE/MATH

See O 7 for details of this session.

HL 6: Focus Session: Tunable Correlations in van der Waals Quantum Materials I (joint session TT/DS/HL)

The library of strongly correlated layered materials has intensively grown, giving now access to the full breadth of symmetry broken emergent phases, ranging from excitonic, to magnetic, superconducting, or Mott insulating ground states. At the same time, also the ways of tuning these correlated phases in 2D are steadily developing, e.g, via twisting or stacking, engineered defects, or applied external fields. Taken together, this nowadays allows for sheer endless possibilities to tailor layered correlated quantum materials on demand opening unprecedented avenues towards both deep insights into emergent phenomena and novel functionalization routes based on many-body properties.

This focus session will highlight recent advancements and breakthroughs achieved in this field, which we expect to be of great interest to the broadest audience and to stimulate discussions crossing field boundaries.

Coordinators: Lennart Klebl (Uni Würzburg, Jonas Profe (Uni Frankfurt), Malte Rösner (Uni Bielefeld), Ursula Wurstbauer (Uni Münster)

Time: Monday 15:00–18:15 Location: HSZ/0003

See TT 12 for details of this session.

HL 7: 2D Materials beyond graphene: Growth, structure and substrate interaction (joint session O/HL/TT)

Time: Monday 15:00–17:45 Location: HSZ/0204

See O 10 for details of this session.

HL 8: Ultra-fast Phenomena I

Time: Monday 15:00–18:15 Location: POT/0006

HL 8.1 Mon 15:00 POT/0006

Lightwave Engineering of Excitonic States in an Atomically Thin Semiconductor — •Omer Kneller[1], Niloufar Nilforoushan[1], Matthias Knorr[1], Markus Borsch[2], Fabian Mooshammer[1], Mackillo Kira[2], and Rupert Huber[1] — [1]Department of Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Department of Electrical Engineering and Computer Science, University of Michigan, Ann Arbor, Michigan 48109, USA

Coherently shaping excitonic states holds great potential for novel optoelectronics and quantum information processing. Yet, their femtosecond-scale coherence time substantially constrains coherent control. Here, intense phase-stable carrier waves of light resonantly drive the excitonic 1s-2p states in monolayer $MoSe_2$ faster than their natural decoherence rate, driving the excitonic system into multiple Rabi oscillations that occur during a single cycle of light. The dynamics are probed by injecting excitons into the 1s state using femtosecond NIR pulses and measuring the induced high-order sideband emission. The signal exhibits surprising spectro-temporal signatures that are reproduced by many-body simulations and a reduced two-level model, exposing the dominant role of the 1s-2p sub-system, even under these extreme driving conditions. An intuitive Floquet analysis links these features to light-induced avoided crossings between higher-order Floquet replicas of the driven two-level system. Our results bridge lightwave electronics in quantum materials, attosecond science, and atomic physics, and establish an exciting new route to shaping many-body quantum correlations at optical clock rates.

HL 8.2 Mon 15:15 POT/0006

Light-Induced Polarization Switching in R-Stacked Bilayer WSe_2 — •Xiangzhou Zhu, Stefono Mocatti, and Matteo Calandra — Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy

Sliding ferroelectricity in two-dimensional van der Waals materials enables polarization control by relative layer motion, offering a promising platform for novel memory devices. Recent works show that strong laser pulses can reverse the polarization of such systems by driving shear phonons, but the required interlayer sliding and structural distortions limit the achievable switching speed. Here, we demonstrate a purely electronic pathway for light-induced po-

larization reversal in rhombohedrally stacked bilayer transition-metal dichalcogenides (TMDs). With constrained density-functional theory (cDFT), we find that photoexcited carrier densities below 0.2 e per unit cell are sufficient to switch the intrinsic ferroelectric dipole without interlayer sliding in WSe_2. This occurs because photoexcitation induces an imbalanced charge redistribution between the layers, which generates a counter-dipole. Using real-time semiconductor Bloch equation simulations, we shows that the total polarization can reverse by light within a few hundred femtoseconds. Furthermore, time-dependent charge analysis reveals that this ultrafast switching is primarily driven by a localized dipole rearrangement around the tungsten sites. These results establish a new mechanism for electronic control in 2D ferroelectrics, relevant for high-speed volatile memory applications.

Funded by the European Union (ERC, DELIGHT, 101052708)

HL 8.3 Mon 15:30 POT/0006

Ultrafast excitonic coherent oscillations in monolayer tungsten disulphide — •Jorge Cervantes Villanueva[1], Davide Sangalli[2], Alberto García-Cristóbal[1], and Alejandro Molina-Sánchez[1] — [1]Institut de Ciència dels Materials (ICMUV), Universitat de València, Catedrático José Beltrán 2, 46980 Paterna, Valencia, Spain — [2]Istituto di Struttura della Materia-CNR (ISM-CNR), Area della Ricerca di Roma 1, Monterotondo Scalo, Italy

Understanding coherent excitonic dynamics in two-dimensional semiconductors is crucial for advancing quantum-optical technologies. Monolayer transition metal dichalcogenides (TMDs) provide an ideal platform due to their strong Coulomb interactions and large exciton binding energies. We perform ab initio pump-probe simulations by propagating the time-dependent density matrix under the influence of overlapping pump and probe fields, capturing the generation and detection of coherent excitons on femtosecond timescales. Focusing on monolayer WS2 with a pump tuned between the A and B excitons, we observe ultrafast oscillations arising from coherent coupling among multiple excitonic states, including the intermediate A* resonance. Exploiting the balance between exciton populations, we propose a scheme to control the coherent response, realizing an optical switch with potential applications in quantum information. These results establish ab initio pump-probe modeling as a predictive tool for characterizing and manipulating coherent excitonic states.

HL 8.4 Mon 15:45 POT/0006

Carrier-envelope phase control of ultrafast photocurrents in layered MoS2 — •Johannes Schmuck[1,2], Björn Sinz[1,2], Nina Pettinger[1,2], Sergey Zherebtsov[1,2], and Alexander W. Holleitner[1,2] — [1]Walter Schottky Institute and Physics Department, Technical University of Munich, Garching, Germany — [2]Munich Center of Quantum Science and Technology, Munich, Germany

We demonstrate carrier-envelope-phase (CEP)-controlled photocurrents in mono-, bi-, and tri-layer MoS2 driven by few-cycle laser pulses. The photocurrent in the two-terminal devices scale quadratically with the field amplitude, indicating perturbative carrier dynamics in the weak-field regime distinct from strong-field tunnelling [1]. Our results extend light-field-sensitive current control from bulk dielectrics, semiconductors, and graphene to two-dimensional transition-metal dichalcogenides, highlighting their potential for electric-field sensitive optoelectronics.

[1] J. Schmuck et al., submitted, arXiv preprint arXiv:2511.08148 (2025).

HL 8.5 Mon 16:00 POT/0006

Development of an ultrafast scanning electron microscope — •Leon Kross[1], Benjamin Schröder[1], Niklas Wemheuer[1], Leon Brauns[1], Murat Sivis[1,2], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]University of Göttingen, 4th Physical Institute, Göttingen, Germany

Ultrafast electron microscopy (UEM) enables the study of structural and electronic dynamics in solid-state materials with nanoscale spatial and femtosecond temporal resolution [1]. While UEM at high (> 30 keV) and low (< 1keV) electron energies is well established, ultrafast experiments in the intermediate energy regime have been less employed thus far, despite their potential to bridge the gap between surface- and bulk-sensitive measurements. Here, we present a new ultrafast scanning electron microscope (USEM), designed to investigate physical phenomena in the energy range from 1 to 30 keV. The modular architecture supports diverse experimental configurations and detection schemes, spanning from standard SEM operation modes - such as secondary- and backscattered-electron imaging - to more advanced techniques including cathodoluminescence or electron diffraction. In this contribution, we show example measurements, highlighting the performance of our USEM and its potential for exploring ultrafast physical phenomena. [1] A. Feist et al. Ultramicroscopy, 176, 63-73 (2017)

HL 8.6 Mon 16:15 POT/0006

Ultrafast X-ray diffraction shows dynamics of phase domains make V2O3 films remember photoexcitation ten thousand times longer — •Oleg Gorobtsov[1,2], Yoav Kalcheim[3,4], Ziming Shao[1], Anatoly Shabalin[3], Nelson Hua[3], Daniel Weinstock[1], Ryan Bouck[1], Mathew Seaberg[5], Diling Zhu[5], Oleg Shpyrko[3], Ivan Schuller[3], and Andrej Singer[1] — [1]Cornell University, USA — [2]University of Tübingen, Germany — [3]University of California San Diego, USA — [4]Technion-Israel Institute of Technology, Israel — [5]SLAC National Accelerator Laboratory, USA

Metal-insulator transitions in vanadium oxides combine electronic and structural phase transformations. Memory effects present during the phase transition in thin V2O3 films make the material a candidate for neuromorphic computing, but what role does the structural phase heterogeneity play in memory? We used an X-ray free-electron laser probe to show that strain feedback on structural phase domain nucleation increases the metal-insulator relaxation time after an optically induced insulator-metal transition from nanoseconds to a hundred microseconds. The dynamic range and precision of the experiment distinguish that the memory follows a stretched exponential law, not a power law. We also provide an experimental basis for the transition incubation times during the first 10 picoseconds after the excitation.

15 min. break

HL 8.7 Mon 16:45 POT/0006

Carrier-envelope phase modulation of ultrafast photocurrents in indium nitride — •Maximilian A. Gruber, Alexandra V. Nemmaier, Johannes Schmuck, Abhilash Ulhe, Gregor Koblmüller, and Alexander W. Holleitner — Walter Schottky Institute and Physics Department, Technical University of Munich, Munich, Germany

Few-cycle laser pulses allow for electronic transport at petahertz frequencies, where the carrier-envelope phase (CEP) controls the direction and strength of the ultrafast photocurrents. While such effects have been studied in graphene, bulk semiconductors and wide-bandgap dielectrics, their realization in group-III nitrides remains largely unexplored. We demonstrate CEPdependent photocurrents in InN devices excited by stabilized 6 fs optical pulses. The response reveals fieldsensitive contributions and strong interface effects close to the contacts of the investigated sample, highlighting the microscopic role of builtin electric fields in device architecture. The results position InN as a promising platform for CEP-controlled ultrafast transport.

HL 8.8 Mon 17:00 POT/0006

Towards studying quasi-particle interactions on the nanoscale — •Philipp Kessler, Matthias Hensen, Victor Lisinetskii, and Tobias Brixner — Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg

Investigating the properties and dynamics of quasi-particles is essential for tailoring material functionality in device fabrication. Nonlinear optical spectroscopy has become a standard tool for probing ultrafast single quasi-particle dynamics. However, the use of high light intensities, intended to improve the signal-to-noise ratio, can also generate multiple quasi-particle excitations, which may interact with each other. As a result, the measured signal consists of overlapping contributions from single- and multi-particle processes, each with distinct dynamics. To address this, our group recently developed the intensity cycling technique, which enables the experimental separation of individual perturbative orders in nonlinear light–matter interaction [1,2]. Here, we report our progress in extending this technique to time-resolved photoemission electron microscopy (PEEM) to study quasi-particle interactions with high spatial resolution. In our PEEM setup [3], we employ a 680 nm pump pulse with variable intensity for excitation and a 340 nm probe pulse for photoemission. This scheme allows us to investigate organic thin films of molecular aggregates, focusing primarily on exciton–exciton annihilation as a probe of exciton diffusion.

[1] P. Malý et al., Nature 616, 280-287 (2023).
[2] J. J. Krich et al., J. Phys. Chem. Lett. 16, 5897-5905 (2025).
[3] B. Huber et al., Rev. Sci. Instrum. 90, 113103 (2019).

HL 8.9 Mon 17:15 POT/0006

Watching polarons form in real time — •Victor Garcia-Herrero and Fabio Caruso — Institute of Theoretical Physics and Astrophysics, Christian-Albrechts University of Kiel, Germany

Polaron formation in pump-probe experiments is a fast, non-equilibrium process arising from the coupled motion of electrons and lattice vibrations, leading to the emergence of a localized quasiparticle. A new first-principles quantum-kinetic approach is introduced to track the real-time dynamics of electrons and the lattice under electron-phonon interactions. We applied this method to the polar insulators MgO and LiF, and determine the characteristic timescales of polaron localization and identify its unique dynamical signatures. The results reveal distinct dynamical signatures of polaron formation and establish clear, practical criteria for its detection in ultrafast pump-probe experiments, providing a direct connection between theory and experiment.

Founded by Marie Skłodowska-Curie Actions (MSCA), TIMES network.

HL 8.10 Mon 17:30 POT/0006

Dynamic control of electron correlations in photodoped charge-transfer insulators — •Thomas C. Rossi[1,2], Nicolas Tancogne-Dejean[3], Malte Oppermann[1,4], Michael Porer[5], Arnaud Magrez[6], Rajesh V. Chopdekar[7], Yayoi Takamura[7], Urs Staub[5], Renske M. van der Veen[2], Angel Rubio[3,8], and Majed Chergui[1,9] — [1]LSU and LACUS, EPFL, Lausanne, Switzerland — [2]PS-ADLU, HZB, Berlin, Germany — [3]MPI for the Structure and Dynamics of Matter, Hamburg, Germany — [4]Department of Chemistry, University of Basel, Switzerland — [5]SLS, PSI, Villigen, Switzerland. — [6]Crystal Growth Facility, EPFL, Lausanne, Switzerland — [7]Department of Materials and Science Engineering, UC Davis, USA — [8]ICC and CCQ, Simons Foundation Flatiron Institute, New York, USA — [9]Elettra-Sincrotrone, Trieste, Italy

Tuning the electronic properties of materials is typically achieved by altering their chemical composition or thermodynamic parameters. An alternative route relies on ultrafast light excitation, which can create transient phases such as light-induced superconductivity and hidden insulator-to-metal transitions. In this talk, I will present evidence of light-driven dynamic screening of electron correlations in a prototypical charge-transfer insulator, nickel oxide (NiO). The excited state, characterized by weakened electron correlations, is metastable for hundreds of picoseconds. The high degree of control achieved over both the energetic and temporal aspects of electronic correlations offers a promising path toward full optical control of the electronic properties of correlated systems and the Mott transition.

HL 8.11 Mon 17:45 POT/0006

Photostriction-Driven Phase Transition in Layered Chiral $NbOX_2$ Crystals: Electrical-Field-Controlled Enantiomer Selectivity — •Jorge Cardenas-Gamboa[1], Martin Gutierrez-Amigo[2], Aritz Leonardo[3], Gregory A. Fiete[4], Juan L. Mañes[3], Jeroen van den Brink[1], Claudia Felser[5], and Maia G. Vergionry[3] — [1]Institute for Theoretical Solid State Physics, IFW Dresden — [2]Department of Applied Physics, Aalto University — [3]Donostia International Physics Center — [4]Northeastern University, Boston — [5]Max Planck Institute for Chemical Physics of Solids

Controlling the handedness of crystal structures is essential for developing next-generation optical, electronic, and information technologies. Yet, achieving reversible and selective control over crystal chirality remains a major challenge. In this work, we demonstrate a two-step pathway for enantiomer selectivity in layered chiral $NbOX_2$ (X = Cl, Br, I) crystals based on photostriction-driven phase transitions. *Ab-initio* simulations reveal that optical excitation is capable of inducing a structural phase transition in $NbOX_2$ from the monoclinic ($C2$) ground state to the higher-symmetry ($C2/m$) structure. In the resulting transient high-symmetry state, an applied electric field breaks the residual inversion-symmetry degeneracy, selectively stabilizing one enantiomeric final state configuration over the other. Our results establish a combined optical-electrical control scheme for chiral materials, enabling reversible and non-contact enantiomer selection with potential applications in ultrafast switching, optoelectronics, and chiral information storage.

HL 8.12 Mon 18:00 POT/0006

Efficient Two-Dimensional Spectroscopy Simulations including Realistic Pulse Shapes, Overlapping, and Time-Ordering Effects — Rémi Gilliot[1,2], •Matteo Russo[1], Alexander Blech[1], Manuel Joffre[2], Christiane Koch[1], and Hélène Seiler[1] — [1]Freie Universität Berlin, Berlin, Germany — [2]Institut Polytechnique de Paris, Palaiseau, France

We present an approach capable of simulating Two-Dimensional Electronic Spectroscopy (2DES) spectra with arbitrary pulse shapes, pulse overlap, and pulse ordering on a standard laptop. Under the assumption of simple dephasing, we show that the 2DES emitted signal - a convolution integral that involves pulses* fields and material response and that is traditionally challenging to evaluate numerically - reduces to a simple product of three independent one-dimensional integrals. This fortunate simplification makes this approach fast and computationally less expensive than others, while still capturing most of the realistic pulse-dependent effects listed above. Finally, we benchmark the effectiveness of this approach on three canonical systems - an anharmonic oscillator, two coupled oscillators, and a dimer model - studying how spectral phase distortions and strongly non-Gaussian pulse shapes, such as those produced by hollow-core fibers, can influence the 2DES emitted signal.

HL 9: Oxide Semiconductors: Growth and Fabrication

Time: Monday 15:00–16:30 Location: POT/0051

HL 9.1 Mon 15:00 POT/0051

Growth of rutile GeO_2 by plasma-assisted suboxide molecular beam epitaxy — Alexander Karg[1], •Satjawoot Phiw-Ondee[1], Manuel Alonso-Orts[1,2], Marco Schowalter[1], Andreas Rosenauer[1,2], Martin Eickhoff[1,2], and Patrick Vogt[3] — [1]Institute of Solid State Physics, University of Bremen, Bremen, Germany — [2]MAPEX Center for Materials and Processes, University of Bremen, Germany — [3]Max Planck Institute for Solid State Research, Stuttgart, Germany

The interest in ultra-wide bandgap (UWBG) semiconductors for high-power electronic applications is rapidly increasing, for which rutile germanium dioxide (r-GeO_2) is a promising material. It possesses excellent properties: a bandgap of 4.6 eV [1], thermal conductivity of 51 W/mK [1], and a breakdown electric field of 7 MV/cm [1] and theoretical bipolar dopability [2].

This work reports on the growth of r-GeO_2 on m-plane Al_2O_3 substrates using plasma-assisted suboxide molecular beam epitaxy, using a SnO_2 buffer, followed by a r-$Ge_xSn_{(1-x)}O_2$ buffer to stabilize the r-GeO_2 phase. The growth of r-GeO_2 on those buffer layers is demonstrated and the responsible nucleation mechanism is investigated in detail. Characterization was performed by atomic force microscopy (AFM) and high resolution X-ray diffraction (HRXRD). Selected r-GeO_2 layers were analyzed by scanning transmission electron microscopy (STEM).

[1]: M. Labed et al., Materials Today 83, 513-537 (2025)
[2]: S. Chae et al., Appl. Phys. Lett. 114, 102104 (2019)

HL 9.2 Mon 15:15 POT/0051

Wafer-scale transfer and integration of tungsten-doped vanadium dioxide films — •Guanyi Li[1,2], He Ma[2], and Peter J. Klar[1] — [1]University of Giessen Institute of Physic, Giessen, 35392, Germany — [2]Beijing University of Technology, Institute of Information Photonics Technology, Beijing 100124, People's Republic of China

The trend in modern optoelectronic devices is towards greater flexibility, wearability, and multifunctionality. This demands more flexible fabrication methods of functional layers. Vanadium dioxide (VO_2), with its metal-insulator transition (MIT) at 68 °C, is of interest for many optoelectronic devices. However, high-quality VO_2 usually needs to be grown at T >450 °C in an oxygen-containing atmosphere implying a low compatibility with many optoelectronic device concepts, e.g., on flexible substrates. Here, we use a layer-by-layer transfer method of wafer-scale tungsten-doped VO_2 films, which enables sequential integration of VO_2 films with different MIT temperatures (down to 40 °C) onto arbitrary substrates. By stacking multiple VO_2 films with different doping levels of W, a quasi-gradient-doped VO_2 architecture can be achieved, effectively broadening the MIT temperature window and reducing the hysteresis of VO_2. Such integrated VO_2 films find a wide scope of applications, e.g., flexible temperature indicator strips, infrared camouflage devices, nonreciprocal ultrafast light modulators, or smart photo actuators. Our work promotes the development of more flexible and tunable optoelectronic devices integrated with VO_2.

HL 9.3 Mon 15:30 POT/0051

Growth and characterization of ultra-wide bandgap oxide semiconductor $LiGa_5O_8$ — •Nazar Masiuta, Sofie Vogt, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix Bloch Institute for Solid State Physics, Semiconductor Physics Group, Leipzig, Germany

Lithium gallium oxide ($LiGa_5O_8$) has been recently grown as an ultra-wide bandgap oxide semiconductor with robust p-type conductivity using mist chemical vapor deposition[1]. This discovery suggests application of the material in high-power electronics by forming p-n junctions with n-type α-Ga_2O_3, β-Ga_2O_3, and isostructural γ-Ga_2O_3. However, establishing the origin of p-type conductivity of lithium gallium oxide remains an experimental challenge[2], while a theoretical prediction argues that neither native nor dopant defects in $LiGa_5O_8$ could be responsible for it[3]. We analyze the influence of pulsed laser deposition growth parameters on the quality of lithium gallium oxide films on different substrates. The structural, optical, and electrical characterization of $LiGa_5O_8$ is performed to determine the type of conductivity and its origin in the fabricated samples.

[1] K. Zhang *et al.*, Adv. Electron. Mater. **11**, 2300550 (2025).
[2] K. Zhang *et al.*, APL Mater. **13**(4), 041104 (2025).
[3] J. L. Lyons, J. Appl. Phys. **135**(16), 165705 (2024).

HL 9.4 Mon 15:45 POT/0051

(N:)CuBi2O4 photocathode thin films for photoelectrochemical water splitting — •Miriam J. Fehrenbach[1,2], Dominic Rapf[1,2], Katarina S. Flashar[1,2], Ian D. Sharp[1,2], and Verena Streibel[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Garching, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Garching, Germany

Photoelectrochemical (PEC) water splitting is a promising pathway to carbon-neutral solar fuels. While metal oxides are well explored as photoanodes, complementary photocathodes remain scarce. Potential candidates are Cu-based oxides, which naturally exhibit p-type conductivity. Among them, copper bismuthate (CuBi*O*) is a promising material [1], combining a visible-light bandgap with high photocurrent onset potentials [2], but suffering from poor charge transport [1]. To address this limitation, we developed a reactive co-sputtering and annealing process to synthesize high-quality, nitrogen-modified CuBi*O* thin films. We systematically examine structural and optical effects of nitrogen incorporation and find a significant improvement in PEC activity. To understand this enhanced performance, we investigate the charge carrier transport properties with (photo)conductivity measurements. [1] J. K. Cooper et al., Chem. Mater., 2021, 33, 3, 934*945. [2] N. T. Hahn et al., J. Phys. Chem. C, 2012, 116, 10, 6459*6466.

HL 9.5 Mon 16:00 POT/0051

High-throughput combinatorial synthesis of perovskite-type materials for solar applications — •Clemens Petersen, Andreas Rosnes, and Holger von Wenckstern — Centre for Materials Science and Nanotechnology, University of Oslo, Norwa

Recently, combinatorial deposition methods have increasingly gained attention due to the high experimental throughput and resource-wise efficiency they offer in materials discovery. Our combinatorial pulsed laser deposition (c-PLD) approach enables the fabrication of material libraries on a single substrate, spanning wide compositional spaces with precise spatial control. Combined with high-throughput characterization techniques (HTC) such as spatially resolved UV-VIS spectroscopy and X-ray diffraction, the properties of complex materials can be rapidly mapped with high chemical resolution and minimal effort. We demonstrate the potential of c-PLD for accelerating the discovery of perovskite oxides for solar-energy-related applications. Using the $SrTiO_3$*$BaTiO_3$ (STO-BTO) system as an example, we showcase rapid screening of structural and optical properties on small area spatially addressable material libraries (SAML) covering the full composition range. In addition, STO-BTO SAMLs enable systematic strain engineering of functional perovskite materials. The tunable band structures and suitability for catalytic processes such as photoelectrolysis and proton-coupled electron transfer render titanate perovskites promising candidates for solar fuel production. Our results underline the capability of c-PLD and HTC workflows to efficiently identify and optimize oxide perovskites for sustainable energy technologies.

HL 9.6 Mon 16:15 POT/0051

Pulsed laser deposition of rutile GeO_2 thin films — •Hannah Dichelle, Sofie Vogt, Marius Grundmann, and Holger von Wenckstern — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik, Germany

Rutile germanium-oxide has recently come into focus as an ultrawide bandgap material which is predicted to offer the possibility of ambipolar doping. [1,2] The stabilization of rutile phase GeO_2 is challenging due to the similar formation energies of the amorphous phase and α-Quarz phase.[2] We present GeO_2 thin films fabricated by pulsed laser deposition at heater temperatures >450°C. To facilitate the crystallization in the rutile phase (Sn, Ge)O_2 buffer layers are grown on sapphire and TiO_2 substrates at heater temperatures >600°C. Both ternary $Sn_xGe_{1-x}O_2$ buffer layers and vertically composition graded buffer layers are used to stabilize the rutile phase. The structural properties of rutile phase GeO2 thin films are investigated as a function of the growth temperature and oxygen pressure.

[1] Chae *et al.*, Appl. Phys. Lett. 114, 102104 (2019)
[2] Shimazoe *et al.*, Jpn. J. Appl. Phys. 64, 050903 (2025)

HL 10: 2D Materials II – Electronic and transport properties (joint session HL/TT)

Time: Monday 15:00–16:30 Location: POT/0081

HL 10.1 Mon 15:00 POT/0081

Ballistic electrostatic graphene superlattices using He ion-milled etching masks — •Rebecca Hoffmann[1], Giulia Piccinini[1], Julien Barrier[1], David Barcons Ruiz[1], Hanan Herzig Sheinfux[1], Takashi Taniguchi[2], Kenji Watanabe[3], Adrian Bachtold[1,4], and Frank H.L. Koppens[1,4] — [1]ICFO-Institut de Ciencies Fotoniques, Castelldefels, Spain. — [2]International Center for Materials Nanoarchitectonics, NIMS, Tsukuba, Japan — [3]Research Center for Functional Materials, NIMS, Tsukuba, Japan — [4]ICREA-Institució Catalana de Recerca i Estudis Avançats, Barcelona, Spain

An electrostatic superlattice is created by applying a periodic electrostatic potential to a material using patterned gates or dielectrics, leading to tunable band structure reconstruction. This approach enables free design of the superlattice geometry and lattice period. While high mobility has been observed, signatures of ballistic transport (e.g. negative resistance in cross geometry, transverse magnetic focusing) remain to be reported. Here, we present a nanofabrication technique combining Helium ion milling of etching masks with damage-free etching of graphite gates [1]. Using these gates in a graphene heterostructure creates an electrostatic superlattice which preserves graphene's high mobility. We report superlattice features. The high electronic quality is confirmed by transverse magnetic focusing and device-size limited mean free path.

[1]D. Barcons Ruiz, et al., Nat. Commun. 13, 6926 (2022)

HL 10.2 Mon 15:15 POT/0081

Tomographic flow regime in the 2D Corbino disk geometry — •Grigorii Starkov — Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany

2D materials offer a unique test ground to study electron transport regimes dominated by the electron-electron collisions. This makes them the perfect platform to observe the electron hydrodynamic flows.

Not so long ago, it has been realized that precisely in 2D, the electron collisions constrained due to Pauli blocking result in the appearance of the long lived collective modes with odd angular character. The corresponding novel transport regime has been dubbed "tomographic".

In the recent experiment [2], magnetoresistance in Corbino-shaped graphene devices was used to disentangle different contributions to the electron transport and to determine viscosity. The obtained temperature-dependence thereof has been linked to the tomographic flow. However, the analysis is based on the bulk expressions for the conductivity and does not treat boundary corrections in detail. At the same time, boundary layers have been shown to be anomalously large in the tomographic flow regime [3].

To take into account the boundary effects, I analyze the magnetoresistance in the 2D Corbino disk geometry across different regimes, using the linearized Boltzmann equation.

[1] P. Ledwith et al, Phys. Rev. Lett. 123, 116601 (2019) [2] Y. Zeng et al, arXiv:2407.05026 (2025) [3] N. Ben-Schachar, J. Hoffmann, arXiv:2503.14431 (2025)

HL 10.3 Mon 15:30 POT/0081

Pulsed-gate spectroscopy of the electron-hole block- ade in bilayer graphene double quantum dots — •Lars Mester[1,2], Hubert Dulisch[1,2], Katrin Hecker[1,2], Konstantinos Kontogeorgiou[3], Samuel Möller[1,2], Leon Stecher[1], Kenji Watanabe[4], Takashi Taniguchi[5], Fabian Hassler[3], Christian Volk[1,2], and Christoph Stampfer[1,2] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Aachen, Germany — [2]PGI-9, Forschungszentrum Jülich, Jülich, Germany — [3]JARA- Institute for Quantum Information, RWTH Aachen University, Aachen, Germany — [4]Research Center for Functional Materials, Na- tional Institute for Materials Science, Namiki, Japan — [5]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Namiki, Japan

Pauli blockade is an established read-out mechanism for quantum-dot (QD) spin qubits. Using bilayer graphene (BLG) as a platform offers advantages such as a tunable valley degree of freedom. Recently, a strong spin-valley blockade was demonstrated in an electron-hole BLG double quantum dot (DQD) using time-averaged transport measurements. Here, we employ pulsed-gate spectroscopy by pulsing between the (0e, 0h) and (1e, 1h) charge configurations. Comparison with sim- ulations allows us to identify unconventional higher-order tunneling as the dominant blockade-lifting mechanism, with timescales governed by QD-lead coupling and the number of accessible states. Our results provide direct access to blockade-lifting dynamics in a BLG DQD, offering relavant insights for the development of future BLG-based qubits.

HL 10.4 Mon 15:45 POT/0081

Temperature Dependent Electrical Transport in Thin $SnSe_2$ — •Lars Thole[1], Aarti Lakhara[2], Preeti A. Bhobe[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Department of Physics, Indian Institute of Technology Indore, Khandwa Road, Indore, Simrol, 453552, India

The two-dimensional material $SnSe_2$ shows special temperature dependent behavior [1], which has not been understood to its full capacity as of now.

We fabricated thin samples of $SnSe_2$ and investigated its electrical transport behavior in regards to its temperature dependence [2]. These samples show a metal-insulator transition with a metallic state for higher temperatures. The low-temperature transport regime is dominated by variable-range hopping. Additionally, the influence of defect states in these samples is investigated by looking at the thickness dependence for different samples [3].

[1] C. Guo, et al., Appl. Phys. Lett. 109, 203104 (2016).

[2] A. Lakhara, L. Thole, R. J. Haug, and P. Bhobe. arXiv: 2507.14536 (2025).
[3] A. Lakhara, L. Thole, R. J. Haug, and P. Bhobe. Phys. Rev. B 112, 235401 (2025).

HL 10.5 Mon 16:00 POT/0081

Polarization resolved Electron Spin Resonance in two-dimensional electron systems — •Daniiar Khudaiberdiev[1], Alexey Shuvaev[1], Michail Glazov[2], Anton Shchepetilnikov[3], Viacheslav Muravev[3], Christian Reichl[4], Werner Wegscheider[4], and Andrei Pimenov[1] — [1]Institute of Solid State Physics, Technische Universität Wien, 1040 Vienna, Austria — [2]St. Petersburg, Russia — [3]Chernogolovka, Russia — [4]Laboratory for Solid State Physics, ETH Zurich, CH-8093 Zurich, Switzerland

Electron spin resonance (ESR) has long served as a powerful probe of g-factor anisotropy, spin-orbit interactions, hyperfine coupling, and collective many-body spin phenomena in two-dimensional electron systems (2DESs). Most prior studies detect ESR in the photoresistance of Hall bars, where the excitation-field distribution and polarization are distorted, complicating the analysis of the excitation conditions.

In contrast, we report polarization-resolved ESR in sub-THz transmission using a quasi-optical setup and large-area samples that ensure high polarization purity. First we study the 2DES hosted in a 4.5-nm AlAs quantum well with a single isotropic valley. The selection rules indicate that Dresselhaus spin-orbit coupling mediates the electric-dipole-active spin absorption. Further we examine systems with more complex spectra such as wide AlAs wells with an active pseudospin, HgTe and InAs quantum wells with low effective mass and strong spin-orbit coupling enhancing the effects.

HL 10.6 Mon 16:15 POT/0081

First-Principles Investigation of Electronic Transport in 2D GaSe: Backward Diodes, p-i-n FETs, and Double-Gate MOSFETs — •Dogukan Hazar Ozbey and Engin Durgun — UNAM - National Nanotechnology Research Center and Institute of Materials Science and Nanotechnology, Bilkent University, Ankara, Turkey

In this study, we present a comprehensive first-principles investigation of charge transport in monolayer GaSe nanodevices by combining density functional theory with the nonequilibrium Green's function (DFT + NEGF) formalism. Three representative architectures, namely p–n junctions, p–i–n field-effect transistors (FETs), and double-gate MOSFETs, are systematically analyzed. Our calculations reveal that GaSe p–n junctions display an unconventional backward diode response, in which reverse currents within the ±1 V window exceed forward currents owing to tunneling-assisted transport, as evidenced by the projected local density of states. When configured as p–i–n FETs, electrostatic gating allows selective control over tunneling conduction. Moderate gate biases suppress the reverse current, whereas stronger gating reactivates and amplifies it. Finally, double-gate GaSe MOSFETs with channel lengths of approximately 5 nm exhibit competitive figures of merit that meet or surpass the ITRS-2028 high-performance benchmarks, achieving an on/off ratio of 1.2×10^4, intrinsic delay time of 0.24 ps, and power–delay product of only 0.06 fJ·μm^{-1}. Our results highlight GaSe as a single 2D semiconductor capable of integrating backward-diode behavior with high-speed transistor operation.

HL 11: Focus Session: Quantum Emitters in 3D Semiconductors

Quantum emitters in 3D semiconductors play a crucial role in many applications. In this focus session, we focus on the latest developments for their use in quantum technologies. In addition to the well-known NV center in diamond, there are a number of other defect centers in various semiconductor systems that hold great potential for quantum sensing, quantum cryptography, and/or quantum information technology. Today's research focuses on the discovery of new centers, their properties, synthesis, and their microscopic origin. For the latter, ab initio methods are often used, and the material systems span silicon, nitrides, carbides, and other semiconductors with large band gaps.

Organized by Carsten Ronning and Jan Meijer

Time: Monday 15:00–18:15 Location: POT/0251

Invited Talk HL 11.1 Mon 15:00 POT/0251

Quantum Repeater Hardware made from Silicon Carbide — •Jörg Wrachtrup — Center for Applied Quantum Technologies, University of Stuttgart

Distributing entanglement via quantum repeaters is a formidable challenge. Memory-based approaches require quantum emitters that couple strongly to optical fields, and at the same time demand stationary qubits with excellent coherence properties. Colour centres in solids meet these requirements remarkably well and are therefore leading contenders in the field. However, existing solutions are either technically demanding or result in limited network efficiency.

Silicon carbide (SiC) offers several advantages over current approaches. Most notably, SiC is a wafer-scale material with excellent nanophotonic properties and hosts defects with outstanding spin coherence. In this talk, I will highlight recent progress in incorporating colour centres into nanophotonic structures and achieving efficient photon extraction. In addition, the electron spins of these colour centres can be coupled to nuclear spin qubits with exceptional coherence properties. I will discuss this coupling and its use as quantum memories for repeaters.

Invited Talk HL 11.2 Mon 15:30 POT/0251

Diamond based quantum sensing for drug testing — •Romana Schirhagl — University Medical Center Groningen, Groningen, the Netherlands

Free radical generation plays a key role in the mechanisms of action of many different drugs. Additionally, free radical generation offers a powerful biomarker to quantify the drug efficacy. However, free radicals are difficult to measure since they are short lived and reactive. Diamond based quantum sensing offers a possible solution to this problem. We have demonstrated recently that we can predict which drugs might work in clinical samples. Here we can either measure stress responses [1] (as for instance caused by anti-cancer drugs or anti-biotics) or reduction of oxidative stress [2] (as caused by anti-inflammatory drugs, certain inhibitors or anti-oxidants). We tested synovial fluid from rheumatoid arthritis and osteoarthritis patients. We can clearly differentiate the two groups which differ in their responsiveness to Piroxicam. Such ex-vivo measurements can be used for diagnostic purposes, to predict the effectiveness of a drug or to elucidate its mechanism of action. In my talk I will show different examples of how quantum sensing can be used in drug development.

1 Tian, Y., Nusantara, A.C., Hamoh, T., Mzyk, A., Tian, X., Perona Martinez, F., Li, R., Permentier, H.P. and Schirhagl, R., 2022. ACS Applied Materials & Interfaces, 14(34), pp.39265-39273.

2 Sigaeva, A., Shirzad, H., Martinez, F.P., Nusantara, A.C., Mougios, N., Chipaux, M. and Schirhagl, R., 2022. Small, 18(44), p.2105750.

Invited Talk HL 11.3 Mon 16:00 POT/0251

The oxygen-related ST1 centre in diamond: a room temperature coherently controllable electron spin — •Sebastien Pezzagna — Applied Quantum Systems, Universität Leipzig, Leipzig, Germany

The development of quantum information and technologies has rapidly evolved from the beginning of the century. Nowadays, there exists a variety of defects and host crystals which are suitable for applications in quantum computing, sensing or communication, such as the nitrogen-vacancy (NV) centre in diamond. However, the reliable and scalable employment of such a system requires the ability to produce it on demand together with a deep understanding of its optical and spin properties, as well as charge states and close by environment.

In this presentation, we will discuss the so-called ST1 centre in diamond, one of the few defect centres possessing a coherently controllable electron spin at room temperature. We will first show how we could identify the nature of the ST1 centre and how it can then be produced on demand. We will then emphasize the large spin readout contrast and charge state stability which characterise the ST1 centre, and how this compares to the well-known NV centre. Finally, we will highlight the peculiarities of the ST1 centre, supported by optical spectroscopy and by investigations of the hyperfine interactions with surrounding carbon-13 nuclear spins and with the oxygen-17 nuclear spin within the centre itself.

15 min. break

Invited Talk HL 11.4 Mon 16:45 POT/0251

Silicon quantum emitters emitting in the optical telecommunication range for scalable quantum photonic circuits — •Yonder Berencén — Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany

Silicon has recently emerged as a promising host for single-photon emitters operating at telecom wavelengths, offering a pathway toward scalable quantum photonic technologies on a CMOS-compatible platform. In this invited talk, I will provide an overview of the most relevant intrinsic and extrinsic-based quantum emitters in silicon, including the W, G, T, and C centers as well as erbium. I will discuss their optical and spin properties, deterministic creation via broad-beam ion implantation and focused ion beam implantation, and recent progress toward realizing spin-optical interfaces in the optical telecom bands. Particular emphasis will be placed on single-emitter spectroscopy, demonstration of optically detected magnetic resonance (ODMR) in silicon at telecom wavelengths, and the integration opportunities enabled by silicon*s mature photonic and electronic fabrication ecosystem. Finally, I will outline a roadmap toward fully monolithic silicon quantum photonic integrated circuits that combine single emitters with on-chip photonic routing and a groundbreaking approach for silicon-based single-photon detectors at the telecom range.

Invited Talk HL 11.5 Mon 17:15 POT/0251

Advances in materials processing for quantum sensing — •Adam Gali — HUN-REN Wigner Research Centre for Physics, Budapest, Hungary — Budapest University of Technology and Economics, Budapest, Hungary

For more than a decade, our first-principles studies have suggested that neutral divacancy defects in silicon carbide (SiC) could provide such an alternative. These defects can be excited in the infrared and emit in the second biological window, making them intrinsically attractive for biological sensing. The next step is to engineer the SiC surface and introduce shallow divacancy species suitable for nanoscale sensing. Under ambient conditions, however, SiC readily oxidizes and forms a high density of optical and paramagnetic defects at the interface, necessitating new materials-processing strategies. We have shown with first-principles calculations that the ODMR contrast of divacancy centers can be enhanced through strain engineering, a prediction verified experimentally by our collaborators. Additionally, we proposed replacing the native oxide with carbon-chain terminations to prevent oxidation. Our simulations revealed that such surfaces serve as ideal hosts for shallow divacancy quantum sensors capable of detecting external paramagnetic species [1]. This theoretical proposal has since been experimentally demonstrated by our collaborators, paving the way toward non-invasive, room-temperature quantum sensor devices.

[1] Non-invasive bioinert room-temperature quantum sensor from silicon carbide qubits, Pei Li et al., Nature Materials, 24, 1913 (2025).

HL 11.6 Mon 17:45 POT/0251

Generation of Vacancy-Based Colour Centres in 4H-Silicon Carbide for Quantum Nanophotonics with Optically Active Spins — •Leonard K.S. Zimmermann[1,2], Jonah Heiler[1,2], Samuel C. Eserin[3], Matthias Rupp[1], Ella B. Schneider[3], Jean-Nicolas Audinot[1], Steven K. Clowes[3], Ben N. Murdin[3], Stephan Kucera[1], and Florian Kaiser[1,2] — [1]Luxembourg Institute of Science and Technology (LIST), Esch-sur-Alzette, Luxembourg — [2]University of Luxembourg, Esch-sur-Alzette, Luxembourg — [3]Advanced Technology Institute, University of Surrey, United Kingdom

Silicon carbide (SiC) has emerged as a promising colour centre platform for scalable quantum systems based on nanophotonics and -electronics. Integration into nanophotonic circuits requires sub-micron three-dimensional positioning control of colour centres, achievable via ion implantation to create vacancies followed by thermal annealing. Spin-optical quantum coherence properties vary significantly with implantation parameters. We present initial results from an ongoing implantation-annealing study for generating VSi and VSiVC colour centres in 4H-SiC. Helium and Neon are implanted with varied doses at different energies, and different annealing processes for colour centre formation are investigated. We summarise single-emitter yield and show basic spin coherence measurements for the different processes. Our study highlights parameters necessary for optimal generation conditions of colour centres in 4H-SiC.

HL 11.7 Mon 18:00 POT/0251

Controlled generation of color centers in MBE-grown AlN for quantum photonics applications — •Meysam Saeedi[1], Duc V. Dinh[1], Andrey N. Anisimov[2], Mingyun Yuan[1], Georgy V. Astakhov[2], and Alberto Hernández-Mínguez[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., 10117 Berlin, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany

The large electronic band gap of aluminium nitride (AlN), its compatibility with CMOS technology, and the presence of defect centers acting as quantum light sources in the visible spectral range, make this material attractive for applications in integrated quantum photonics. In this contribution, we demonstrate the controlled generation of optically active defect centers in AlN thin films grown on 4H-SiC by molecular beam epitaxy (MBE). To this end, we compare the photoluminescence (PL) spectra of pristine AlN samples grown under both N-rich and Al-rich conditions with their corresponding PL spectra after H-ion irradiation and annealing. We show that achieving high-purity single-photon emitters in samples grown under N-rich conditions is hindered by a broad background PL, primarily arising from native oxygen-related defect complexes already present in as-grown samples. However, the PL background is reduced by more than one order of magnitude by turning the MBE growth conditions from N-rich to Al-rich regimes. These results outline a clear pathway toward the engineering of integrated, high-purity quantum emitters in epitaxial AlN.

HL 12: Heterostructures, Interfaces and Surfaces: Photonics

Time: Monday 16:45–18:30 Location: POT/0051

HL 12.1 Mon 16:45 POT/0051

Surface patterning for high index contrast AlOx/GaAs distributed Bragg reflectors — •Frederike Jaeschke[1,2], Yurii Kutovyi[1,2], Nils von den Driesch[1,2], Serhii Darahan[3], Christoph Krause[1], Benjamin Bennemann[1], Frank Vewinger[3], and Alexander Pawlis[1,2] — [1]Peter Gruenberg Institute, Forschungszentrum Juelich GmbH, Juelich, Germany — [2]JARA-Fundamentals of Future Information Technology, Juelich-Aachen Research Alliance, Aachen, Germany — [3]Institut für Angewandte Physik, Universitaet Bonn, Bonn, Germany

Enhancing the refractive index contrast between the constituent materials in a distributed Bragg reflector (DBR) leads to stopband broadening and an increase in the attainable reflectivity for a given number of layer pairs, thereby mitigating the impact of growth-induced thickness variations on optical properties. One promising approach involves the post-growth wet-oxidation of AlAs to amorphous AlOx, which substantially increases the index contrast relative to conventional AlAs/GaAs stacks. In this talk, we present optimization of the AlAs/GaAs DBR growth parameters alongside different substrate patterning approaches which facilitate controlled lateral oxidation for micrometer-scale AlOx/GaAs pillar structures. We compare the optical properties of wet-oxidized AlOx/GaAs and as-grown AlAs/GaAs DBRs to explore the potentials and limitations of such pre-structuring concepts for realizing high index contrast DBRs with decreased growth times and improved layer thickness accuracy.

HL 12.2 Mon 17:00 POT/0051

Improving Photoelectrochemical Nitrate Reduction on Copper (I) Oxide Electrodes — •Maximilian Christis[1,2], Jasmin Zitzmann[1,2], Saswati Santra[1,2], and Ian Sharp[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Germany

The photoelectrochemical (PEC) nitrate reduction reaction (NO_3RR) offers a green approach for simultaneous production of ammonia (NH_3) and removal of the wastewater pollutant nitrate (NO_3*) in ambient conditions. Copper (I) oxide (Cu_2O) was recently reported to be active for both electrochemical (EC) and PEC NO_3RR, but its practical application is limited by stability issues. Thus, optimal reaction conditions that balance NH_3 selectivity and catalyst stability remain to be established. In the current investigation, we find that alkaline electrolytes enhance Cu_2O-catalyzed PEC NO_3RR compared to neutral conditions, and higher NH_3 selectivity is achieved at lower applied potentials. However, under illumination and at potentials < 0.3 V vs. RHE, the catalyst rapidly reduces to metallic Cu, favoring EC rather than PEC NO_3RR. To address this challenge, we are exploring possible strategies to reduce in-situ decomposition of Cu_2O photocathodes, aiming to enable their long-term use for solar NH_3 synthesis.

HL 12.3 Mon 17:15 POT/0051

InGaN/GaN nanowire arrays for photoelectrochemical biosensors — •Hannah Nell, Genrietta Steingelb, Rudolfo Hötzel, Ruben Neelissen, Stephan Figge, Tim Grieb, and Martin Eickhoff — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

Group III-nitride materials are known for their stability under physiological conditions, making them promising candidates for use as electrochemical biosensors [1]. In this work, we analyse the simultaneous detection by photoluminescence (PL) and photocurrent measurements of InGaN/GaN nanowire (NW) arrays, enabling sensitive and selective sensing of redox-active biomolecules. However, the performance of the NW photoelectrode is constrained by non-radiative surface recombination of photogenerated carriers at the semiconductor-electrolyte interface, leading to irreversible photooxidation of the NW surface, mainly driven by non-passivated surface states. The deposi-

tion of ultra-thin metal oxide films is a possibility to suppress such effects. The influence of TiO2 as a surface coating on the sensor properties was analysed by photoelectrochemical characterisation, demonstrating how surface modifications can affect the sensor performance in biochemical environments. [1] G. Steinhoff, et al., Appl. Phys. Lett. 83, 177 (2003)

HL 12.4 Mon 17:30 POT/0051

Metal-oxide passivation for high-efficiency photoelectrochemical devices — •Negin Mogharehabed[1], Mohammad Amin Zare Pour[1,2], Christian Höhn[3], Roel van de Krol[3], Thomas Hannappel[2], and Agnieszka Paszuk[1] — [1]BMFTR Junior Research Group PARASOL, Technische Universität Ilmenau, Germany — [2]Fundamentals of Energy Materials, Technische Universität Ilmenau, Germany — [3]Institute for Solar Fuels, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

Thin metal-oxide protection layers are crucial in highly efficient III-V photoelectrochemical (PEC) devices to suppress interfacial recombination and ensure long-term stability. Here, we study TiO_2 layers deposited on AlInP/GaInP(100) photoabsorbers, examining how surface preparation prior to atomic layer deposition and the Ti-precursor chemistry affect the chemical composition and band alignment at the TiO_2/III-V heterointerface, as well as the TiO_2 bulk and surface properties. Before TiO_2 deposition, the native oxide on AlInP(100) was removed by wet-chemical etching. TiO_2 films were grown using either TTIP or $TiCl_4$ with H_2O at various substrate temperatures. X-ray photoelectron spectroscopy was used to characterize the interface and TiO_2 bulk composition. We observe precursor-dependent differences in contaminant species in the TiO_2 bulk, at the surface, and at the TiO_2/III-V heterointerface, while their concentration is strongly influenced by deposition temperature and post-growth annealing. Finally, we correlate precursor choice and initial surface condition with TiO_2 layer stability in aqueous electrolytes under PEC-relevant conditions.

HL 12.5 Mon 17:45 POT/0051

Lab-Based NAP-XPS for Probing Photoelectrochemical Interfaces: The Case of $CuBi_2O_4$ — •Katarina S. Flashar[1,2], Miriam Fehrenbach[1,2], Gaurav Anand[3], Dominic Rapf[1,2], Barbara A. J. Lechner[3], Ian D. Sharp[1,2], and Verena Streibel[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Garching, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Garching, Germany — [3]Chemistry Department, TUM School of Natural Sciences, Technical University of Munich, Garching, Germany

Understanding complex (photo)electrochemical conversion processes at functional interfaces requires in situ and operando characterization. A tool enabling such investigations is near-ambient pressure X-ray photoelectron spectroscopy (NAP-XPS). In this contribution, we discuss the implementation of an open liquid cell for (photo)electrochemical measurements at our recently installed, lab-based NAP-XPS system (SPECS). As a photoelectrochemical case study, we examine sputter-deposited copper bismuthate ($CuBi_2O_4$) thin film photocathodes in contact with water-based electrolytes. We thereby extend previous NAP-XPS studies on light- and gas-dependent changes in surface chemistry of $CuBi_2O_4$ [1] to the solid|liquid interface under illumination. These investigations demonstrate the capability of our lab-based NAP-XPS to probe functional interfaces of energy materials under working conditions, offering an accessible and flexible alternative to synchrotron-based measurements. [1] F. E. Oropeza et al., ACS Appl. Energy Mater. 2019, 2, 6866 - 6874.

HL 12.6 Mon 18:00 POT/0051

Correlative Atomic Force Microscopy to Understanding Local Charge Transport in Photoanodes — •Sven Doll and Johanna Eichhorn — Technical University of Munich, Garching, Germany

Efficient photosystems for solar-to-chemical energy conversion are often based on nanostructured semiconductor architectures. In these material systems, the nanoscale properties frequently dominate the performance at the macroscale. Therefore, local understanding of their charge transfer and transport properties is decisive for optimizing their efficiency and stability.

To this end, we correlate Kelvin probe force microscopy (KPFM) and (photo)conductive atomic force microscopy (AFM) to study the local band bending, charge accumulation, as well as variations in the generated surface photovoltage and (photo)conductivity. However, analyzing nanostructured materials with complex morphologies is not trivial, because effects such as topographic crosstalk can significantly influence the results obtained. To overcome these issues, we leverage 2nd eigenmode and heterodyne KPFM measurements with improved resolution and sensitivity compared to conventional tapping mode KPFM techniques. For $BiVO_4$, one of the most extensively studied metal oxide photoanode materials, we compare different KPFM modes and correlate the results with local conductivity measurements to gain insights into local semiconductor properties at grain boundaries or different crystal facets. Overall, the gained nanoscale insights will put forward the development of rational design strategies to enhance the macroscale durability and efficiency of solar energy conversion systems.

HL 12.7 Mon 18:15 POT/0051

Persistent UV-Induced Work Function Control at Atomic Layer Deposited TiO_2 /Ta_2O_5 Bilayer Interfaces — •Julius Kühne[1,2], Tim Rieth[1,2], Katarina S. Flashar[1,2], Johannes Dittloff[1,2], Lukas Wolz[2], Johanna Eichhorn[2], Verena Streibel[1,2], and Ian D. Sharp[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Am Coulombwall 4, 85748 Garching — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Am Coulombwall 4, 85748 Garching

While atomic layer deposition (ALD) enables precise fabrication of ultrathin metal-oxide films, the mechanisms governing charge-carrier dynamics and band alignment at their interfaces often remain poorly understood. Oxide bilayers grown by ALD offer a versatile platform to characterize and tune defects that dictate interface energetics and charge transfer. Here, we examine the optical tuning of interface energetics in ultrathin ALD TiO_2/Ta_2O_5 bilayer films. A persistent -0.4 eV work-function (WF) shift is observed via contact potential difference (CPD) measurements after 275 nm illumination, with polarity reversal upon bilayer sequence inversion. This response arises from long-lived deep-trap filling, suggesting oxygen-vacancy migration. Capacitance-voltage (C-V) profiling, in-plane transport, and Kelvin probe force microscopy (KPFM) confirm vertical and lateral charge redistribution, while X-ray photoelectron spectroscopy (XPS) probe defect states. The results indicate that WF modulation originates from charge trapping by deep-trap states at the interface, offering insight into defect-driven effects in oxide heterointerfaces.

HL 13: 2D Materials III – Interlayer excitons

Time: Monday 16:45–18:30 Location: POT/0081

HL 13.1 Mon 16:45 POT/0081

Robust Interlayer Exciton Interplay in twisted Van der Waals Heterobilayer and Heterotrilayer on a Broadband Bragg Reflector up to Room Temperature — •Bhabani Sankar Sahoo, Shachi Machchhar, Avijit Barua, Martin Podhorsky, Chirag Chandrakant Palekar, and Stephan Reitzenstein — Technische Universität Berlin, Berlin, Germany

The MoSe2/WSe2/WSe2 Heterotrilayer (HTL) shows higher interlayer exciton (IX) emission intensity compared to the MoSe2/WSe2 heterobilayer (HBL) due to the additional WSe2 monolayer in the HTL, which improves interlayer coupling and provides additional radiative pathways. However, its coupling strength and thermal stability with increasing temperature remain unexplored. Here, we fabricate HTL and HBL using H-type stacking with twist angle of 55 and 50 for the MoSe2/WSe2 and WSe2/WSe2 heterostructures (HS) on the chirped distributed Bragg reflectors (cDBRs) centered at 800 nm. Photoluminescence (PL) emission at 4K shows that HTL exhibits more than 10-fold higher intensity compared to HBL. The temperature-dependent valley polarization reveals the interplay of triplet and singlet IX in the PL emission of the HBL and Indicates the influence of band modulation on the PL emission of the HTL. The temperature-dependent lifetime further provides insights into the different decay processes in both the HS, highlights the variations in optical performance between HTL and HBL HS with temperature. Additionally, through the combined effect of controlled stacking angles and the use of cDBR substrate, we successfully achieve room temperature IX across both regions of HS.

HL 13.2 Mon 17:00 POT/0081

Ring-shaped Interlayer Exciton Ensembles in $MoSe_2/WSe_2$ Heterostructures by Laguerre-Gaussian Excitation — •Mirco Troue[1], Johannes Figueiredo[1], Gabriel Mittermair[1], Jonas Kiemle[1], Hendrik Lambers[2], Ana Senkić[2], Ursula Wurstbauer[2], and Alexander Holleitner[1] — [1]Walter Schottky Institute and Physics Department, TU Munich, Am Coulombwall 4a, 85748 Garching, Germany — [2]Institute of Physics, Münster University, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Transition metal dichalcogenide monolayers exhibit strong light-matter interactions, which promotes them as ideal candidates for novel 2D optoelectronic applications. A vertical stacking into van der Waals heterostacks leads to the formation of long-lived interlayer excitons in adjacent layers. We report on ring-shaped ensembles of interlayer excitons in $MoSe_2/WSe_2$ heterostructures as excited by an optical Laguerre-Gaussian mode. The excitation is achieved with the help of a spatial light modulator. A hyperspectral analysis of the exciton photoluminescence suggests that the excitation scheme generates a non-uniform momentum distribution that favors the accumulation of high-energy excitons in the rings' center. We discuss the mechanisms leading to such a distribution, includ-

ing exciton-exciton interaction, phase-space filling, and incomplete thermalization.

HL 13.3 Mon 17:15 POT/0081

Exciton-Exciton Interactions in Van der Waals Heterobilayers — •Tommy Schulz[1], Alexander Steinhoff[2], and Frank Jahnke[1] — [1]University of Bremen, Bremen, Germany — [2]Carl von Ossietzky University Oldenburg, Oldenburg, Germany

Optically excited van der Waals heterobilayers hosting long-lived interlayer excitons provide a compelling platform for exploring correlated electronic states. In this work, we compute the exciton energy shift as a function of excitation density and temperature. This shift arises from a subtle interplay of various many-body interaction processes, each of which contributes either a blue- or a redshift, corresponding to repulsive or attractive interactions, respectively. By incorporating the fermionic substructure of excitons as well as dynamical screening effects, we show that the commonly assumed dominant repulsive dipole-dipole interaction is almost perfectly compensated. This finding challenges the simple picture of a purely bosonic exciton gas. Moreover, we identify a crossover from attractive to repulsive behavior at elevated exciton densities. Comparing these results - obtained using first-principle band structures and Coulomb matrix elements - with those from a simpler two-band model highlights the importance of a material-realistic description of the electronic states.

HL 13.4 Mon 17:30 POT/0081

Optical Injection and Detection of Long-Lived Interlayer Excitons in van der Waals Heterostructures — •Anna Seiler, Alperen Tügen, Arthur Christianen, Martin Kroner, and Atac Imamoglu — ETH Zurich, Switzerland

Interlayer excitons, electron-hole pairs spatially separated between two layers of 2D materials, have gained attention for their potential to enable the exploration of bosonic quantum phases. A promising strategy to stabilize these excitons is to use transition metal dichalcogenide (TMD) bilayer structures, where the two TMD layers are separated by a few layers of hexagonal boron nitride (hBN), effectively isolating itinerant electrons and holes. While these systems have primarily been studied through transport measurements, challenges such as difficulties in making ohmic contacts to TMD monolayers and the lack of photoluminescence have limited their broader exploration. Here, we demonstrate optical generation of dipolar interlayer excitons in TMD bilayers separated by up to seven hBN layers. We observe that the 2s excitons in the individual layers remain intact in the presence of opposite charges in both layers, suggesting that the oppositely charged carriers are strongly bound, forming stable interlayer excitons. We measure exciton lifetimes up to ten microseconds, underscoring their potential for studying exotic quantum phases such as Bose-Fermi mixtures and excitonic condensates [1]. These phenomena can be accessed through optical spectroscopy, enabling future exploration.

[1] A. Tüğen, A. M. Seiler, et al., Phys. Rev. Lett. DOI: https://doi.org/10.1103/stgs-2s58

HL 13.5 Mon 17:45 POT/0081

Influence of hBN spacer layers on atomic reconstruction in $MoSe_2$/WSe_2 heterostructures probed by electron microscopy — •Johannes Figueiredo[1,2], Kaiyuan Chen[3], Aubrey Penn[4], Mirco Troue[1,2], Sebastian Loy[1,2], Frances M. Ross[3], Julian Klein[3], and Alexander Holleitner[1,2] — [1]Walter Schottky Institute, TU Munich — [2]MCQST — [3]Massachusetts Institute of Technology — [4]MIT.nano

Atomically thin hexagonal boron nitride (hBN) tunnelling barriers in transition metal dichalcogenide (TMD) heterobilayers have recently facilitated the observation of macroscopic interlayer exciton phases interpreted as possible condensation and superfluid phenomena. However, such hBN spacer layers are also expected to modify moiré-driven atomic reconstruction. Here, we resolve local stacking configurations, lattice relaxation patterns and twist-angle variations across encapsulated $MoSe_2$/WSe_2 heterobilayers using a combination of high-angle annular dark-field scanning transmission electron microscopy (HAADF STEM), convergent-beam electron diffraction and four-dimensional STEM. Our analysis shows that the presence and thickness of the hBN spacer layers alter the balance between elastic relaxation and interlayer registry, producing a reconstruction landscape that differs qualitatively from that of directly contacted $MoSe_2$/WSe_2 bilayers. We also discuss how the resulting changes in structural homogeneity tune the moiré potential experienced by interlayer excitons and outline the implications for realizing spatially uniform macroscopic exciton phases in TMD-based quantum devices.

HL 13.6 Mon 18:00 POT/0081

Spin-bright interlayer exciton and trion ground state in Janus transition metal dichalcogenide bilayers from first-principles — •Franz Fischer[1,2], Carl Emil Mørch Nielsen[1], Marta Prada[1], and Gabriel Bester[1] — [1]University of Hamburg, Institute of Physical Chemistry, 22761 Hamburg, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, 22761 Hamburg, Germany

We investigate bilayer Janus transition metal dichalcogenides using ab initio many-body screened configuration interaction calculations [1] and find that MoSSe–WSSe and WSSe–WSSe, with Se–S interfaces, exhibit spin-allowed interlayer exciton and trion ground states [2], in contrast to the spin-forbidden ground states of conventional transition metal dichalcogenides bilayers. This distinctive behavior is driven by the intrinsic structural asymmetry and interface-induced polarization, which significantly modify the electronic band structure. Moreover, we demonstrate that external mechanical strain allows to tune the optical properties of these excitons, enabling precise control over their brightness and potential applications in optoelectronic devices.

[1] Mørch Nielsen, C.E., Fischer, F. & Bester, G. *npj 2D Mater. Appl.* **9**, 11 (2025)
[2] Mørch Nielsen, C.E., Fischer, F., Prada, M. & Bester, G. *2D Mater.* **12** 045015 (2025)

HL 13.7 Mon 18:15 POT/0081

Interplay of excitonic species in vertical and lateral transition metal dichalcogenide heterostructures — •Sai Shradha[1], Md. Tarik Hossain[2], Nicole Engel[1], Luc Oswald[1], Julian Führer[1], Daria Markina[1], Andrey Turchanin[2], and Bernhard Urbaszek[1] — [1]Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 6-8, D-64289 Darmstadt, Germany — [2]Institute of Physical Chemistry, Friedrich Schiller University Jena, Lessingstr. 10, D-07743 Jena, Germany

The properties of transition metal dichalcogenides (TMDs) can be extended beyond those offered by individual monolayers by combining different monolayers to create heterostructures. Vertically stacked heterostructures host quasiparticles such as interlayer and Moiré excitons. In lateral heterostructures (LHs), where monolayers of different materials are covalently bonded in the plane of their atoms, unidirectional exciton transport and the formation of charge-transfer excitons can be realized [1]. Chemical vapour deposition (CVD) has been a key fabrication technique for LHs. This work investigates composite CVD-grown $MoSe_2$-WSe_2 heterostructures consisting of both lateral and vertical interfaces, providing a single platform to study exciton dynamics across different interface types. Optical spectroscopy reveals efficient interlayer coupling in such structures, resulting in a uniquely strong interlayer exciton emission. Several spectroscopy techniques, including magneto-optics, are employed to characterize and shed light on exciton dynamics in such systems.

[1] S. Shradha et. al., arXiv, 2510.21422 (2025)

HL 14: Focus Session: Tunable Correlations in van der Waals Quantum Materials II (joint session TT/DS/HL)

Time: Tuesday 9:30–10:45 Location: HSZ/0105

See TT 27 for details of this session.

HL 15: Organic Semiconductors: Optics and Photonics

Time: Tuesday 9:30–12:00 Location: POT/0006

HL 15.1 Tue 9:30 POT/0006

Accessing 'Slow' Dynamics in Photocatalysts with PIAS — •Maria Ferree[1], Rebecca Gröninger[2], Tianhao Xue[1], Thomas Bein[1], Bettina Lotsch[2], and Frédéric Laquai[1] — [1]Dept. Physical Chemistry, LMU München, Germany — [2]Max Planck Institute for Solid State Research, Stuttgart, Germany

Quasi-steady-state Photoinduced Absorption Spectroscopy (PIAS) is a highly sensitive tool for probing long-lived excited states and charge carriers in semiconductors. We showcase PIAS capabilities by studying diverse systems, ranging from conjugated polymers and COF-based films to nanoparticle dispersions. PIAS is often overshadowed as researchers default to sophisticated Transient Absorption (TA) Spectroscopy. However, low-frequency modulated excitation

with lock-in signal detection capture extremely weak changes in transmission induced by polarons or triplet states with lifetimes ranging from nanoseconds to seconds - dynamics that remain largely inaccessible by TA, but highly relevant for diffusion-limited processes, e.g. photocatalysis. Frequency-dependent measurements provide insight into lifetimes and concentrations of long-lived species. Whilst Time-resolved Photoluminescence (TRPL) can further reinforce the conclusions obtained from PIAS by extracting exciton recombination kinetics. Our studies of organic semiconductor-based photocatalysts are a reminder that PIAS is a powerful, often more suitable method complementary to ultrafast spectroscopy and other characterisation techniques. It provides unique access to 'slow' excited-state dynamics through relatively straightforward data acquisition and processing.

HL 15.2 Tue 9:45 POT/0006

Subwavelength OLED pixels based on plasmonic electrodes — •Leo Siebigs[1], Cheng Zhang[2], Björn Ewald[1], Luca Steinbrecher[2], Maximilian Rödel[1], Thomas Fleischmann[1], Monika Emmerling[2], Bert Hecht[2], and Jens Pflaum[1] — [1]Experimental Physics 6, University of Würzburg, 97074 Würzburg — [2]Experimental Physics 5, University of Würzburg, 97074 Würzburg

Next-generation display technologies, such as augmented and virtual reality, demand the continued miniaturisation of individual pixels. A novel approach towards achieving the necessary ultra-high resolution involves subwavelength organic light-emitting diode (OLED) pixels based on plasmonic nanoelectrodes. The nanoelectrode acts as an optical antenna, ensuring efficient light-outcoupling to the far-field and control over the emission characteristics by adjusting the antenna geometry. However, upon scaling the pixel dimensions below the wavelength of light, sharp nanoelectrode contours dominate the device operation. As a result (i) filament growth leads to rapid device failure and (ii) spatially imbalanced charge-carrier transport and recombination limits the external quantum efficiency (EQE). We address these challenges by selectively passivating the nanoelectrode edges with an insulating layer and defining the active area via a nanoaperture. As proof-of-concept, efficient and stable hole-injection is shown in hole-only devices based on gold nanoelectrodes. For the first time, we demonstrate light extraction from individually addressable 300 nm x 300 nm plasmonic OLED pixels with a maximum luminance of 3000 cd m^{-2} and 1% EQE. C., Zhang et al., Sci. Adv. 2025, DOI: 10.1126/sciadv.adz8579

HL 15.3 Tue 10:00 POT/0006

Near infrared OLEDs for neuroimplants — •Sabina Hillebrandt[1], Sumit Mohapatra[1], Ahmed Gaber Abdelmagid[2], Konstantinos C. Daskalakis[2], Andreas Mischok[1], and Malte C. Gather[1,3,4] — [1]Humboldt Centre for Nano- and Biophotonics, University of Cologne, Germany — [2]Department of Mechanical and Materials Engineering, University of Turku, Finland — [3]School of Physics and Astronomy, University of St Andrews, United Kingdom — [4]CECAD, University of Cologne, Germany

OLEDs offer spectral tunability, mechanical flexibility, and compatibility with scalable thin-film fabrication, making them strong candidates for biointegrated photonic technologies. Near-infrared (NIR) OLED emission can penetrate deep into tissue and may enable neuromodulation without the need for genetic interventions.

We present the development of high-brightness, top-emitting NIR OLEDs specifically engineered for implantable neurotechnology. Using optimized emitter-host combinations, microcavity tuning, and customized charge-transport layers, these devices exhibit peak emission above 800 nm with no measurable output below 700 nm, thereby reducing off-target excitation and tissue scattering. The devices achieve power densities approaching 0.1 mW/mm^2, levels relevant for neuromodulation, while maintaining both thermal stability and robust operational performance. To further refine spectral purity and directional control, we integrate strong-coupling architectures, yielding polariton OLEDs with angular-stable NIR emission above 800 nm even on flexible, implantable polymer substrates.

HL 15.4 Tue 10:15 POT/0006

Aggregation enhanced singlet emission in a purely organic emitter with thermally activated delayed fluorescence — •Jiacheng Gong, Xin Zhou, Kaiwen Guo, Toulik Maitra, Denis Andrienko, Gert-Jan Wetzelaer, Paul W. M. Blom, and Yungui Li — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Purely organic thermally activated delayed fluorescence (TADF) emitters have gained great attentions in the field of organic light-emitting devices. However, the long-lived triplet exciton contributes to efficiency roll-off and device degradation at high current densities. Great efforts have been made to accelerate reverse intersystem crossing (rISC), while there are less studies on the increase of singlet radiative transition rate (krS). Herein, based on the benchmark TADF emitter CzDBA, it is found that it exhibits a larger krS in neat film, which is ~ 4 times faster than that in toluene with similar dielectric environment. The modelling of excited-state dynamics for electrically excited TADF emitters demonstrates that the increased krS reduces triplet and singlet densities simultaneously, while retaining high charge-to-photon conversion efficiency. Furthermore, time-resolved photoluminescence and steady-state absorption spectroscopic analysis shows that the broadened absorption feature increases the oscillator strength and hence increases krS in terms of Strickler-Berg relation. Gaussian disorder model is further applied to PL excitation spectra, and a larger disorder factor from the film samples implies that the large disorder of energetic landscape may contribute to the enhanced krS.

HL 15.5 Tue 10:30 POT/0006

Spectral diffusion of charge-transfer states in organic donor:acceptor blends due to carrier relaxation — •Giacomo Cotelli[1], Anna Köhler[1], and Reinder Coehoorn[2] — [1]University of Bayreuth, Bayreuth, Germany — [2]Eindhoven University of Technology, Eindhoven, The Netherlands

Blends of small-molecule organic semiconductors may display emission from an intermolecular charge transfer (CT) excited state. An aspect that is not well understood so far is the spectral diffusion of such CT states. We present a comprehensive study of CT state spectral diffusion in two- and three-component blends, using kinetic Monte Carlo simulations. We disentangle the effects of the CT state lifetime, charge carrier energetic disorder and blend composition on the emission spectra. Furthermore, we highlight similarities and differences between the emission of photogenerated CT states in films and electrically generated CT states in OLEDs.

HL 15.6 Tue 10:45 POT/0006

Direct Prediction of Organic Light-emitting Diode Efficiency Roll-off from Photophysical Parameters of Thermally Activated Delayed Fluorescence Emitters — •Kaiwen Guo, Yungui Li, and Paul Blom — Max Planck Institute for Polymer Research, Mainz, Germany

Severe efficiency roll-off significantly limits the practical performance of organic light-emitting diodes (OLEDs) at high luminance, especially for the devices based on thermally activated delayed fluorescence (TADF) emitters. Although numerous TADF emitters have been developed and investigated over last decade, in molecular scale the intrinsic molecular-origin of roll-off still remains unclear. In this work, we establish a direct correlation between device roll-off and intrinsic photophysical properties of TADF emitter, and analytically derive the roll-off as a function of exciton generation rate.

We propose an integrated methodology to extract complete set of photophysical parameters of TADF emitter, including the rates of exciton decays, spin conversion kinetics and bimolecular annihilation coefficients. Notably, we reveal that the roll-off behavior in TADF based OLED is not solely governed by bimolecular annihilation processes, but also influenced by the lifetime of delayed fluorescence. This knowledge enables us to predict the severity of roll-off directly from optical measurements and provides insight for further molecule designing.

15 min. break

HL 15.7 Tue 11:15 POT/0006

OLED-based implants for neurostimulation — •Sumit Mohapatra[1], Falko Fuhrmann[2], Julian F. Butscher[1,3], Sabina Hillebrandt[1,3], Martin Fuhrmann[2], and Malte C. Gather[1,3,4] — [1]Humboldt Centre for Nano- and Biophotonics, Department of Chemistry, University of Cologne, Germany — [2]Neuroimmunology and Imaging Group, DZNE, Bonn, Germany — [3]School of Physics and Astronomy, University of St Andrews, UK — [4]CECAD, University of Cologne, Germany

Light-based neurostimulation allows precise manipulation of neural circuits, yet delivering light to deep tissue remains a challenge. OLEDs combine spectral tunability, mechanical flexibility, and thin-film integration, enabling fabrication of neural probes for localized stimulation.

We advance this approach by integrating OLEDs onto magnetoelectric substrates to create fully wireless neuromodulation platforms, which are 200 μm-thick, contain 300*500 μm^2 OLEDs delivering mean power densities of 0.04 mW/mm^2. Tunable kilohertz-range resonances allow clustered multi-pixel operation, while thin-film encapsulation ensures biocompatibility and protection in a physiological environment. We also introduce a flexible OLED-based neuroprobe by integrating OLEDs onto 15 μm-thick commercial electrophysiology arrays. Using these pre-validated implantable platforms, they are transformed into μOLED arrays with 28 individually addressable μOLEDs (50 μm diameter, 300 μm pitch), achieving power density up to 0.1 mW/mm^2 at 7 V. In vivo optogenetic experiments using μ-OLEDs in mice confirm effective neuronal activation, verified by two-photon calcium imaging.

HL 15.8 Tue 11:30 POT/0006

Exploring Molecular Stability in Organic Solar Cells: A Combined DFT and ML Approach — •Muhammad Waqas and Harald Oberhofer — Chair for Theoretical Physics VII and Bavarian Center for Battery Technologies, University of Bayreuth

The stability of organic solar cells (OSCs) remains a significant challenge in the field. In this work, we present a data-driven approach that integrates density functional theory (DFT) and machine learning (ML) to identify molecular parameters that influence device stability. For this purpose, we compute different

optical and electronic parameters by using DFT and time-dependent DFT and check their influence on the lifetime (T80) of OSCs. The first step is to collect lifetime data from the already published literature for different OSC materials. The second step involves DFT and TD-DFT calculations for the selected molecules, thereby generating a dataset. This dataset serves as a foundation for training the ML models. Based on the DFT-generated data, we train ML models that can help us recognise the most influential parameters that affect the stability of OSCs. Furthermore, based on the insights gained from the ML models, we can explore the chemical space to find other molecules that can be used to prepare more stable devices.

HL 15.9 Tue 11:45 POT/0006

Accurate characterization of next-generation photodiodes — Siddhartha Saggar[1,2], Giedrius Puidokas[2], and •Caroline Murawski[1,2] — [1]Institute of Solid-State Electronics, TUD Dresden University of Technology, 01062 Dresden, Germany — [2]Kurt Schwabe Institute for Sensor Technologies, 04736 Waldheim, Germany

Photodiodes based on organic and emerging semiconductor materials have demonstrated high potential for optical sensing in biomedicine, imaging applications, and light-based data transmission. During the last decade, concerns have arisen regarding the reliable reporting of the device performance, especially under low illumination conditions. This work addresses these concerns and provides a robust framework for measuring and reporting standardized photodetection metrics. We have developed a measurement setup including a highly sensitive electrometer, calibrated optical filters, and light sources with narrowband emission spectra. For operation of the setup, we provide open-source Python scripts and outline protocols suitable for accurate characterization of steady-state photodetecting metrics.

HL 16: Focus Session: Quantum Emitters in 2D Semiconductors

Quantum emitters are fundamental building blocks in the development of scalable quantum communication networks. They provide capabilities for single-photon generation, quantum memory, and entanglement distribution*essential components for quantum key distribution, quantum repeaters, and future quantum internet infrastructure. Two-dimensional (2D) materials have recently emerged as a highly promising platform for quantum photonics. Their atomically thin nature enables strong light-matter interaction, high tunability, and seamless integration with photonic and electronic environments. Moreover, the reduced dielectric screening and strong excitonic effects inherent to 2D materials provide unique opportunities to engineer and control localized excitonic states that act as quantum emitters. This combination of physical richness and technological compatibility places 2D materials at the frontier between fundamental quantum optics and device-level quantum technologies. To advance the field, it is essential to understand both the microscopic theoretical principles and the engineering challenges associated with integrating such systems into communication networks.

Organized by Michael Lorke, Iris Niehues and Tobias Heindel

Time: Tuesday 9:30–12:45 Location: POT/0081

Invited Talk HL 16.1 Tue 9:30 POT/0081

Tailoring the performance of WSe_2 quantum emitters via cavity quantum electrodynamics and coherent driving — •Ivan Solovev — Institute of Physics, Carl von Ossietzky University of Oldenburg, Oldenburg, Germany

The ability to create scalable arrays of bright and easily-fabricated single photon sources has sparked keen interest in Van der Waals materials, rendering them a promising platform for emerging quantum technologies. Here I will provide an overview how their performance can be substantially improved via integration into a tunable microcavity as well as exploiting resonant excitation schemes. The implementation of the monolithic Fabry-Pérot open cavity, operating in a weak coupling regime, enables the observation of phenomena such as Purcell enhancement of radiative decay, strain-induced tuning of the emitter energy and two-photon interference. An impact of phonons on dephasing and resulting indistinguishability will be discussed. Furthermore, the selective excitation in a coherent manner is achieved via resonant driving, leading to the observation of Rabi oscillations.

Invited Talk HL 16.2 Tue 10:00 POT/0081

Deterministic single-photon emitters in 2D materials — •Ursula Wurstbauer — University of Münster, Germany

Single-photon emitters (SPEs) play a pivotal role as building blocks for quantum technologies. In two-dimensional (2D) materials, SPEs can deterministically be generated, externally manipulated and monolithically integrated. The properties of SPEs in atomically thin membranes are strongly dependent on the host materials and differ e.g. between TMDCs and hBN but also on the emitters origin, like defects, strain or moiré-potentials in twisted structures [1,2]. SPEs can be generated on-demand and on-chip with high lateral precision in the prototypical TMDC monolayer MoS2 by defect engineering utilizing focused helium ions [3]. These defect states in TMDCs interact with the electronic bands, whereas some defects in hBN show color center like behavior [1]. Following a general introduction, we focus on generation and characterization of rather monoenergetic SPEs in hBN by Argon ion irradiation [4]. We gratefully acknowledge A. R. Bhuiyan, R. Schmidt, A. Michaelis de Vasconcellos, R. Bratschitsch and Harry Mönig for fruitful collaboration. [1] S. Michaelis de Vasconcellos et al. Physica status solidi b259, 2100566 (2022). [2] M. Brotons-Gisbert, et al. MRS Bulletin 49, 914-931 (2024). [3] J. Klein et al. ACS Photonics, 8, 2, 669-677 (2021). [4] A. R. Bhuiyan et al.

Invited Talk HL 16.3 Tue 10:30 POT/0081

Resolving atomic and electronic structure of point defects in MoS_2 by first-principles calculations and scanning tunneling microscopy — •Hannu-Pekka Komsa — University of Oulu, Oulu, Finland

A unique advantage of 2D materials is that the defects in them are always at or very near to the surface, which can be highly beneficial in quantum emitter and quantum sensing applications. Importantly, this also enables direct characterization and manipulation of the defects with surface-sensitive techniques, such as scanning tunneling microscopy (STM). Since STM probes mainly the electronic structure, defect identification often requires comparison to results from first-principles calculations.

I will present our recent investigations on the electronic structure of a few common point defects in 2D MoS_2, such as S vacancies, Mo and Fe adatoms, and C substitutional on S site, combining first-principles calculations and experimental STM results from University of Cologne and Karlsruhe Institute of Technology. I will first discuss the computational aspects that were found to be important in achieving good agreement with experiments. A careful analysis and comparison of the computational and experimental results then allow us to infer defect identity, charge state, defect-defect interactions, magnetic moment, and dynamic effects such as defect transformations among Jahn-Teller configurations, defect charging, and spin lifetimes. Finally, benefiting from the atomic manipulations inside STM, rational atom-by-atom fabrication of defect structures can be envisioned.

15 min. break

Invited Talk HL 16.4 Tue 11:15 POT/0081

Polarization dynamics of isolated defects in hexagonal boron nitride — Serkan Paçal[1], Çağlar Samaner[1], Furkan Ağlarcı[1], Ömer S. Tapşın[1], and •Serkan Ateş[1,2] — [1]Department of Physics, Izmir Institute of Technology, Izmir, Turkey — [2]Faculty of Engineering and Natural Science, Sabanci University, Istanbul, Turkey

Single-photon sources (SPSs) are indispensable for quantum information technologies like Quantum Key Distribution. The practical success of these applications critically depends on the high purity and long-term stability of the emitted light's polarization state, which serves as the information-carrying quantum bit (qubit). Understanding and controlling polarization dynamics, therefore, presents a universal challenge for establishing reliable solid-state quantum interfaces. We propose using hexagonal Boron Nitride (hBN) defect centers as a

promising new platform for SPSs exhibiting strong, stable single-photon emission at room temperature, making it an ideal model system. In this work, we specifically investigate the polarization properties of hBN defect centers. We analyze the dynamics and temperature dependence of the polarization degree, focusing on the influence of electron-phonon interactions. Our results offer crucial insights that enable the development of targeted strategies to enhance the polarization stability of single-photon emitters, thereby facilitating more robust quantum optical systems.

Invited Talk HL 16.5 Tue 11:45 POT/0081

Defect-driven quantum emission in 2D materials — •Magdalena Grzeszczyk — IFIM, NUS, 117544, Singapore

Carbon-doped hexagonal boron nitride (hBN:C) provides a compelling 2D analogue to classical wide-bandgap hosts such as ruby (Cr:Al2O3), where isolated impurity centers give rise to sharp, stable optical transitions. These point defects have emerged as robust and manipulatable single-photon emitters (SPEs). By combining a broad suite of experimental techniques with advanced theoretical modeling, we introduce a consistent assignment of the observed excitations in hBN:C to the most likely underlying defect complexes. The described defect states residing in close proximity to the surface present an ideal sensors of local fields at the nanoscale. An example of how the local dielectric environment strongly modulates these centers, producing distinct spectral shifts will be discussed. Additionally, these defect states can be electrically excited in hBN-based light-emitting diode structures, providing a route toward integrated quantum emitters in van der Waals devices. Finally, ZnPS3 will be introduced as an emerging new host of SPEs. As a representative member of a broader family of layered MPX3 compounds, such as MnPS3 and FePS3, this emergent host opens new platform for future exploration of SPEs with intrinsic magnetic tunability.

HL 16.6 Tue 12:15 POT/0081

Nanoscale magnetic field sensing with spin defects in hexagonal boron nitride — •Korbinian Felber, Timo Strobl, Paul Konrad, Andreas Sperlich, and Vladimir Dyakonov — Experimental Physics 6, Julius-Maximilians-Universität Würzburg (JMU), 97074 Würzburg, Germany

The development of quantum sensors based on solid-state spin defects is a vibrant research area, yet most host materials are three-dimensional, making it challenging to position the sensing spins in close proximity to a target sample. This limitation was recently overcome in 2020 with the discovery of the negatively charged boron vacancy (V_B^-) in the two-dimensional van der Waals material hexagonal boron nitride (hBN). Exfoliating spin-active hBN flakes provide coherent spin manipulation in an atomically thin host. Using optically detected magnetic resonance (ODMR), these hBN spin defects provide sensitive readout of local magnetic fields, temperature, and strain, making functional hBN layers an ideal platform for exploring fundamental questions in 2D magnetism. In this study, we assemble a vdW heterostructure by stacking active hBN on top of a 2D ferromagnet. By employing spin-relaxometry techniques, we probe nanoscale magnetic fluctuations near the Curie temperature of the exfoliated ferromagnet. Our results highlight the potential of hBN-based quantum sensors for characterizing local magnetic properties in vdW heterostructures, offering substantial benefits for the design of next-generation 2D devices.

HL 16.7 Tue 12:30 POT/0081

Ion-beam induced quantum emitters in hexagonal boron nitride — •Jan Böhmer, Annkathrin Köhler, Hannes Simon, Lucas Böhme, and Carsten Ronning — Friedrich Schiller University, Jena, Germany

Defect centers in solid-state materials are emerging as highly promising candidates for realizing robust quantum light sources. Among these, hexagonal boron nitride (hBN) has attracted significant interest due to its potential for hosting room-temperature single photon emitters (SPEs). We utilize ion-beam irradiation to introduce optically active defect centers into hBN, offering a controlled and tunable method for engineering defect centers. We have investigated intrinsic and extrinsic ion-beam induced defect centers in exfoliated hBN flakes: Micro-photoluminescence spectroscopy (μ-PL) was employed to characterize the spectral properties of the induced emitters, while second-order correlation measurements ($g^{(2)}$) were performed to demonstrate the single-photon emission behavior and determine the quantum nature of the sources. Additionally, in-situ electrical measurements were used to monitor the reaction of the hBN flakes to irradiation in real-time. The results demonstrate that ion-beam irradiation can be successfully utilized for creation of quantum emitters in hBN. This work contributes to the ongoing effort to develop reliable, solid-state single photon emitters for quantum applications.

HL 17: Quantum Dots and Wires: Rings, Wires and Transport

Time: Tuesday 9:30–12:15 Location: POT/0251

HL 17.1 Tue 9:30 POT/0251

Growth of hexagonal Silicon Germanium quantum rings — •Marvin Marco Jansen[1], Mette F. Schouten[1], Denny Lamon[1], Wouter H.J. Peeters[1], Marcel A. Verheijen[1,2], and Erik P.A.M. Bakkers[1] — [1]Department of Applied Physics, Eindhoven University of Technology, Groene Loper 19, 5612AP Eindhoven, The Netherlands — [2]Eurofins Materials Science BV, High Tech Campus 11, 5656 AE Eindhoven, The Netherlands

Developing a silicon-based laser represents a key step toward commercially viable photonic circuits. A promising route is the recently discovered hexagonal silicon germanium (hex-SiGe) grown as shells around gallium arsenide (GaAs) nanowires (NWs), which has demonstrated efficient direct band-gap emission. In addition, type-I band alignment was demonstrated in hex-SiGe/Ge quantum wells (QWs), pushing the system closer to lasing. Theory predicts that combining hexagonal/cubic Ge(Si) QWs could further enhance optical performance. Here, we investigate the growth of hex-SiGe/Ge QWs on GaAs NWs that alternate between wurtzite (WZ) and zinc blende (ZB) crystal phases, forming ring-shaped hexagonal Ge QWs. These quantum rings feature two types of confinement: crystal-phase-induced axial confinement and radially controlled alloy composition. We explore several different WZ/ZB superlattice designs and TEM analysis confirms successful integration of hexagonal/cubic SiGe alloys and SiGe/Ge QW shells on the designed superlattices. Our results establish crystal-phase superlattice NWs as a promising platform realizing hex-Ge quantum rings and marking progress towards a hex-SiGe laser.

HL 17.2 Tue 9:45 POT/0251

A road to parallelisation - spin qubits as single electron pumps — •Dustin Wittbrodt[1], Johannes Christian Bayer[1], Lars Schreiber[2], Janne Lehtinen[3], and Frank Hohls[1] — [1]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany — [2]JARA Institute for Quantum Information, Forschungzentrum Juelich, Germany — [3]SemiQon Technologies Oy, Espoo, Finland

The main workhorse of low current Ampere realization is the Single Electron Pump (SEP), which generates quantized currents based on the quantized transport of single charge carriers. The result are currents in the fA-pA range, measureable with a precision of as low as 0.1 ppm. For further improvement of accuracy and current output, parallelization of pumps is the necessary next step. Semiconductor spin qubit devices offer an interesting solution. In addition to sharing the same central building unit, the quantum dots, spin qubits also offer the possibility of incorporating CMOS logic and taking advantage of a mature, high-yield industry for large scale SEP manufacturing, thus allowing for the implementation of a high number of pumps with minimal control inputs. Various Si and Si-compound spin qubit technology platforms are being tested as SEP candidates, within the EU-funded AQuanTEC project. The focus of the activities includes the characterisation of these spin qubits in DC measurements and then in a series of AC measurements to characterise the pumping behaviour of these devices. We present the results of this effort here, offering a perspective on the potential application of Qubit technology for broader use as quantum metrological instruments.

HL 17.3 Tue 10:00 POT/0251

Using full counting statistics to identify interactions in the electron dynamics in a self assembled quantum dot — •Johann Zöllner, Hendrik Mannel, Daniel Oppers, Axel Lorke, Martin Geller, and Jürgen König — Faculty of Physics and CENIDE, University of Duisburg-Essen

We study interactions and electron dynamics in a self-assembled quantum dot using full counting statistics. Each tunneling event identified with a resonance-fluorescence-based continuous measurement [1]. Full counting statistics provides much more information than just the average current through the system. The details of the probability distribution obtained from full counting statistics depends on whether interactions play a role in electron transport or whether it can be modeled by noninteracting fermions [2,3]. This is reflected in sign changes of the factorial cumulants calculated from the probability distribution. Factorial cumulants are a measure for fluctuations and are particularly suited to characterize discrete distributions. We identify these sign changes predicted by theory in the experimental data. In this way, simply by observing individual tunneling events between the dot and a reservoir, we have gained information about the electron dynamiks like spin relaxation between Zeeman-split energy level and the presence of interactions.

[1] A. Kurzmann *et al.*, PRL **122**, 247403 (2019)
[2] D. Kambly *et al.*, PRB **83**, 075432 (2011)
[3] P. Stegmann *et al.*, PRB **92**, 155413 (2015)

HL 17.4 Tue 10:15 POT/0251

Effective Hamiltonians for Ge/Si core/shell nanowires from higher-order perturbation theory — Sebastian Miles[1], A. Mert Bozkurt[1], •Dániel Varjas[2,3,4], and Michael Wimmer[1] — [1]QuTech and Kavli Institute of Nanoscience, Delft University of Technology — [2]IFW Dresden and Würzburg-Dresden Cluster of Excellence ct.qmat — [3]Max Planck Institute for the Physics of Complex Systems — [4]Budapest University of Technology and Economics

We theoretically explore the electronic structure of holes in cylindrical Germanium/Silicon core/shell nanowires using a perturbation theory approach. The approach yields a set of interpretable and transferable effective low-energy model parameters for the lowest few sub-bands up to fifth order in perturbation theory for various experimentally relevant growth directions. In particular, we are able to resolve higher-order cross terms, e.g., the dependency of the effective mass on the magnetic field. Our study reveals orbital inversions of the lowest sub-bands for low-symmetry growth directions, leading to significant changes of the lower order effective coefficients. We demonstrate a reduction of the direct Rashba spin-orbit interaction due to competing symmetry effects for low-symmetry growth directions. Finally, we find that the effective mass of the confined holes can diverge, yielding quasi flat bands interesting for correlated states. We show how one can tune the effective mass of a single spin band allowing one to tune the effective mass selectively to its divergent points.

HL 17.5 Tue 10:30 POT/0251

Improving optical quality in highly strained GaAs/$In_xAl_{1-x}As$ core/shell nanowires — Xiaoxiao Sun, •Alexej Pashkin, René Hübner, Finn Moebus, Yuxuan Sun, Andreas Worbs, Slawomir Prucnal, Shengqiang Zhou, Stephan Winnerl, Manfred Helm, and Emmanouil Dimakis — Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

III-V semiconductor nanowires are promising for applications in photonics, electronics, and sensing. In lattice-mismatched GaAs/$In_xAl_{1-x}As$ core/shell nanowires, tensile strain in the GaAs core enables substantial bandgap tuning across the near-infrared spectrum. However, $In_xAl_{1-x}As$ shells are typically grown at low temperatures, which compromises their structural quality and induces non-radiative recombination. We present two strategies to mitigate it. The first employs a dual-shell architecture in which an intermediate $Al_yGa_{1-y}As$ shell spatially separates carriers in the GaAs core from the $In_xAl_{1-x}As$ shell [1]. Optimizing the spacer thickness significantly enhances photoluminescence efficiency and extends emission lifetimes. The second strategy focuses on optimizing the shell growth conditions. We show that higher growth temperatures improve the core/shell interface quality, reducing non-radiative recombination and carrier scattering, with optimal performance near 500°C [2]. This allows a simple single-shell structure to approach the performance of the more complex dual-shell design.

[1] X. Sun et al., *Adv. Funct. Mater.* **34**, 2400883 (2024).
[2] X. Sun et al., *Appl. Phys. Lett.* **127**, 182107 (2025).

HL 17.6 Tue 10:45 POT/0251

Quantum dot as a model system for a Hund's coupled impurity — •Olfa Dani[1], Johannes C. Bayer[1,2], Timo Wagner[1], Gertrud Zwicknagl[3], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Hannover, Germany — [2]Physikalisch-Technische Bundesanstalt, Braunschweig, Germany — [3]Institut für Mathematische Physik, Technische Universität Braunschweig, Braunschweig, Germany

In this work, we investigate electron transport through the third shell [1] of a gate-defined GaAs quantum dot, where the exact electron number (N) is determined using a quantum point contact and tuned in a controlled manner by changing the applied gate voltages of the device [2]. For N = 7-11, the addition energy shows a triangular evolution with a maximum at half-filling. This trend is reproduced by model calculations including Hund's rule exchange. In the same filling range, a zero-bias anomaly (ZBA) characteristic of the Kondo effect appears. Its width and amplitude display a similar triangular dependence, reflecting the particle-hole symmetry of the three spin-degenerate orbitals. The pronounced ZBA is attributed to the contribution of both the Kondo resonance and low-energy Hund satellite excitations associated with degenerate orbitals observed in the spectral function [3]. The quantum dot is viewed as a multi-orbital Kondo impurity with Hund's interaction and serves as a model system for a Hund's coupled impurity.

[1] L. P. Kouwenhoven, et. al., Rep. Prog. Phys. 64 (2001).
[2] T. Wagner, et. al., Nat. Phys.15 (2019).
[3] O. Dani, et. al., arXiv: 2505.21675 (2025).

15 min. break

HL 17.7 Tue 11:15 POT/0251

Quantum stochastic resonance in a single-photon emitter — •H. Mannel[1], J. Zöllner[1], E. Kleinherbers[2], M. Zöllner[1], N. Schwarz[1], F. Rimek[1], A. Ludwig[3], A. Lorke[1], J. König[1], and M. Geller[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, 47057 Duisburg, Germany — [2]Department of Physics and Astronomy, University of California, Los Angeles, California 90095, USA — [3]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany

Classical stochastic resonance (SR) describes how noise can enhance the response of a driven bistable system. Recently, it has been extended to the quantum regime, where fluctuations originate from single tunneling events [1]. Building on optical real-time charge detection in self-assembled quantum dots [2], we demonstrate quantum stochastic resonance in a single InAs/GaAs quantum dot, weakly tunnel-coupled to an electron reservoir. Periodic modulation of the gate voltage synchronizes the electron tunneling with the external drive, while resonance fluorescence provides a fully optical, high-resolution readout of the charge state. From the full counting statistics of the tunneling events, we observe a pronounced narrowing of the distribution at the resonance condition, marking the transition from stochastic to increasingly deterministic transport [3].

[1] T. Wagner et al., Nat. Phys. 15, 330 (2019).
[2] A. Kurzmann et al., Phys. Rev. Lett. 122, 247403 (2019).
[3] H. Mannel et al., Commun Phys 8, 404 (2025).

HL 17.8 Tue 11:30 POT/0251

Spin relaxation dynamics of the excited triplet state in self-assembeld quantum dots — •Carl Nelson Creutzburg[1], Arne Ludwig[2], Andreas D. Wieck[2], Martin Geller[1], and Axel Lorke[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]Chair of Applied Solid State Physics, Ruhr-University Bochum, Germany

The two-electron triplet state in self-assembled quantum dots (QDs) can pair with the singlet ground state to form an electrically addressable spin qubit candidate. Using such qubits for quantum information processing requires long coherence times T_2, ultimately limited by the spin relaxation time T_1. While T_1 has predominantly been probed using optical techniques, we here present an all-electrical approach to access the spin relaxation dynamics.

The QDs are embedded in an inverted high-electron-mobility transistor, allowing controlled electron tunneling between the dots and a coupled two-dimensional electron gas (2DEG), which also serves as a sensitive charge detector. Using time-resolved transconductance spectroscopy [1] with a three-level pulse sequence, we observe the relaxation from the excited triplet to the singlet state as a function of the charging interval. A rate-equation analysis yields the spin relaxation time T_1. This approach provides an independent and complementary route to previous studies [2] and may help refine key assumptions.

[1] B. Marquardt et al., Nature Commun. 2, 209 (2011)
[2] K. Eltrudis et al., Appl. Phys. Lett. 111, 092103 (2017)

HL 17.9 Tue 11:45 POT/0251

CMOS Compatible Short-Channel Junctionless Nanowire Transistors — •Sayantan Ghosh[1,2], Alessandro Puddu[1,2], Slawomir Prucnal[1], Yordan M. Georgiev[1], Ahmad Echresh[1], and Artur Erbe[1,2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Technische Universität Dresden, 01069 Dresden, Germany

The demand for miniaturized, high-speed, and energy-efficient electronics is pushing conventional planar transistors to their scaling limits, where short-channel effects and fabrication complexity constrain performance. Junctionless nanowire transistors (JNTs) offer a promising alternative through simplified architecture, strong electrostatic control, and CMOS compatibility. Using uniformly doped channels and eliminating pn-junctions, JNTs reduce process complexity and improve scalability for next-generation nanoelectronics. In this work, short-channel silicon JNTs were fabricated on SOI substrates using a CMOS-compatible top-down method. The devices use 20 nm-wide n-type Si nanowires with channel lengths from 1000 nm to 50 nm. Back-gate operation shows clear ambipolar behaviour, while top-gate operation yields the unipolar response characteristic of true JNTs. The 50 nm device achieves a current on/off ratio > 5 orders of magnitude and a subthreshold swing of around 200 mV/dec, demonstrating strong potential for low-power nanoscale technologies.

HL 17.10 Tue 12:00 POT/0251

Majorana bound states in 1D superconducting nanowires: detection, transport, and braiding — •Suhas Gangadharaiah — Indian Institute of Science Education and Research Bhopal India

Majorana bound states (MBSs) have emerged as promising candidates for robust quantum computation due to their topological protection. However, similar tunneling conductance features for both the MBSs and certain types of Andreev bound states have turned out to be a major obstacle in the verification of the presence of MBSs in semiconductor-superconductor heterostructures. In this talk, we will first discuss our protocol to probe properties specific to the MBSs and use it to distinguish the topological zero-bias peak (ZBP) from a trivial one [1]. We will next consider the dynamical transport of MBSs in the semiconductor-superconductor heterostructure in a realistic scenario involving noisy conditions and their role in inducing diabatic errors. We will discuss the scaling laws that relate these errors to the drive time [2]. Finally, we will discuss our ongoing work on MBS braiding in a trijunction geometry composed of three connected Kitaev chains.

1. Dibyajyoti Sahu, Vipin Khade, and Suhas Gangadharaiah. Effect of topological length on bound state signatures in a topological nanowire. Phys. Rev. B, 108:205426, Nov 2023.

2. Dibyajyoti Sahu and Suhas Gangadharaiah. Transport of Majorana bound states in the presence of telegraph noise. Physical Review B, 111(23):235306, June 2025.

HL 18: Nanomechanical systems (joint session HL/TT)

Time: Tuesday 10:00–12:45 Location: POT/0051

HL 18.1 Tue 10:00 POT/0051

Mechanical characterization of freely-suspended crystalline YIG nanodevices — •Jonny Qiu[1,2], Matthias Grammer[4,5], Sebastian Sailler[6], Sebastian T. B. Goennenwein[6], Michaela Lammel[6], Hans Huebl[3,4,5], and Eva Weig[1,2,3] — [1]TUM School of Computation, Information and Technology, Garching, Germany — [2]Zentrum für Quantum Engineering, Garching, Germany — [3]Munich Center for Quantum Science and Technology, Munich, Germany — [4]TUM School of Natural Sciences, Garching, Germany — [5]Walther-Meißner-Institut, BAdW, Garching, Germany — [6]University of Konstanz, Department of Physics, Konstanz, Germany

Efficient quantum transduction, the reciprocal conversion of quantum signals from one energy level to another, is an ongoing challenge in quantum network applications. Engelhardt et al. [1] proposed a microwave to optical converter (MWOC) that co-localizes microwave, magnetic and elastic excitations within a suspended optomechanical crystal (OMC) made of crystalline yttrium iron garnet (YIG).

In this talk, we report our progress towards realizing the MWOC and present freely-suspended YIG nanodevices. We fabricated YIG cantilevers and beams using an electron beam lithography process and a subsequent crystallization by annealing approach. Piezo-driven interferometric spectroscopy reveals the mechanical response modes of these devices, from which we extract Young's modulus and internal stress to design the OMC as a MWOC. We visualize and thus confirm the corresponding mode shapes via laser doppler vibrometry.

[1] F. Engelhardt, et al., Phys. Rev. Appl. 18, 044059 (2022).

HL 18.2 Tue 10:15 POT/0051

Sensing local temperature changes of a silicon nitride nanomembrane under large-amplitude vibration — •Valentin Barth, Mengqi Fu, and Elke Scheer — University of Konstanz, Konstanz, Germany

In MEMS and NEMS, changes in environmental conditions (e.g., a global change in temperature [1]) can alter the motion properties of silicon nitride (SiN) membranes. Vibrational motion may cause the membrane to experience local heating effects.

SiN square membranes (side length: 450 μm, thickness: 500 nm) are used and driven with a piezoelectric actuator. The motion is monitored using digital holographic microscopy. The measurements are carried out with a strong drive, resulting in vibration amplitudes on the order of hundreds of nanometers. Local temperatures are measured via the Seebeck effect using permalloy ($Ni_{81}Fe_{19}$) and gold as thermocouple, which provides a sensitivity of 20 μV/K and is suitable for micrometer-scale measurements [2]. To improve the signal-to-noise ratio and suppress unwanted contributions, the measurement is performed with a lock-in amplifier, where the temperature signal is demodulated at twice the drive frequency. The measured temperature depends on both the position of the thermometer and the vibration amplitude, with values reaching up to 0.5 mK. Besides the temperature signal of the membrane, signals caused by vibrations from neighboring membranes (distanced 1.5 mm) are also detected.

[1] F. Yang et al., Sens. Actuators A Phys. 354, 114307 (2023).
[2] F. L. Bakker et al., J. Appl. Phys. 111, 084509, (2012)

HL 18.3 Tue 10:30 POT/0051

FEBID and FIBID nanowire field emitters integrated with microcantilevers - fabrication and characterization — •Ewelina Gacka[1,2], Gregor Hlawacek[1], Krzysztof Kwoka[2], Tomasz Piasecki[2], Bartosz Pruchnik[2], René Hübner[1], and Teodor Gotszalk[2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328, Dresden, Germany — [2]Department of Nanometrology, Wroclaw University of Science and Technology, 50-370, Wroclaw, Poland

Because micro- and nanomechanical systems are continuously evolving, there is a need to leverage various fabrication technologies. A scanning electron microscope with a gallium focused ion beam, as well as a helium ion microscope, were used to integrate platinum-carbon (Pt-C) and tungsten-carbon (W-C) nanowire field emitters with microcantilevers, serving as deflection sensors. Pt-C and W-C nanocomponents were fabricated using an additive, direct-writing method - focused-electron-/ion-beam-induced deposition (FEBID/FIBID)[1,2]. After growth calibration, the field emission behavior was studied in situ inside a vacuum chamber. The deposited Pt-C and W-C materials were characterized using Kelvin probe force microscopy and transmission electron microscopy. [1] T. Piasecki et al., Nanotechnology 35 (2024), doi: 10.1088/1361-6528/ad13c0. [2] E. Gacka et al., Measurement 234 (2024), doi: 10.1016/j.measurement.2024.114815.

HL 18.4 Tue 10:45 POT/0051

Optimization of Faraday Cage Angled Etching and Its Application Prospects in Silicon Carbide — •Wuzheng Ge[1,2], Ciaran Fowley[1], Jens Zscharschuch[1], Claudia Neisser[1], Artur Erbe[1,2], Philipp Bredol[3], Felix David[3], and Eva Weig[3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany — [2]Dresden University of Technology, Faculty of Electrical and Computer Engineering, 01069 Dresden, Germany — [3]Technical University of Munich, Chair of Nano and Quantum Sensors, 85748 Munich, Germany

This work presents the optimization of a Faraday Cage Angled Etching (FCAE) approach for ICP-RIE. By reshaping the plasma potential through the cage's mesh geometry, FCAE steers ions along the cage-wall normal, enabling controllable ion incidence angles. Reproducible 3D triangular cross-section structures were demonstrated on silicon, confirming the effectiveness of ion-direction tuning. The results were also applied to silicon carbide nanomechanical resonators. The enhanced directional ion flux enables direct fabrication of free-standing, stress-free structures in bulk, undoped SiC. This capability offers new pathways for advanced SiC-based MEMS.

15 min. break

HL 18.5 Tue 11:15 POT/0051

Probing Mechanical Nonlinearities with Quantum Dots — •Noah Spitzner, Jona Richter, Emeline Denise Sophie Nysten, Matthias Weiss, and Hubert Krenner — Universität Münster, Münster, Germany

The coupling of quantum dots to mechanical resonances is a well-established approach to investigate the behaviour of mechanical resonators and crystals. Within that approach, the quantum dots (QDs) act as point-like sensors sensitive to dynamical changes to their lattice constant. Vibrations in the host structure modulate the emission energy of the quantum dot, enabling readout of mechanical modes via ultrafast optical detectors. In our hybrid structures, mechanical excitation is achieved by integrating the QD-membrane onto a lithium niobate substrate equipped with finger-like electrodes called interdigitated transducers (IDTs). Applying a radio-frequency (RF) signal to the IDTs generates surface acoustic waves, which propagate on the surface of the substrate, coupling to quantum dots in their path.

This hybrid platform was taken a step further by structuring the QD-membrane into rings hosting mechanical resonances. Frequency sweeps of the RF signal applied to the IDT revealed sharp resonances in the emission-energy modulation exclusively for the quantum dots located within the rings. Interestingly, the resonances appear over a large region of SAW frequencies from 200 MHz to 900 MHz. Moreover, we detect clear signatures of a nonlinear mechanical response e.g. asymmetric lineshapes in the time-modulated optical signal of the QD when the external drive by the IDT is increased.

HL 18.6 Tue 11:30 POT/0051

Dry processing of 3C-silicon carbide nanostring resonators — •Felix David[1,2,3], Yannick Klass[1], Philipp Bredol[1,2,3], and Eva Weig[1,2,3] — [1]Technische Universität München, School of Computation, Information and Technology, Garching, Germany — [2]Technische Universität München, Zentrum für QuantumEngineering (ZQE), Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), München, Germany

We fabricate string resonators from strongly stressed 3C-silicon carbide (SiC) grown on a silicon substrate. In conventional fabrication processes, electron-beam lithography with PMMA is employed to define a metallic hard mask for the subsequent dry etching step via a liftoff process. This requires some wet-chemical process steps, such as HF etching and metal removal, which can destroy samples. Here, we describe an alternative process that avoids all wet-chemical process steps, enabling superior quality. It involves the use of a negative electron-beam resist as an etch mask, as well as the completely reactive-ion etching-based release of the nanostrings. The dry-processed nanostrings can be fabricated with a high yield and exhibit high mechanical quality factors at room temperature. Due to its high reliability, combined with high process speed, it also allows for quick adaptation to new projects, such as multilayer and hybrid mechanical systems.

HL 18.7 Tue 11:45 POT/0051

The best of two worlds: hexagonal boron nitride exfoliated on stressed silicon carbide string resonators — •Philipp Bredol[1], Felix David[1], Junhui Wu[2], Andrey N. Anisimov[2], Takashi Taniguchi[3], Kenji Watanabe[3], Georgy V. Astakhov[2], Artur Erbe[2], and Eva M. Weig[1] — [1]TU Munich, Chair of Nano and Quantum Sensors, 85748 Munich, Germany — [2]HZDR, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

The boron vacancy (VB) of hexagonal boron nitride (h-BN) is a promising single photon emitter for applications in quantum technologies. Nanomechanical control of the VB would greatly enhance its versatility in such applications, therefore nanomechanical h-BN resonators are of great interest. Here we demonstrate that h-BN can be exfoliated on a chip with a pre-stressed silicon carbide thin-film and subsequently patterned into nanomechanical string resonators with high tensile stress. The resulting h-BN covered string resonators have high mechanical quality factors due to dissipation dilution and show the optically detected magnetic resonance signature of the VB of h-BN. Our fabrication approach allows to decouple the choice of the defect hosting 2D-material from the engineering of the mechanical mode and paves the way to nanomechanical control of single photon emitters in h-BN and other 2D materials.

HL 18.8 Tue 12:00 POT/0051

Cavity optomechanics with van der Waals materials — •Aloysius Farrel[1,3], Lukas Schleicher[1,3], Irene Sánchez Arribas[1,3], Leonard Geilen[2,3], Alexander Musta[2,3], Alexander Holleitner[2,3], and Eva Weig[1,3] — [1]Chair of Nano and Quantum Sensors, TU Munich, Germany — [2]Walter Schottky Institute, TU Munich, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany

Freely suspended two-dimensional materials are promising platforms for hybrid quantum systems that combine mechanical, optical, and electronic properties. Coupling the optical and mechanical modes of the resonators would be the first step towards such hybrid quantum system.

Here, we present studies of the mechanical resonators with van der Waals materials, such as hBN, on a SiN membrane. We map the spatial mechanical modes of the freestanding and supported 2D materials. Furthermore, we observe an optical nonlinearity in our high-finesse fiber optic cavity setup, which could couple to the mechanical modes. This result helps us understand the optomechanical coupling of the system and leads the way for a hybrid quantum device by incorporating quantum emitters in the system.

HL 18.9 Tue 12:15 POT/0051

Imaging GHz surface acoustic waves in epitaxial graphene cavities — •Mingyun Yuan[1], Alberto Hernández-Mínguez[1], Yi-Ting Liou[2], Jens Herfort[1], Joao M. J. Lopes[1], and Paulo V. Santos[1] — [1]Paul-Drude-Institut, Leibniz Institut im Forschungsverbund e.V., Berlin, Germany — [2]Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

The imaging of sound has fascinated scientists and the public alike, dating back to Chladni's demonstrations in the 19th century. Nowadays, it is possible to image mechanical vibrations at the nanoscale, enabling direct probing of propagation, scattering and diffraction for high-frequency acoustic waves with short wavelengths. Here, we present the imaging of GHz surface acoustic waves (SAWs) in an epitaxial monolayer graphene nanostructure, based on thermal decomposition of SiC, using atomic-force microscopy (AFM). We observe a near-perfect strain transfer that gives rise to rich acoustic patterns in the phononic cavity formed by the graphene nanostructure. Furthermore, the enhanced acoustic intensity in the graphene region indicates a waveguiding effect, with graphene serving as an atomically thin, embedded shorting layer. Within the cavity, signatures of quantum chaos are observed. The high spatial resolution of AFM enables the investigation of SAW strain transferred onto 2D materials with high precision. The results also demonstrate an epitaxial nanophononic platform for both functional acoustic devices and fundamental studies of quantum phenomena.

HL 18.10 Tue 12:30 POT/0051

Nonlinear vibrational dynamics locally probed by time-resolved electron diffraction — •Kai Nettersheim[1], Alexander Schröder[1], and Sascha Schäfer[1,2] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Regensburg Center for Ultrafast Nanoscopy (RUN), Regensburg, Germany

Nonlinear dynamics of micro- and nanoscale electro-mechanical systems can be observed using electrical or optical methods. However, these approaches are often limited in their spatial resolution, which leaves the underlying mechanics only partially accessible. Recent advances in ultrafast electron microscopy (UTEM) enable the highly localized probing of nanoscale oscillators, allowing to retrieve detailed information about their atomic structure and material defects.

Utilizing stroboscopic UTEM imaging techniques, we present the characterization of nonlinear mode dynamics in free-standing silicon membranes employing an event-based electron detector with nanosecond temporal resolution [1]. The high-Q resonator is excited using an optical pulse train driving the sample into the nonlinear regime. Due to the use of event-based converged electron beam diffraction (CBED), phase-accurate measurements of the nanoscale structural motion are provided. Whereas at weak driving, the oscillator displays a simple Duffing-type bistability, higher harmonic overtones as well as period doubling dynamics emerge at higher driving amplitudes.

[1] A. Schröder et al., Ultramicroscopy 256, 113881 (2024)

HL 19: Graphene: Growth, structure and substrate interaction (joint session O/HL)

Time: Tuesday 10:30–12:30 Location: HSZ/0201

See O 33 for details of this session.

HL 20: Poster I

Time: Tuesday 18:00–20:00 Location: P1

HL 20.1 Tue 18:00 P1

Defect-Mediated Electronic Reconstruction in Li-TFSI-Passivated Layered InI Crystals — •Abdulsalam Aji Suleiman[1,2], Ali Karatutlu[1,3], and Aydan Yeltik[4] — [1]Department of Engineering Fundamental Sciences, Sivas University of Science and Technology, Sivas 58000, Türkiye — [2]Sivas Cumhuriyet University Nanophotonics Application and Research Center (CÜNAM), Sivas 58140, Türkiye — [3]Institute of Materials Science Nanotechnology, National Nanotechnology Research Center (UNAM), Bilkent University, Ankara 06800, Türkiye — [4]Department of Material Science and Nanotechnology Engineering, TOBB University of Economics and Technology, Ankara 06560, Türkiye

Layered indium iodide (InI) is a van-der-Waals semiconductor whose bandgap (1.6-2.8 eV) enables strong light-matter coupling but suffers from iodine-vacancy defects that limit stability. Surface passivation with lithium bis(trifluoromethanesulfonyl)imide (Li-TFSI) modifies near-surface electrostatics and bonding, improving optical and transport properties. Photoluminescence shows stronger emission and longer carrier lifetimes, consistent with reduced non-radiative recombination. Soft-X-ray absorption spectroscopy at the HESEB beamline probes F, N, O, C K-edges and I M4,5-edges, revealing how TFSI-ions coordination alters In-I bonding and orbital hybridization. These results link chemical passivation and defect energetics, outlining a route to stable halide-based optoelectronic devices.

HL 20.2 Tue 18:00 P1

Tensor network methods for electron-hole complex in nanoplatelets — •Bruno Hausmann and Marten Richter — Institut für Physik und Astronomie, Technische Universität Berlin, Germany

Nanoplatelets are colloidally grown, atomically thin, rectangular semiconductor nanostructures. Excitons in nanoplatelets are solutions of a four-dimensional Schrödinger equation. This is especially true as the structure is in between the weak and strong confinement regimes. Solving this equation is computationally expensive compared to the typical two-dimensional Wannier equation under weak confinement. Going beyond excitons to trions and biexcitons, the memory size of the discretized wavefunctions grows exponentially with the particle number. Tensor network methods have successfully been applied to solve high-dimensional eigenvalue problems. Here we adapt them to the eigenvalue equation for excitons and trions by decomposing the real-space wavefunctions into quantics tensor trains (QTT). Operators that transform the indices, e.g. shift operators in finite differences, become binary circuits, e.g. an addition network.

We were able to compute ground and excited states together with their energies for platelet dimensions between strong and weak confinement with a resolution (up to 2048 grid points per dimension) infeasible to implement without tensor networks. For illustration, eigenenergies, oscillator strengths, and various wavefunction projections were calculated.

HL 20.3 Tue 18:00 P1

Markovian vs. Full Quantum-Kinetic Approach to Phonon-Assisted Incoherent Exciton Formation in Atomically Thin Semiconductors — •Leonard Schneider, Andreas Knorr, and Henry Mittenzwey — Nichtlineare Optik und Quantenelektronik, Institut für Physik und Astronomie, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

Excitonic coherence decay and incoherent exciton formation in atomically thin semiconductors such as monolayer transition metal dichalcogenides are strongly influenced by the coupling between charge carriers and lattice vibrations. Based on Heisenberg's equations of motion, we derive the microscopic dynamics of excitonic transitions and incoherent exciton occupations coupled via phonon-assisted processes. For a consistent quantum-kinetical approach, we go beyond the usual one-phonon processes and include up to two-phonon-assisted and phonon-population-assisted transitions, which corresponds to a truncation of the hierarchy problem within a fourth-order Born approximation. We numerically evaluate the full quantum kinetics for the dephasing- and incoherent-exciton-generation dynamics and compare it to the corresponding Markovian limit. The corresponding influence of memory effects and multi-phonon processes is discussed in detail.

HL 20.4 Tue 18:00 P1

Far- and near-field photoluminescence of interlayer excitons in MoS2/WS2 heterostructures — •Johannes Holters and Iris Niehues — Institute of Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Monolayers of transition-metal dichalcogenides show intense photoluminescence (PL) at room temperature due to their high exciton binding energies. Recently, heterostructures composed of two vertically stacked monolayers have gained significant attention because of the emergence of novel quantum phenomena within these materials. Of particular interest are interlayer excitons, where, in contrast to intralayer excitons, electron and hole reside in different layers of the heterostructure. Strain, nanobubbles, Moiré effects and other local inhomogeneities can localize the appearance of these interlayer excitons to several nanometer. Here we use a scattering-type scanning near-field microscope (s-SNOM) to investigate the photoluminescence (PL) of interlayer excitons in a MoS2/WS2 heterostructure with a spatial resolution below the diffraction limit. The obtained tip-enhanced PL (TEPL) images are compared to standard confocal microscopy images. Both intra- and interlayer excitons are visible in far- and near-field images. In the TEPL images an enhanced PL signal is observed in the form of arcs around nanobubbles. These features can be assigned to interference effects caused by the interaction of the far-field light with the tip. Additionally, it is found that the intensity of the interlayer exciton PL strongly depends on the polarization of the exciting laser as well as the distance between tip and sample in the TEPL setup.

HL 20.5 Tue 18:00 P1

Optical Properties of CrSBr/TMD heterostructures — •Nicole Engel[1], Luc Oswald[1], Sai Shradha[1], Lukas Krelle[1], Daria Markina[1], Zdenek Sofer[2], and Bernhard Urbaszek[1] — [1]Institute for Condensed Matter Physics, TU Darmstadt, Darmstadt, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Czech Republic

Monolayer transition metal dichalcogenides (TMDs) exhibit several fascinating properties. These characteristics can be further expanded by creating heterostructures with CrSBr. CrSBr is an antiferromagnetic semiconductor which exhibits promising magnetic interactions with monolayer TMDs. The magnetic order of CrSBr influences the optical properties of $MoSe_2$ and WSe_2, facilitating charge transfer processes [1,2]. This work investigates CrSBr/TMD heterostructures using low-temperature optical spectroscopy with applied magnetic fields to probe excitonic properties. Understanding the optical and valley properties of CrSBr/TMD heterostructures will be relevant for the development of spintronic and valleytronic devices and show a great potential for light harvesting and enhancement of emission from 2D-materials.

[1] C. Serati de Brito et. al., Nano Lett. 2023, 23, 11073-11081
[2] J. de Toledo et. al., Nano Lett. 2025, 25, 13212-13220

HL 20.6 Tue 18:00 P1

Optical Properties of Interlayer Excitons in Transition Metal Dichalcogenide Heterostructures — •Luc Frederik Oswald[1], Sai Shradha[1], Nicole Engel[1], Julian Führer[1], Md. Tarik Hossain[2], Lukas Krelle[1], Daria Markina[1], Andrey Turchanin[2], and Bernhard Urbaszek[1] — [1]Institute for Condensed Matter Physics, TU Darmstadt, Darmstadt, Germany — [2]Institute for Physical Chemistry, Friedrich Schiller University, Jena, Germany

Interlayer excitons (IXs) in van der Waals heterostructures arise from electrons and holes confined in different monolayers, forming long-lived quasi particles with strong spin-valley coupling. In $MoSe_2/WSe_2$ systems, type-II band alignment and conduction-band splitting give rise to multiple IX states whose optical signatures are highly sensitive to temperature, lattice vibrations, and magnetic fields. This work investigates the optical response of an hBN-encapsulated, $MoSe_2/WSe_2$ lateral-vertical heterostructure grown via chemical vapour deposition (CVD). A combination of temperature-dependent photoluminescence, excitation-spectroscopy approaches, and magneto-optical measurements is used to probe the formation, evolution, and valley properties of interlayer excitons in this hybrid geometry. Together, they reveal characteristic interlayer emission features, their excitation pathways, and signatures of spin-layer hybridization.

HL 20.7 Tue 18:00 P1

Study of irradiation-induced deep-level defects in transition metal dichalcogenides MX2 (M = Mo,W; X = S, Se) — •Andrii Bodnar, Łukasz Gelczuk, and Paweł Scharoch — Departament of Semiconductor Materials Engineering, Wroclaw University of Science and Technology, Wybrzeze Wyspianskiego 27, Wroclaw 50-370, Poland

This work presents comprehensive density functional theory (DFT) calculations investigating native point defects in pristine and alpha-particle-irradiated MX_2 materials, where M represents Mo or W and X represents S or Se. The calculations focused on identifying deep-level defects and their charge transition levels, with subsequent experimental validation through deep level transient spectroscopy (DLTS) measurements. The satisfactory agreement between state-of-the-art DFT-calculated defect levels and DLTS experiments confirmed the reliability of the computational methodology and enabled identification of the origins of experimentally observed defect levels.

The validated DFT approach employing the HSE06 hybrid functional, which accurately predicts band gaps and eliminates self-interaction errors present in other approaches, was applied to calculate charge transition levels of defects in bulk MX_2 that are experimentally challenging to measure directly using DLTS. Using DFT-generated data, deep-level defects induced by alpha-particle irradiation in bulk MX_2 were identified and defect evolution under different irradiation doses was tracked.

HL 20.8 Tue 18:00 P1

Influence of hBN encapsulation on the degradation process of Hittorf phosphorus — •Maximilian Scharpey[1], Daniel Wigger[2], Nicolas Pajusco[3], Iker Herrero[3], Rainer Hillenbrand[3], and Iris Niehues[1] — [1]Institute of Physics, University of Münster, Germany — [2]Department of Physics, University of Münster, Germany — [3]CIC nanoGUNE BRTA, Donostia-San Sebastián, Spain

The van-der-Waals material Hittorf phosphorus (HP, violet phosphorus) has attracted increasing interest due to its promising semiconducting properties including high charge carrier mobility, a tuneable bandgap, and high optical absorption in the visible [1]. However, its degradation poses significant challenges for device applications. Here, we investigate the influence of hexagonal boron nitride encapsulation on the optical properties of thin flakes of mechanically exfoliated HP. By comparing photoluminescence and nanoscale Fourier transform infrared spectroscopy of encapsulated and non-encapsulated HP samples over a period of days, we gained insight on the degradation process. In addition, we used scattering-type scanning near field optical microscopy to localize the origin sites of degradation under the encapsulation layer with a resolution beyond the diffraction limit. These findings contribute to a deeper understanding of the degradation process of HP, which will play a crucial role in stabilizing this material for future applications.

[1] Ahmad et al., Adv. Funct. Mater. **34**, 2410723 (2024)

HL 20.9 Tue 18:00 P1

Graphene/WSe_2 heterostructures for optical investigation of proximity spin-orbit coupling — •Ernst Knöckl, Matthias Klein, Alexander Holleitner, and Christoph Kastl — Walter Schottky Institute, School of Natural Sciences, Technical University of Munich

We investigate proximity-induced spin-orbit coupling (SOC) in graphene/WSe_2 heterostructures using the circular photogalvanic effect (CPGE) as a symmetry-selective, experimentally simple optical probe of spin-valley-locked band textures [1]. By measuring helicity-dependent photocurrents as a function of gate voltage, excitation energy, and device geometry, we aim to disentangle Rashba and valley-Zeeman SOC contributions and to extract their magnitude and sign as a function of the graphene-WSe_2 twist angle. A key requirement is the fabrication of large, clean, and field-effect-gateable graphene/TMDC heterostructures. To this end, we demonstrate a modified dry-transfer process based on specifically prepared polydimethylsiloxane (PDMS) stamps [2]. We further determine the relative twist angle using Raman spectroscopy and second-harmonic generation (SHG) spectroscopy.

[1] Kiemle, Jonas, et al. ACS nano 16.8, 12338-12344 (2022)
[2] Jain, A. et al. Nanotechnology 29.26, 265203 (2018)

HL 20.10 Tue 18:00 P1

Transport measurements in thin layers of $HfTe_5$ — •Freddy Sack[1], Christopher Belke[1], Sonja Locmelis[2], Lina Bockhorn[1], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität, 30167 Hannover, Germany

Hafnium pentatelluride ($HfTe_5$) gained interest due to its topological insulator behavior and the pronounced anisotropy arising from highly disparate electron and hole masses. In recent works, a thickness dependent band gap was observed [1]. In contrast to the small band gap found in bulk $HfTe_5$, single layers are predicted to be quantum spin hall insulator with a large band gap [1-4]. In this study, we investigate temperature dependent transport properties of thin layers of $HfTe_5$ from 5 K to 270 K. Gate dependent measurements for different magnetic fields are utilized to characterize thin flakes with a thickness less than 50 nm and to investigate the resistance anomaly.

[1] C. Belke et al., 2D Mater. 8, 0350292021 (2021)
[2] K.C Dogan et al., Nanoscale, 16, 11262 (2024)
[3] Ling-Xioa Zhao et al., Chinese Phys. Lett. 34 037102 (2017)
[4] Bo Fu et al., Phys. Rev. Lett. 125, 258801 (2020)

HL 20.11 Tue 18:00 P1

Spectroscopic Imaging Ellipsometry at Cryogenic Temperatures Reveals Peak Splitting in 2D Polar Silver — •Ulrich Limberg[1], Jakob Henz[1], Siavash Rajabpour[2], Alexander Vera[2], Arpit Jain[2], Joshua A. Robinson[2], Su Ying Quek[3], and Ursula Wurstbauer[1] — [1]Institute of Physics, Munster, Germany — [2]MatSE PennState, Pennsylvania, USA — [3]Centre of Advanced 2D Materials, Signapore, Signapore

Two-dimensional (2D) polar metals are a new class of atomically thin materials created by confinement heteroepitaxial growth, where metallic species such as silver are intercalated between epitaxial graphene and a 6H-SiC substrate [1]. Silver intercalation leads to two competing semiconducting monolayer phases, the metastable Ag(1) and the stable Ag(2), each showing distinct opto-electronic behaviour [2].

Spectroscopic imaging ellipsometry (SIE) enables spatially resolved analysis of the complex dielectric function of both phases. Using temperature-dependent SIE from 5 K to room temperature, we investigate the modification of the linear light-matter interaction of 2D polar Ag with temperature. At low temperatures, we detect a splitting of the characteristic absorption peak of Ag(2). The experimentally determined dielectric function agrees well with theoretical predictions [2].

[1] N. Briggs et al., Nat. Mater. 19.6, 637-643 (2020).
[2] A. Jain et al. in preparation (2025).

HL 20.12 Tue 18:00 P1

Structural and Electrical Characterization of Graphene Thin Films from Dispersions — •Yasaman Jarrahi Zadeh[1], Lars Grebener[2], Shaghayegh Pourdahrany[3], Muhammad Ali[4], Nicholas Wilson[5], Mohaned Hammad[2], Günther Prinz[1], Martin Geller[1], Michael A. Pope[5], William Wong[3], Hartmut Wiggers[4], Doris Segets[2], and Axel Lorke[1] — [1]Faculty of Physics, and CENIDE, University of Duisburg-Essen, Germany — [2]Institute for Energy and Materials Processes, and CENIDE, University of Duisburg-Essen, Germany — [3]Department of Electrical and Computer Engineering, and WIN, University of Waterloo, Canada — [4]Institute for Combustion and Gas Dynamics, and CENIDE, University of Duisburg-Essen, Germany — [5]Department of Chemical Engineering, and WIN, University of Waterloo, Canada

Graphene powders were produced by microwave-plasma synthesis and sonicated into ethanol or water with carboxymethyl cellulose (CMC) or di-n-dodecyl dimethylammonium bromide (DDDA) stabilizers. Using ultrasonic spray coating or Langmuir deposition, thin films were deposited on sapphire and characterized by SEM, Raman spectroscopy, and transport measurements. Water-based CMC dispersions produced the most uniform films. Raman spectra showed good structural quality (judged by the intensity ratio $I_{2D}/I_G \sim 1.5$). CMC-stabilized spray-coated films (0.1 wt%) achieved the highest conductivity (2.5 mS) and mobility (11 cm^2/V.s). DDDA films were more porous with lower mobility, while multilayer Langmuir films reached higher mobility (19 cm^2/V.s) but reduced conductivity.

HL 20.13 Tue 18:00 P1

Raman polarization switching in CrSBr — Priyanka Mondal[1], Daria Markina[1], •Lennard Hopf[1], Lukas Krelle[1], Sai Shradha[1], Julian Klein[2], Mikhail Glazov[3], Iann Gerber[4], Kevin Hagmann[1], Regine v. Klitzing[1], Kseniia Mosina[5], Zdenek Sofer[5], and Bernhard Urbaszek[1] — [1]Institute for Condensed Matter Physics, TU Darmstadt — [2]Department of Materials Science and Engineering, Massachusetts Institute of Technology — [3]St. Petersburg, Russia — [4]Université de Toulouse, INSA-CNRS-UPS, LPCNO — [5]Department of Inorganic Chemistry, University of Chemistry and Technology Prague

In recent years, few-dimensional nanomaterials have sparked significant interest within the solid-state research community due to their novel properties and possible applications in quantum technologies. Layered CrSBr has attracted particular interest due to its quasi 1D nature, strong electron-phonon interaction and air-stability. This work probes the optical anisotropy using polarization resolved photoluminescence and Raman spectroscopy on mono and few-layer CrSBr. These techniques are sensitive to the crystal orientation and reveal the intricate dependence of phonon polarization on excitation energy. Additionally, a clear thickness dependence of the electronic and vibrational properties is found. These results shed light on the complex electron-phonon and photon-phonon interactions in CrSBr opening new avenues for future application in optoelectronic devices.

HL 20.14 Tue 18:00 P1

Tuning carrier type and electrical properties of 2D alloy transistion metal dichalcogenides — •Axel Printschler, Md Tarik Hossain, Nhat Lam Duong, Julian Picker, Rahul Sharma, Christof Neumann, Muhammad Sufyan Ramzan, Caterina Cocchi, and Andrey Turchanin — Friedrich Schiller University Jena, Germany

Two-dimensional (2D) transition metal dichalcogenide (TMD) alloys offer a powerful platform for engineering material properties beyond the limitations of their constituents. Controlling the electronic characteristics of TMDs is crucial for the development of advanced electronic and optoelectronic devices and functional circuitry. This study focuses on the electronic properties of monolayer $(V_xW_yMo_{1-x-y})S_2$ alloys synthesized via a liquid-precursor-based chemical vapor deposition (CVD) approach. We investigate the charge transport in these materials using field-effect transistor (FET) devices. Our electrical measurements demonstrate a controlled transition from n-type to p-type semiconducting behavior, culminating in a metallic state for high vanadium concentrations. This change is supported by density functional theory (DFT) calculations. The tunability, directly correlated with the alloy composition, provides a reliable strategy for tailoring the electronic character of 2D TMDs and underscores their significant potential for application in next-generation electronic devices.

HL 20.15 Tue 18:00 P1

Many-body effects and intervalley coupling mechanisms in monolayer transition metal dichalcogenides — •Oleg Dogadov[1,2], Henry Mittenzwey[3], Thomas Deckert[4], Micol Bertolotti[2], Daniele Brida[4], Giulio Cerullo[2,5], Andreas Knorr[3], and Stefano Dal Conte[2] — [1]Fritz Haber Institute, Berlin, Germany — [2]Politecnico di Milano, Milan, Italy — [3]Technische Universität Berlin, Berlin, Germany — [4]University of Luxembourg, Luxembourg — [5]CNR-IFN Milan, Italy

The strongly bound excitons and the spin-valley locking effect make monolayer (1L) transition metal dichalcogenides (TMDs) an ideal platform to study intra- and intervalley many-body effects. Despite extensive studies conducted during the last years, a unified description of the competing many-body interactions and intervalley coupling processes in 1L-TMDs is lacking. Here, we apply broadband helicity-resolved transient absorption spectroscopy combined with a microscopic theory based on the excitonic Bloch equations to investigate coherent optical response and valley polarization dynamics in 1L-WSe_2. We unambiguously unravel competing valley-dependent contributions of two- and four-particle correlations to the coherent optical response of the studied material. By exploring the valley (de)polarization dynamics, we dissect the roles of individual intervalley coupling mechanisms, including Coulomb exchange and Dexter-like interaction, as well as phonon-assisted scattering, providing a consistent picture of the processes governing spin-valley dynamics in 1L-TMDs.

HL 20.16 Tue 18:00 P1

Unconventional Nanopatterning of 2D Materials for Future Nanoelectronics — •Tawat Chen[1,2], Poonam Borhade[3], Ya-Ping Hsieh[4], and Mario Hofmann[1] — [1]Department of Physics, National Taiwan University, Taipei, 10617 Taiwan — [2]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 3, 07743 Jena, Germany — [3]Institute of Physics, Academia Sinica, Taipei, 10617 Taiwan — [4]Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, 10617 Taiwan

Two-dimensional (2D) materials offer a promising pathway to surpass the physical scaling limits of silicon-based electronics in the post-Moore era. However, fabricating high-resolution nanofeatures on these materials using conventional photolithography is constrained by Rayleigh's diffraction limit and escalating processing costs. In this work, we demonstrate nanopatterning techniques that overcome these limitations. First, we utilize a self-expansion double patterning (SEDP) process to generate nanometer-scale features through a self-limiting, temperature-controlled oxidation mechanism, enabling the fabrication of graphene nanoribbons with precise control. Second, to achieve high-density patterning without standard lithography, we investigate the formation of porous anodic aluminum oxide (AAO) via anodization, successfully creating porous arrays with a diameter of 37 nm. Finally, we discuss the physical mechanisms governing these formation processes and their potential for the scalable, high-throughput fabrication of next-generation 2D material devices.

HL 20.17 Tue 18:00 P1

Universality of Raman spectroscopy for determining twist angle in diverse systems — •Ana Senkić[1], Nicolai Leonid Bathen[2], Thorsten Deilmann[1], Hendrik Lambers[1], Lara Blinov[1], Aleksandar Matković[3], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]Israel Institute of Technology, Haifa, Israel — [3]Chair of Physics, Department Physics, Mechanical Engineering, and Electrical Engineering, Montanuniversität Leoben, Leoben, Austria

Twisted bilayers of transition metal dichalcogenides form moiré superlattices, resulting in electronic moiré minibands [1]. Correlated phases hosted in these structures are prone to twist disorder given by lateral fluctuations of the moiré cell size [2]. We investigated this lateral twist inhomogeneity on twisted WSe2 bilayers using comprehensive correlative lateral force microscopy and Raman spectroscopy [3].

In this work, we expand the topic by investigating different twisted systems: artificially stacked fully encapsulated WSe2 bilayers, MoSe2/WSe2 heterobilayers and CVD-grown MoS2 bilayers. Moiré phonon frequencies obtained from Raman spectroscopy maps are utilized to determine the twist angle over micrometer-sized areas in these systems. Additionally, Raman mapping facilitates fast and non-destructive identification of homogeneous, high-quality regions in encapsulated and gated structures.

[1] N. Saigal, et. al., Phys. Rev. Lett. 133, 046902 (2024) [2] S. Shabani et al. Nat. Phys. 17, 720-725 (2021) [3] N.L. Bathen et al. in preparation

HL 20.18 Tue 18:00 P1

Nonlinear interference in a CrSBr BIC metasurface — •Fabian Glatz[1], Thomas Weber[2], Till Weickhardt[1], Luca Sortino[2], Andreas Tittl[2], and Giancarlo Soavi[1] — [1]Friedrich Schiller University Jena — [2]Ludwig Maximilians University of Munich

The active electrical [1] and all-optical [2] modulation of the nonlinear optical (NLO) response of layered materials has attracted great interest for nanophotonic applications. Ferroic layered materials, such as CrSBr, offer an alternative and powerful approach for NLO tuning thanks to temperature-dependent phase transitions [3]. Here, we present a new method where NLO modulation arises from interference effects between bound states in the continuum (BIC) resonances and the bulk NLO susceptibility of a CrSBr nanophotonic device. To achieve this, we patterned exfoliated CrSBr flakes into metasurfaces that exhibit BICs and investigated their NLO response. By varying the dimensions of the metasurface, we obtain direct control over the energy, linewidth and Q-factor of the BIC resonances [4]. When the energy of the BIC resonance is close to that of the CrSBr exciton, we further observe a strong modulation in third harmonic generation (THG), characterized by both constructive and destructive interference depending on the energy of the emitted TH signal. These results allow us to retrieve the real and imaginary parts of the BIC-resonance, and they further demonstrate a new powerful approach for NLO engineering at the nanoscale. *[1] Soavi et al. Nat. Nanotech. 13, (2018). [2] Klimmer et al. Nat. Photon. 15, (2021). [3] Wang et al. Nat. Com. 14, (2023). [4] Weber et al. Nat. Mater. 22, (2023).*

HL 20.19 Tue 18:00 P1

Surface acoustic wave spectroscopy on low dimensional semiconductor materials — •Paul Hollatz, Felix Ehring, Paromita Bhattacharjee, Emeline Nysten, and Hubert Krenner — Intitute of Physics, University of Münster, Germany

For future technologies, low-dimensional quantum materials such as 2D transition metal dichalcogenides (TMDCs), 1D Nanowires, or 0D Quantum Dots (QDs) are of highest relevance.

Studying the properties of such semiconductor nanomaterials can be achieved by various methods, including the combination of surface acoustic wave (SAW) spectroscopy and photoluminescence (PL) measurements, which provides unique access to carrier dynamics.

In this approach, SAWs operating in the MHz to GHz regime enable on-chip integration due to their micro- to nanometer wavelengths.

Here, we show that interaction of a SAW with co-integrated materials via its strain and the electrical field enables contact-free sensing and manipulation of their optical properties.

When combined with time-integrated and time-resolved PL measurements, it reveals excitation pathways and charge-carrier behaviour, offering deeper insight into the fundamental processes that govern these materials and paving the way for advanced optoelectronic applications.

HL 20.20 Tue 18:00 P1

Interfacial Electronic Coupling in WS2-PyMACl van der Waals Heterostructures — •Mohammed Adel Aly[1,2], Dominik Muth[3], Bettina Wagner[4], Martin Koch[2], Johanna Heine[4], and Marina Gerhard[3] — [1]Institute of Physics and Center for Nanotechnology, University of Münster, 48149 Münster, Germany — [2]Department of Physics and Marburg Centre for Quantum Materials and Sustainable Technologies, Semiconductor Photonics Group, Philipps-Universität Marburg, 35032 Marburg, Germany — [3]Department of Physics and Marburg Centre for Quantum Materials and Sustainable Technologies, Semiconductor Spectroscopy Group, Philipps-Universität Marburg, 35032 Marburg — [4]Department of Chemistry and Marburg Centre for Quantum Materials and Sustainable Technologies, Philipps-Universität Marburg, 35032 Marburg, Germany

Interfacial coupling in mixed van der Waals systems enables tuning of the optical response of 2D semiconductors. We investigate heterostructures based on monolayer WS2 and few-layer organic crystalline pyrenemethylammonium chloride (PyMACl). Time-resolved photoluminescence shows a pronounced shortening of the PyMACl emission lifetime, indicating efficient interfacial coupling. Polarization-resolved measurements show a clear polarization anisotropy in WS2 within the heterostructure, pointing to symmetry breaking induced by the organic crystal. These observations demonstrate electronic coupling across the interface and highlight ionic organic crystals as functional substrates for tailoring excitonic behavior in 2D materials.

HL 20.21 Tue 18:00 P1

Optical Properties of a Transition-metal Dichalcogenide - ZnO Nanowire Field-effect Transistor — •Yashvi Bulsara[1], Maximilian Tomoscheit[1], Omid Ghaebi[1], Edwin Eobaldt[1], Carsten Ronning[1], and Giancarlo Soavi[1,2] — [1]Institute of Solid State Physics, University of Jena — [2]Abbe Center of Photonics, University of Jena

Transition-metal dichalcogenide (TMD) monolayers combined with zinc-oxide (ZnO) nanowires (NW) represent a promising platform for electrically tunable nanophotonic devices. ZnO NWs can be used as nanoscale lasers, supporting waveguiding, field amplification and being the gain medium at the same time. A further major step towards the success and broad applicability of NW lasers, is the possibility to actively tune their laser properties via external stimuli, such as the piezo-electric effect[1]. Recently, we have demonstrated that coupling of ZnO NWs to monolayer TMDs leads to an increase of the lasing intensity threshold[2]. Building on this approach, in this poster I will propose a device where the laser emission of a ZnO NW can be electrically tuned by coupling it to a TMD based field-effect transistor. Besides the main idea and device architecture, I will present preliminary results of device fabrication and characterization.

[1] M. Zapf, Nano Lett., 2017, 17 (11), 6637-6643
[2] E. Eobaldt, Nanoscale, 2022,14, 6822-6829.

HL 20.22 Tue 18:00 P1

Optical Properties of He^+-Irradiated CrSBr — •Alison Pfister[1], Daria Markina[1], Shengqiang Zhou[2], Regine von Klitzing[1], Kseniia Mosina[3], Zdenek Sofer[3], and Bernhard Urbaszek[1] — [1]Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 6-8, D-64289 Darmstadt, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstraße 400, 01328 Dresden, Germany — [3]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Technicka 5, 166 28 Prague 6, Czech Republic

CrSBr, a van der Waals layered magnet, exhibits rich interactions among quasiparticles, involving photons, excitons, and spins. Although antiferromagnetic in its bulk pristine form with ferromagnetic intralayer order, irradiation with He^+ ions drives CrSBr into a ferromagnetic state, enabling novel optical behaviour without applying an external magnetic field. We probe the optical response using polarization-resolved Raman spectroscopy together with absorption and photoluminescence excitation (PLE) measurements. Pronounced changes in Raman intensity and polarization alongside marked variations in absorption near the Curie temperature, and resonant features in PLE spectra were observed. Analysis of Raman tensor evolution and anomalous temperature-dependent behaviour of excitons in absorption highlights intricate coupling between lattice, electronic, and magnetic states, positioning CrSBr as an attractive platform for exploring quasiparticle physics in 2D magnets and related quantum technologies.

HL 20.23 Tue 18:00 P1

Creating Chalcogenide Aeromaterials through Atomic Layer Deposition — •Vladimir Ciobanu[1], Alejandra Ruiz-Clavijo[2], Tudor Braniste[1], Sebastian Lehmann[2], Niklas Wolff[3], Dongho Shin[2], Eduard Monaico[1], Rainer Adelung[3], Lorenz Kienle[3], Kornelius Nielsch[2], and Ion Tiginyanu[1] — [1]Technical University of Moldova, Chisinau, Moldova — [2]Leibniz Institute of Solid State and Materials Research, Dresden, Germany — [3]Kiel University, Kiel, Germany

In this work, we report the development of SnS2 and SnSe2 aeromaterials synthesized via ALD on sacrificial ZnO microtetrapod templates. The ALD process enables conformal coating of the 3D ZnO microtetrapod network with precise thickness control. The resulting SnS2 and SnSe2 shells retain the original tetrapodal morphology after selective ZnO removal in acid, forming a hollow microtubular structure with the wall thickness of about 50 nm and very high porosity. Structural characterization by XRD revealed that the as-deposited films are amorphous, while post-deposition annealing in a S or Se atmosphere at 250 °C induces crystallization of SnS2 or SnSe2. SEM demonstrated uniform coverage and preservation of the porous aeromaterial network. TEM revealed the presence of SnSx or SnSex phases with multidomain. These results highlight the

capability of ALD to fabricate crystalline, compositionally controlled, and geometrically complex chalcogenide aeromaterials with strong potential for photoactive and catalytic applications. Acknowledgements: We thank the BMFTR and NARD for the funding of ProMoMo project DEHYCONA.

HL 20.24 Tue 18:00 P1

Creating Chalcogenide Aeromaterials through Atomic Layer Deposition — •Vladimir Ciobanu[1], Alejandra Ruiz-Clavijo[2], Tudor Braniste[1], Sebastian Lehmann[2], Niklas Wolff[3], Dongho Shin[2], Eduard Monaico[1], Rainer Adelung[3], Lorenz Kienle[3], Kornelius Nielsch[2], and Ion Tiginyanu[1] — [1]Technical University of Moldova, Chisinau, Moldova — [2]Leibniz Institute of Solid State and Materials Research, Dresden, Germany — [3]Kiel University, Kiel, Germany

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HL 20.25 Tue 18:00 P1

Investigating few-layer 3R-MoS_2 on top of laser-written waveguides — •Elisabeth Grune[1], Alina Schubert[1], Karoline Becker[1], Rico Schwartz[1], Andreas Thies[2], Alexander Szameit[1], Takashi Taniguchi[3], Kenji Watanabe[3], Matthias Heinrich[1], and Tobias Korn[1] — [1]Insitute of Physics, University of Rostock, Rostock, Germany — [2]Ferdinand-Braun-Institut, Leibniz-Institut für Höchstfrequenztechnik, Berlin, Germany — [3]National Institute for Material Science, Tsukuba, Japan

The properties of 3R-MoS_2, ranging from photoluminescence to second-harmonic generation, have attracted increasing scientific interest in recent years. Our goal is to couple these optical properties evanescently to an laser-written optical waveguide running along the substrate's surface. As a first step, we manufactured a system containing an hBN-encapsulated few-layer 3R-MoS_2 flake on top of a surface waveguide and investigated its photoluminescence signal in several optical geometries at room temperature as well as under cryogenic conditions. We find that when exciting the sample from above, the waveguide itself emits an unexpectedly high background fluorescence signal compared to the 3R-MoS_2 flake. We also use the waveguide itself to excite the flake, yet find that the previous fluorescence also dominates the spectrum. We discuss strategies for mitigating improving the present structures.

HL 20.26 Tue 18:00 P1

Transport simulations of bilayer graphene/WSe_2 electron-hole double quantum dots with spin-orbit coupling — •Nikita Berg[1,2], Hubert Dulisch[1,2], Roxana Anghel[1,2], Simone Sotgiu[1,2], Christian Volk[1,2], and Christoph Stampfer[1,2] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University — [2]Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich

The electron-hole (e-h) symmetry in bilayer graphene (BLG) gives rise to robust spin-valley blockade in double quantum dots (DQDs) operated in the e-h regime. This enables the system to serve as a sensitive probe for blockade-breaking mechanisms. BLG/WSe_2 heterostructures offer electrostatic tunability of proximity-induced spin-orbit coupling (SOC) through the layer selectivity of the electron and hole wave functions in BLG. In this system, one possible spin-blockade-breaking mechanism arises from Rashba-type SOC, which can mediate spin-flip tunneling between the dots.

We present a master-equation-based steady-state transport simulation framework that accounts for coherence effects in e-h BLG double quantum dots. Using this approach, we show that Rashba-mediated spin-flip tunneling produces a distinctive dependence of the e-h blockade lifting on the angle of the applied in-plane magnetic field. This predicted angular dependence provides a clear and experimentally testable signature of induced Rashba spin-orbit coupling in BLG/WSe_2 heterostructures.

HL 20.27 Tue 18:00 P1

Active Fabri-Perot interferometer cavity stabilization for high-resolution spectroscopy of low-light single-photon emitters — •F. Stechemesser[1], F. Schaumburg[1], C. Dietrich[2], H. Mannel[1], A. Rodriguez[2], J. König[2], C. Steiner[3], P. Pesch[3], A. Lorke[1], G. Prinz[1], M. Geller[1], and A. Kurzmann[2] — [1]Faculty of Physics, University of Duisburg-Essen and CENIDE, Germany — [2]Physikalisches Institut Fachgruppe Physik, Universität zu Köln, Germany — [3]Fachgruppe Physik, RWTH Aachen, Germany

Single-photon emission from solid-state quantum emitters, such as quantum dots and defects in 2D materials, with narrow linewidths is one of the key ingredients for future applications in quantum information processing. In photoluminescence spectroscopy, the linewidths of such emitters can be determined using a grating spectrometer. However, in resonance fluorescence and at low laser excitation intensity, such spectrometers reach their limits regarding resolution and optical sensitivity. We introduce an actively stabilized, narrow-linewidth (free spectral range of 30 GHz) Fabry-Perot interferometer (FPI) that is stabilized using the light from a frequency-tunable diode laser. The quantum emitter photons are sent through the FPI, which is scanned across the emitter resonances. This approach enables measurements on a single photon detector (APD) with extended integration times. The single photon sensitivity of an APD can then be used to resolve low-intensity optical resonances of the different quantum emitters with a resolution down to 60 MHz. We show first results of single photon emission from InAs quantum dots and defects in WSe_2 monolayers.

HL 20.28 Tue 18:00 P1

Temperature-Dependent Studies of Interlayer Exciton in PbI2/WS2 Heterostructure — •Tobias Manthei[1], Bhabani Sahoo[1], Ajay Kumar[2], Abhishek Misra[2], Chirag Palekar[1], and Stephan Reitzenstein[1] — [1]Institut für Physik und Astronomie, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany — [2]Department of Physics, Indian Institute of Technology Madras, Chennai 600036, India; Center for 2D Materials Research and Innovation, IIT Madras, Chennai 600036, India

We present temperature-dependent studies of interlayer exciton in PbI2/WS2 heterostructure. The interlayer exciton formed in such heterostructures consist of electron and hole situated at gamma point in Brillouin zone of respective materials. Hence these dipolar exction are twist angle independent and momentum direct while emitting at room temperature. Taking advantage of the stable nature of the interlayer exciton we investigated radiative lifetime along with polarisation as function of the temperature. We observe relatively long radiative lifetime at low temperature compared to room temperature. Furthermore, we measured the polarisation of the interlayer exciton, which suggests that the emission is elliptically polarised, with peak splitting occurring at high temperatures. This provides insight into spin-valley dynamics. Our studies establish solid foundation for further light-matter interaction experiments related to room temperature interlayer excitons integrated in microcavity.

HL 20.29 Tue 18:00 P1

Effective Theory of Feshbach Resonances in Two-Dimensional Semiconductors — •Maximilian Wolf and Richard Schmidt — Institut für Theoretische Physik, Universität Heidelberg, 69120 Heidelberg, Germany

Feshbach resonances in two-dimensional semiconductor bilayer systems have recently been demonstrated through experiments and first-principles calculations. Motivated by these findings, we introduce an effective model that captures the essential physics of these resonances. We show how the model parameters can be fixed directly from experimental data, enabling us to derive analytical scattering phase shifts and propagators in the few-body limit. With these results, observables at finite chemical potential can be computed using standard many-body techniques. As an example, we evaluate the exciton absorption spectrum in TMD materials and compare our predictions with experimental observations.

HL 20.30 Tue 18:00 P1

Manipulation of hybrid interlayer excitons in homobilayer MoS_2 — •Ankur Arora, Mathias Federolf, Atanu Patra, Subhamoy Sahoo, Monika Emmerling, Anuj Kumar Singh, Simon Betzold, and Sven Höfling — Lehrstuhl für Technische Physik, Julius-Maximilians-Universität Würzburg, Würzburg, Germany

Van der Waals (vdW) heterostructures of transition metal dichalcogenide materials provide a versatile platform for novel excitonic phenomena. Homobilayer MoS_2 is particularly attractive, as its hybrid interlayer excitons (hIX) possess a permanent dipole moment with high oscillator strength, even at room temperature and exhibit tunability via the quantum-confined Stark effect under an external DC electric field. In this work, we investigated the optical properties of hIX in homobilayer MoS_2, which is electrically contacted with few-layer graphene (FLG) and encapsulated in hexagonal boron nitride (hBN). The hBN encapsulation improves the optical response by narrowing the excitonic linewidths, revealing the effect of the dielectric environment. By applying a vertical electric field, we show the Stark splitting of the peaks of the hIX. The vdW heterostructure is transferred onto a distributed Bragg reflector (DBR) with pre-patterned contacts forming a half-cavity design. This architecture serves as a critical first step toward the fabrication of a full microcavity, enabling the exploration of strong light-matter coupling. Our results pave the way for electrically tuning these dipolar hIX polaritons inside a microcavity for fundamental studies on exciton condensates and exciton polariton-induced superconductivity.

HL 20.31 Tue 18:00 P1

SH modulation in a TMD-graphene heterostructure — •Raja Hoffmann[1], Lisa Suchomel[1], Omid Ghaebi[1], Till Weickhardt[1], and Giancarlo Soavi[1,2] — [1]Friedrich-Schiller-Universität Jena, Germany — [2]Abbe Center of Photonics, Jena, Germany

One of the most fascinating properties of layered materials is arguably the possibility to combine them in heterostructures with engineered electronic and optical properties. In the field of nonlinear optics, a clear example is the emergence of second harmonic generation (SHG) in layered heterostructures realized by combining centrosymmetric materials. In such samples, interface broken space inversion symmetry can be engineered in different ways depending on the choice of materials and twist angle. An interesting example, which has been investigated recently in Ref.[1], are heterostructures composed of bilayer TMDs and monolayer graphene. As charges move from the TMD into the graphene, an imbalance between the bottom and top layers in the TMD bilayer leads to breaking of the inversion symmetry.

Building on these previous seminal results, we further investigate a bilayer TMD-monolayer graphene gated device, focusing in particular on both gate and all-optical tuneability of its engineered SHG. With this, we aim to add another prototype sample to the growing list of nonlinear nanophotonic devices based on layered materials and displaying ultrafast tunable optical properties [2,3].

[1] Zhang et al. Science Advances 9, 4571 (2023).
[2] Ghaebi et al. Advanced Science 11, 2401840 (2018).
[3] Klimmer et al. Nature Photonics 15, 837-842 (2021).

HL 20.32 Tue 18:00 P1

Electrical and optical studies of twisted graphene bilayers — •Anselm Watschke, Monica Kolek Martinez de Azagra, and Thomas Weitz — I. Physikalisches Institut, University of Goettingen

As a van der Waals heterostructure, twisted bilayer graphene shows rich angle-dependent electronic behavior, including magic-angle superconductivity [1] and near-30° interlayer decoupling [2], motivating efforts to tune its electrical properties through multiple degrees of freedom. Furthermore, in situ quantum twisting microscope measurements revealed the angle dependent tunneling current for small regions of twisted bilayer graphene [3].

In this work, we fabricated devices incorporating a locally twisted bilayer graphene region, enabling simultaneous investigation of the off-angle regime and adjacent monolayer domains. Encapsulation in hexagonal boron nitride was used to maintain the intrinsic behavior of graphene, and vibrational and electronic properties were subsequently examined through Raman spectroscopy and gate-tunable transport measurements.

[1] Cao, Y., Fatemi, V., Fang, S. et al. Nature 556, 43*50 (2018). https://doi.org/10.1038/nature26160
[2] H. Schmidt, T. Lüdtke, P. Barthold, E. McCann, V. I. Fal'ko, R. J. Haug; Appl. Phys. Lett. 27 October 2008; 93 (17): 172108. https://doi.org/10.1063/1.3012369
[3] Inbar, A., Birkbeck, J., Xiao, J. et al. Nature 614, 682*687 (2023). https://doi.org/10.1038/s41586-022-05685-y

HL 20.33 Tue 18:00 P1

Laser induced oxidation of thin layered MoS2 — •Aniketa Anampally, Gerhard Berth, Klaus Jöns, and Henry Hübschmann — Paderborn University, Germany

Transition metal dichalcogenides (TMDs) have gained great attention within the growing field of 2D materials. Due to their inherent semiconductor properties, materials like molybdenum disulfide (MoS2) have been implemented in many components of photonic and optoelectronic devices [1,2]. Precise structural modification has been proven to exhibit significant benefits to build tailored devices on the nanoscale [3]. In this work nonlinear microscopy is utilized for in-situ probing and laser oxidation of mechanically exfoliated 2H-MoS2. Precise locally resolved oxidation has been performed by second harmonic microscopy. The arising layer number dependency of this treatment is investigated further supported by polarization resolved analysis.

HL 20.34 Tue 18:00 P1

Optimization of quantum dot in nanowire for efficient emission in telecom spectral range — •Tomasz Gzyl[1], Giada Bucci[2], Valentina Zannier[2], Paweł Mrowiński[1], Anna Musiał[1], Elisa García-Tabarés[3], Ileana Florea[4], Beatriz Galiana[3], Lucia Sorba[2], Wojciech Rudno-Rudziński[1], and Grzegorz Sek[1] — [1]Wrocław University of Science and Technology, 50-370 Wrocław, Poland — [2]NEST Istituto Nanoscienze CNR and Scuola Normale Superiore, 56127 Pisa, Italy — [3]Universidad Carlos III de Madrid, 28903 Getafe, Spain — [4]CNRS-CHREA, 06560 Valbonne, France

One of the promising platforms for realization of a single photon source emitting in telecom wavelengths is an InAs(P) quantum dot (QD) embedded in a nanowire (NW), designed to enhance extraction efficiency and directionality of QD emission. Chemical Beam Epitaxy technique is employed to grow the QD within novel zinc-blende InP NW or wurzite InAsP NW. Here, we present numerical simulations of the QD-NW system, using finite-difference time-domain method to find optimal NW geometry for maximal extraction efficiency, within numerical aperture of 0.4 used in experiment and taking into account parameters space limited by the growth technology. To verify the calculations and further guide the growth of optimized structures, we performed microphotoluminescence measurements as a function of excitation power on samples with different composition and NW shell diameter. The structural quality of the samples was confirmed using Scanning Transmission Electron Microscopy with Energy Dispersive X-ray Spectroscopy.

HL 20.35 Tue 18:00 P1

Electrostatic Inter-Layer Coupling Between Self-Assembled Quantum Dot Layers — •Jan Lange[1], Lukas Berg[1], Laurin Schnorr[1], Charlotte Rothfuchs-Engels[2], Nikolai Bart[2], Severin Krüger[2], Sven Scholz[2], Arne Ludwig[2], Andreas Wieck[2], and Thomas Heinzel[1] — [1]Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität, Bochum, Germany

In this study, transient capacitance spectroscopy is used to examine the coupling between self-assembled quantum dots (SAQDs) - made of InAs in a GaAs heterostructure - in spatially separated layers. A rate equation model was developed, incorporating self-consistent band bending calculations, to describe the impact of the inter-layer coupling on the charge transfer processes. Here, also effects caused by the wetting layer are described and included into the model. The findings indicate that the coupling arises from the electrostatic field generated by the charged quantum dots in the adjacent layer as well as charge in a wetting layer, providing a quantitative explanation for the altered electron capture and emission dynamics.

HL 20.36 Tue 18:00 P1

Illumination Response of Electron Capture and Emission Dynamics in Self-Assembled Quantum Dots — •Till Draxler[1], Jan Lange[1], Julia Avdeev[1], Sven Scholz[2], Arne Ludwig[2], Andreas Wieck[2], and Thomas Heinzel[1] — [1]Condensed Matter Physics Laboratory, Heinrich-Heine University Düsseldorf — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum

InAs Self Assembled Quantum Dots (SAQDs) are nanoscale semiconductor structures that confine charge carriers in all three spatial dimensions, leading to discrete, atom-like energy levels. Using Deep Level Transient Spectroscopy (DLTS) the influence of infrared irradiation with photon energies in respect to the bandgap energies of GaAs and InAs on the electron transfer dynamics is studied. To maintain a proper illumination of the SAQDs, semi-transparent NiCr Schottky gates are manufactured instead of classical Au gate.

HL 20.37 Tue 18:00 P1

Optimized quantum dot emitters for telecom applications: from growth to diode integration — •Tobias Bruggesser, Ponraj Vijayan, Patrick Pietrantuono, Sergej Vollmer, Philipp Noack, Justus A. Unfried, Ulrich Pfister, Michelle Weiss, Simone L. Portalupi, Michael Jetter und Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen, University of Stuttgart, Germany

Quantum communication and quantum computing applications require a reliable high-purity single photon source. Stranski-Krastanov grown indium arsenide (InAs) quantum dots (QDs) are among the most widely studied candidates, as they possess high purity, brightness, and indistinguishability. When embedded in a GaAs semiconductor matrix, these QDs emit in the near-infrared region (≈ 900 nm), and this can be shifted to the technologically important telecom C-band (1530-1565 nm) by introducing an InGaAs metamorphic buffer (MMB) beneath the QDs to engineer the strain. Our group has previously developed a thin InGaAs MMB based on a non-linear grading of the indium content with a so-called jump-convex-inverse (jci) design. This design is compatible with optical device fabrication, as it can be incorporated into a high-quality 1λ-cavity structure. In this work, we present our approach towards integrating these telecom C-band emitting InAs QDs into a p-i-n diode structure. Our goal is to control the charge carrier environment of the QDs, improve their optical properties, and achieve fine-tuning of the emission energy via the quantum-confined Stark effect.

HL 20.38 Tue 18:00 P1

Design and optimization of photonic nanostructures for embedding GaAs quantum dots emitting at 780 nm — •Mrunmayee Deodhar[1], Ponraj Vijayan[1], Katharina Dahler[1], Ulrich Pfister[1], Michelle Weiss[1], Melina Peter[2], Ailton José Garcia Jr.[2], Thomas Oberleitner[2], Michael Jetter[1], Simone Luca Portalupi[1], Armando Rastelli[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen (IHFG), Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, Germany — [2]Institute of Semiconductor and Solid State Physics, Johannes Kepler University Linz, 4040 Linz, Austria

Droplet-etched GaAs quantum dots (QDs) are a promising source for single and highly indistinguishable photons. Their optical properties like a narrow wavelength distribution, short decay times, linewidths close to the Fourier limit, and the resulting highly indistinguishable photons make them highly appealing for

several quantum technologies. We demonstrate the integration of these QDs into photonic nanostructures such as single-mode waveguides, multimode interference splitters, and Bragg grating waveguides. We also present simulations and describe the fabrication process used to realize these photonic nanostructures.

HL 20.39 Tue 18:00 P1

Auger-recombination in no-wetting layer InAs self-assembled quantum dots — •M. Rasulyar[1], H. Mannel[1], F. Rimek[1], A. Ludwig[2], A. Lorke[1], and M. Geller[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, 47057 Duisburg, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany

The Auger-Meitner effect is a non-radiative recombination pathway in which the energy of an electron-hole pair is transferred to a third carrier. In colloidal quantum dots, this mechanism is known to suppress radiative emission, while in self-assembled InAs/GaAs quantum dots, both non-radiative Auger processes [1] and radiative Auger-like channels [2] have been reported. However, as Auger recombination is a dephasing effect in quantum dot-based single-photon devices, we study the influence of the confining potential on the non-radiative Auger recombination rate.

We investigate the Auger-Meitner dynamics in a no-wetting layer quantum dot incorporated in a gate-tunable p-i-n diode. Under resonant excitation of the trion transition, we observe a pronounced quenching of the resonance-fluorescence signal. The intensity reduction is quantitatively explained by the competition between the electron emission rate and the electron tunneling-in rate. The Auger recombination rate is in the order of $1\,\mu s^{-1}$ and in accordance with previous measurements with a rate of $\gamma_a = 2.3\,\mu s^{-1}$ [1]. [1]A. Kurzmann et al., Nano Lett. 16, 3367 (2016). [2]M. Löbl et al., Nat. Nanotechnol. 15, 558-562 (2020). [3]M. Löbl et al., Commun. Phys. 2, 93 (2019).

HL 20.40 Tue 18:00 P1

Single-electron charging events on double quantum dots in InSb nanowires — •Kanji Furuta[1], Marcus Liebmann[1], Fenja Thomsen[1], Sasa Gazibegovic[2], Diana Car[2], Erik Bakkers[2], and Markus Morgenstern[1] — [1]II. Phys. Inst. B, RWTH Aachen Univ., Germany — [2]Dept. of Appl. Phys., Eindhoven Univ., The Netherlands

As a step to develop a single-electron counting tip for a scanning tunneling microscope, we investigate the charge states of a double quantum dot (DQD) formed in an InSb nanowire by monitoring the current through a floating-gate-coupled sensor quantum dot (QD). The DQD and sensor QD are defined electrostatically by bottom finger gates below hexagonal boron nitride (h-BN) used as the gate dielectric. Time-resolved measurements of the sensor QD current reveal single-electron charging events in the DQD. The asymmetric capacitive coupling of the floating gate allows us to identify which dot acquires an electron. The time traces of the double quantum dot movement of individual electrons are analyzed using full counting statistics, from which the Fano factor and factorial cumulants [1] are extracted.

[1] P. Stegmann *et al.*, Phys. Rev. B **92**, 155413 (2015).

HL 20.41 Tue 18:00 P1

Towards a Quantitative Framework for Capacitance-Voltage Spectroscopy in Quantum Dot Ensembles — •Phil Julien Badura[1], Nico Frédéric Brosda[1], Ismail Bölükbaşı[1], Ibrahim Engin[1], Patrick Lindner[1], Sascha René Valentin[1], Andreas Dirk Wieck[1], Björn Sothmann[2], and Arne Ludwig[1] — [1]Fakultät für Physik und Astronomie, Experimentalphysik VI, Ruhr-Universität Bochum, Bochum, Germany — [2]Fakultät für Physik and CENIDE, Universität Duisburg-Essen, Lotharstraße 1, D-47048 Duisburg, Germany

This study investigates an inhomogeneous ensemble of quantum dots coupled to a charge reservoir using capacitance-voltage spectroscopy. Experimental measurements reveal shifts in capacitance peak positions influenced by AC frequency and temperature, with frequency-dependent shifts remaining unexplained by existing models. To address this, we develop a master-equation-based theoretical model incorporating energy-dependent tunneling effects, which successfully reproduces the experimental data. Our findings emphasize the role of energy-dependent tunneling in distinct regimes: at low temperatures, energy-level dispersion dominates, while at high temperatures and frequencies, shifts arise from optimized sequences of in- and out-tunneling events.

HL 20.42 Tue 18:00 P1

Towards the integration of telecom C-band QDs into photonic integrated circuits — •Michelle Weiss, Ulrich Pfister, Ponraj Vijayan, Simon Oberle, Justus Unfried, Philipp Noack, Tobias Bruggesser, Sergej Vollmer, Raphael Joos, Michael Jetter, Simone L. Portalupi, and Peter Michler — Institut für Halbleiteroptik und Funktionelle Grenzflächen (IHFG), University of Stuttgart, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, Germany

Photonic integrated circuits (PICs) pave the way to the realization of several quantum technologies on a small footprint, which makes them highly desirable for applications in quantum communication, computing, simulation and sensing. Silicon and silicon nitride are leading materials for PICs due to the high quality optical components and low optical propagation losses. Due to the indirect bandgap of silicon most of the single-photon sources (SPSs) are based on probabilistic implementations. However, the probabilistic generation of the photons can limit the scalability and requires the use of high laser powers, which is a potential drawback regarding the integration of on-chip detectors. In this regard, In(Ga)As quantum dots (QDs) are promising candidates as on-demand SPSs with high single-photon purity. For their integration on low-loss PICs, several approaches already exist, like monolithic integration techniques and hybrid approaches used for interfacing with silicon-based platforms. We present the progress on various PIC integration techniques for InGaAs QDs grown on a metamorphic buffer layer and so emitting in the telecom C-band.

HL 20.43 Tue 18:00 P1

Aharonov-Bohm interferometry with interacting quantum dots — •Oliver Oing, Alexander Hahn, Jürgen König, and Fred Hucht — Theoretische Physik, Universität Duisburg-Essen

We describe an Aharonov-Bohm interferometer consisting of two leads and two tunnel-coupled quantum dots with on-site Coulomb interaction using first order perturbation theory in the tunnelling strength. In earlier work, a diagrammatic approach was chosen. The complexity of the diagrams for arbitrary parameters limited the calculations to symmetric systems in energies and couplings. By developing a systematic routine in *Mathematica* to generate all possible diagrams, we can explore a wider range of system configurations. Eleven system parameters can be arbitrarily tuned, namely the finite Coulomb interactions, the quantum dot level energies as well as the tunneling strengths, magnetic flux, bias voltage and temperature, enabling us to describe both symmetric and asymmetric systems. A finite bias voltage makes it possible to explore the non-linear response regime. The routine calculates density matrix elements and uses these to obtain the occupations of the quantum dots, the current and the conductance through the system. With this, we compare to analytic results and numerically exact results obtained with the TraSPI method [1].

[1] S. Mundinar, A. Hahn, J. König, A. Hucht, Phys. Rev. B **106**, 165427 (2022)

HL 20.44 Tue 18:00 P1

Characterization of Quantum Dots after Rapid Thermal Annealing in Photonic Layer Structures — •Jasper Ullrich, Severin Krüger, Elias Kersting, and Arne Ludwig — Universitätsstraße 150, Bochum 44801

Rapid thermal annealing (RTA) is an effective post-growth technique for engineering the structural and optoelectronic properties of InGaAs quantum dots (QDs). Short, high-temperature pulses induce controlled interdiffusion that blueshifts the emission wavelength, reduces inhomogeneous broadening, and modifies carrier confinement. In this work, we investigate how specific annealing conditions*temperature, duration, and ambient environment*govern these changes and, in particular, how they influence the oscillator strength of confined excitonic transitions. We expect to show that optimized RTA parameters significantly enhance radiative coupling of QDs, leading to increased oscillator strength and faster emission dynamics. These results would provide a systematic framework for tailoring the optical performance of InGaAs QDs for quantum-light sources, high-speed emitters, and infrared photonic devices.

HL 20.45 Tue 18:00 P1

Ohmic contact for charge tuning devices — •Krupali Dobariya[1], Tom Fandrich[1], Yiteng Zhang[1], Arijit Chakraborty[1], Sulabh Shrestha[1], Doaa Abdelbarey[1], Eddy P. Rugeramigabo[1], Michael Zopf[1,2], and Fei Ding[1,2] — [1]Leibniz Universität Hannover Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover, Germany. — [2]Leibniz Universität Hannover Laboratorium für Nano- und Quantenengineering, Schneiderberg 39, 30167 Hannover, Germany.

Semiconductor quantum dots have shown unique properties as deterministic single photon and entangled photon pair sources. Their outstanding optical properties have the potential for use in quantum applications like quantum communication, quantum key distribution and quantum computing. Nevertheless, due to the stochastic nature of the self-assembly growth process, quantum dots typically emit photons with a broad wavelength distribution across the entire chip, posing challenges for applications requiring specific wavelengths. To address this issue, various tuning techniques have been developed. Electrical tuning, in particular, has emerged as an effective method for adjusting the wavelength and mitigating charge noise in semiconductor quantum dots. Here we study the impact of contact fabrication on the emission properties of GaAs quantum dots. We aim to optimize the process of forming ohmic contacts to n- and p-doped GaAs, placing special emphasis on the selection of materials and the reduction of contact resistance. The quality and performance of the electrical contacts are evaluated through the photoluminescence characterization.

HL 20.46 Tue 18:00 P1

Mixed-dimensional Silicon Junctionless Nanowire Transistors with Hexagonal Boron Nitride Gate Dielectrics — •Ahmed Elwakeel[1,2], Sayantan Ghosh[1,2], Alessandro Puddu[1,2], Madhuri Chennur[1,2], Slawomir Prucnal[1], Yordan Georgiev[1], Ahmad Echresh[1], and Artur Erbe[1,2] — [1]1Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Technische Universität Dresden, 01069 Dresden, Germany

The investigation of two-dimensional hexagonal boron nitride (hBN) as a gate dielectric arises from the intrinsic limitations of conventional oxide layers in aggressively scaled devices. Owing to its atomically thin structure, excellent insulating characteristics, and inherently clean surface free of dangling bonds, hBN enables improved electrostatic control and effective channel passivation. In Junctionless Nanowire Transistors (JNTs), which remain strong contenders for extending Moore's Law, the use of hBN offers the potential to suppress interface trap states and enhance carrier transport. In this work, a top-down fabrication approach was employed to define the n-type doped silicon nanowires (C = 1E19 cm-3). Two distinct JNT devices were prepared: one with native oxide and another incorporating a thermally grown oxide. Subsequently, exfoliated hBN flakes were dry-transferred onto both samples as a gate dielectric. The hBN-integrated JNTs with thermally grown oxide exhibited pronounced improvements in subthreshold swing, on-state current, and the ION/IOFF ratio.

HL 20.47 Tue 18:00 P1

Importance of Aluminium Quality for High-Quality Quantum Emitter — •Severin Krüger[1,2], Elias Kersting[1], Phil Badura[1], and Arne Ludwig[1] — [1]Ruhr-Universität Bochum, Bochum, Germany — [2]Sparrow Quantum Aps, Copenhagen, Denmark

InAs quantum dots are regarded as excellent candidates for single photon emitters due to their high photon rates, good single photon properties, and compatibility with scalable and integratable photonic platforms.

Despite remarkable progress for quantum dots emitting at 950 nm, achieving the same results for quantum dots emitting in the important optical fibre transparency window around 1.3 *m has remained a major challenge.

Here we present a routine we used to monitor and improve the quality of aluminium containing layers grown in our MBE. We find that high quality Al in MBE significantly improves the interface quality and smoothness of Al(Ga)As layers by reducting the surface roughness.

These improvements enabled the growth of pristine distributed Bragg reflectors beneath a defect free, charge tunable quantum dot device, emitting near transform-limited single photons in the O-band at 1.3 um.

HL 20.48 Tue 18:00 P1

RoHS-Compliant Nanocrystal LEDs for Flexible Near-Infrared Biomedical Emitters — •Simon Letzer[1], Andrey Iodchik[2], Rabiul Islam[1], Vladimir Lesnyak[2], and Caroline Murawski[1] — [1]Institute of Solid State Electronics, TU Dresden, Germany — [2]Physical Chemistry, TU Dresden, Germany

The near-infrared (NIR) biological window enables deep-tissue access for non-invasive imaging and health monitoring. Wearable emitters for this range require flexible and efficient materials, yet organic LEDs lose performance above 850 nm. Colloidal nanocrystals (NCs) offer a promising alternative for NIR emission, although most efficient systems contain Hg, Cd, or Pb, restricting their use in biomedical settings. We therefore investigate RoHS-compliant NCs for solution-processed NIR emitters. As a baseline, we employed CdHgSe/CdZnS core/shell NCs, which have already demonstrated strong performance in LEDs and provide a reliable platform for optimizing device processing [1]. Film quality is strongly influenced by concentration, solvent, dispense time, spin profile, and baking conditions. High-boiling-point solvents produced uniform macroscopic films, while low-temperature baking and high spin speeds improved nanoscale smoothness. Building on these conditions, we fabricated our first RoHS-compliant devices based on CuInS2/ZnS NCs. Processing parameters were refined for this material, and different transport layers and device architectures were evaluated. These results demonstrate a viable path toward cadmium-free NIR emitters for wearable biomedical sensors.

[1] Adv. Funct. Mater. 2024, 34, 2310067.

HL 20.49 Tue 18:00 P1

Stark Tuning of CsPbBr3 Quantum Dots — •Christopher Borchers[1], Johann Dzeik[1], Maximilian Heller[1], Frederik Benthin[1], Eddy Rugeramigabo[1], Chenglian Zhu[2,3], Ihor Cherniukh[2,3], Gabriele Rainò[2,3], Maksym Kovalenko[2,3], Michael Zopf[1,4], and Fei Ding[1,4] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover — [2]Institute of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zürich, CH-8093 Zürich, Switzerland — [3]Laboratory for Thin Films and Photovoltaics, Empa - Swiss Federal Laboratories for Materials Science and Technology, CH-8600 Dübendorf — [4]Laboratory of Nano and Quantum Engineering, Leibniz University Hannover, Schneiderberg 39, D-30167 Hannover, Germany

CsPbBr3 perovskite quantum dots are bright, solution-processable nanocrystal emitters with size-tunable color and high oscillator strength. Furthermore, they can be fabricated and processed in a cheap and facile way. We investigate electric-field tuning of single dots through the quantum-confined Stark effect to minimize exciton fine-structure splitting and tune separate emitters into resonance with each other. This opens up possibilities of creating entangled photon pairs of super- and subradiance with perovskite quantum dot based photonic devices.

HL 20.50 Tue 18:00 P1

Low temperature dry etching of InAlAs/InP nanostructures for telecom band single photon sources — •Ankita Choudhary[1], Chenxi Ma[1], Yiteng Zhang[1], Eddy Patrik Rugeramigabo[1], Michael Zopf[1,2], and Fei Ding[1,2] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover, Germany — [2]Laboratorium für Nano- und Quantenengineering, Leibniz Universität Hannover, Schneiderberg 39, 30167 Hannover, Germany

Epitaxial InP-based quantum dots are excellent candidates for telecom band single photon sources for long-distance quantum communication. Enhancing photon extraction requires integration into photonic nanostructures through high resolution lithography and dry etching. Conventional chlorine-based ICP-RIE etching of InP is challenging due to competing thermal demands that lead to uncontrollable volatilisation of chlorine byproducts at high temperatures, while low-temperature cyclic methods result in defect-rich interfacial layers.Here we demonstrate low temperature chlorine based etching that circumvents byproduct volatilisation and stoichiometric imbalance and eliminates defect layer formation without intermediate chemical treatments. we demonstrate the fabrication of a submicron truncated cone with smooth sidewalls, enhancing spontaneous emission directionality. The fabricated nanostructure shows 3-4 times improved extraction efficiencies compared to as-grown samples, with an NA of 0.7 detection optics. This process provides a robust pathway for fabricating high-quality photonic nanostructures for quantum telecommunications.

HL 20.51 Tue 18:00 P1

Lateral Electric Field Tuning of Quantum Dots — •Johann Dzeik[1], Christopher Borchers[1], Chenxi Ma[1], Ankita Choudhary[1], Xian Zheng[1], Yiteng Zhang[1], Tom Fandrich[1], Arijit Chakraborty[1], Michael Zopf[1,2], and Fei Ding[1,2] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover, Germany — [2]Laboratorium für Nano- und Quantenengineering, Leibniz Universität Hannover, Schneiderberg 39, 30167, Hannover, Germany

Quantum dots are among the most promising material systems for single photon sources in quantum communication and computation. However, they exhibit a stochastic distribution of emission wavelengths and fine-structure splitting, necessitating post-growth tuning that must be compatible with their fabrication and photonic environment. In this study, we use planar electrodes in parallel and quadrupolar configurations at varying distances to investigate the influence of electric fields on the emission wavelength and fine-structure splitting of GaAs/AlGaAs quantum dots.

HL 20.52 Tue 18:00 P1

SUPER Scheme in Telecom-Wavelength Quantum Dots — •Zenghui Jiang — Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover

Co-authors: Vikas Remesh, Frederik Benthin,Thomas Bracht, Michael Jetter, Simone Portalupi, Doris Reiter, Peter Michler, Michael Zopf, Fei Ding

Abstract:

To obtain the best photon properties from quantum dots (QDs), direct driving between the S-shell and the ground state i.e., resonant excitation is typically required. However, laser filtering under resonant excitation is extremely challenging because the QD emission and the excitation laser lie at essentially the same wavelength. The recently proposed and experimentally demonstrated SUPER scheme addresses this challenge by using two relatively detuned laser pulses to directly drive the two-level system. Since the excitation and emission wavelengths are well separated, the scattered excitation laser can be spectrally filtered much more easily. In our work, we implement a pulse shaper based on a spatial light modulator to generate two well-defined laser pulses from a single broadband pulse for the SUPER scheme. In addition, we investigate SUPER excitation using two narrow-linewidth continuous-wave lasers as a comparison, enabling a clearer understanding of the excitation dynamics and the differences relative to pulsed operation.

HL 20.53 Tue 18:00 P1

Andreev Spin Qubits in Hole-Gas Based Nanowires with Mixed Superconducting Pairing — •Markus Plautz — Norwegian University of Science and Technology, Norway

Ge-based lower-dimensional hole gases proximitized by superconductors represent a promising platform for future quantum technologies, largely related to the complicated p-wave nature of the orbital wavefunctions of the valence band. While standard models often treat the induced superconductivity as purely s-wave, recent microscopic theories indicate that the proximity effect in these sys-

tems is far more complex. They reveal that the strong spin-orbit interaction can induce non-trivial mixed pairing correlations, featuring coexisting s- and p-wave terms.

We calculate the Andreev reflection phases and determine the Andreev bound state (ABS) energy spectrum in the presence of Zeeman and spin-orbit fields. In particular, we show how these odd-parity correlations influence the spin splitting, leading to distinct changes in the qubit energy levels. Furthermore, we discuss the coherent control of the qubit subspace by considering a time-dependent perturbation of the spin-orbit coupling. By deriving the exact transition matrix elements, we construct an effective Hamiltonian for the ASQ and investigate how this mechanism can be utilized to coherently drive the qubit.

HL 20.54 Tue 18:00 P1

Nonequilibrium transport in designed random obstacle arrays — •Frederik Bartels[1], Johannes Strobel[1], Beate Horn-Cosfeld[1], Mihai Cerchez[1], Klaus Pierz[2], Hans Werner Schumacher[2], Dominique Mailly[3], and Thomas Heinzel[1] — [1]Condensed Matter Physics Laboratory, Heinrich Heine University, Düsseldorf, Germany — [2]Physikalisch-Technische Bundesanstalt (PTB), Bundesallee 100, 38116 Braunschweig, Germany — [3]CNRS, Université Paris-Saclay, C2N Marcoussis, 91460 Marcoussis, France

Nonequilibrium transport phenomena in two-dimensional electron systems include Hall field induced resistance oscillations (HIROs), zero resistance states (ZRS), phase inversion of SdH oscillations, and modifications of the giant negative magnetoresistance (GNMR). In our recent work [1], we studied HIROs in two-dimensional electron gases dominated by scattering at artificially introduced, randomly distributed circular obstacles. For sufficiently high obstacle densities, these scatterers dominate the HIROs. The HIRO period increases with obstacle density, indicating a localization of the Hall field around the obstacles and providing an alternative explanation of the scaling factor γ in terms of spatially varying Hall fields. Here, we extend these studies to cross-shaped obstacle geometries designed to enhance backscattering - the central mechanism in the theory of HIROs [2]. The findings may help to establish a more unified understanding of nonlinear resistance oscillations in two-dimensional systems with artificial scatterers. [1] Bartels *et al.* Phys. Rev. B **111**, 165301 (2025), [2] Yang *et al.* Phys. Rev. Lett. **89**, 076801 (2002)

HL 20.55 Tue 18:00 P1

Tenfold Conductance Enhancement in Graphene Nanoscrolls via Interlayer Hopping — •Jia-Cheng Li[1], Yu-An Cheng[2], Ying-Je Lee[2], Xuan-Fu Huang[2], Yu-Jie Zhong[2], Carmine Ortix[3], and Ching-Hao Chang[2] — [1]Program on Key Materials, Academy of Innovative Semiconductor and Sustainable Manufacturing, National Cheng Kung University, Tainan 70101, Taiwan — [2]Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan — [3]Institute for Theoretical Solid State Physics, IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany

Rolling a graphene nanoribbon into a nanoscroll, a radial superlattice, offers a simple yet powerful way to control electronic transport at the nanoscale. In this work, we show that a one-turn nanoscroll exhibits a dramatic enhancement of quantum conductance compared to a flat ribbon, reaching nearly an order of magnitude in our tight-binding transport calculations. This effect does not rely on curvature-induced gauge fields or external perturbations. Instead, it arises purely from interlayer hopping at the overlapping edges of the scroll, which hybridizes the zigzag edge states and reconstructs the low-energy band structure. The resulting collapse of the flat bands reduces the density of states and shifts the Fermi level upward at fixed carrier density, activating multiple propagating modes. As the number of turns increases, these effects gradually weaken. Our findings identify nanoscrolls as a tunable geometry-driven platform for engineering transport in low-dimensional carbon systems.

HL 20.56 Tue 18:00 P1

Top-Down Fabrication and characterization of Al-Si-Al Nanowire Schottky barrier field-effect transistors — •Banafsheh Aghvami[1], Alessandro Puddu[1,2], Ahmed Elwakeel[1,2], Sayantan Ghosh[1], Ahmad Echresh[1], and Artur Erbe[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstrasse 400, Dresden, 01328, Germany — [2]Technische Universität Dresden, Dresden, 01069, Germany

In Schottky barrier field-effect transistors (SBFETs), the channel length plays a crucial role in device performance. Shorter channels lead to lower channel resistance, stronger electrostatic gate control, reduced threshold voltage, and improved ON/OFF current ratios. However, to achieve sub-100 nm channel lengths using conventional top-down patterning approaches is extremely challenging due to resolution limits, line-edge roughness, and probable alignment errors. In contrast, the Al-Si-Al solid-state exchange process via rapid thermal annealing (RTA) enables the formation of well-defined and self-aligned short silicon channels. In this study, electron beam lithography (EBL) is used to define nanowire structures into HSQ resist. Then, the patterned structures will be transfered into the silicon layer by Inductively Coupled Plasma-Reactive Ion Etching (ICP-RIE). The Aluminium metal contacts will be formed by sputtering deposition. Scanning Electron Microscopy (SEM) will be employed to analyse the Al-Si-Al heterostructure. In addition, the performance of fabricated SBFETs will be evaluated by electrical characterisation using back-gated configuration.

HL 20.57 Tue 18:00 P1

Organic LEDs for optogenetic cochlear implants — •Nirbhika Nandakumar and Caroline Murawski — Dresden University of Technology, Dresden, Germany

Recent studies have highlighted the potential of optogenetic cochlear implants (oCIs) to surpass the spatial resolution limitations of conventional electrical stimulation by utilizing confined light to activate genetically modified auditory neurons [1]. Existing oCI prototypes predominantly use micro-LEDs, which can generate high optical power but are constrained by thermal load, rigidity, and limited scalability toward dense stimulation arrays [2]. In this work, we investigate organic light-emitting diodes (OLEDs) as alternative light sources for next-generation oCIs. Bottom-emitting OLEDs were fabricated and experimentally characterized with respect to spectral emission, efficiency, and achievable optical power density. The micro-cavity was designed by complementary optical simulations to generate a forward-directed, spatially confined illumination capable of efficiently reaching the intended spiral ganglion neurons. An implant design is proposed based on the geometry of the cochlea, required pixel size, and spacing. The combined experimental and simulation results establish OLEDs as promising alternatives to micro-LEDs for integration into future oCI architectures.

[1] A. Huet et al., Annu. Rev. Neurosci. 47, 103 (2024).
[2] L. Jablonski et al., J. Neural Eng. 22, 046034 (2025).

HL 20.58 Tue 18:00 P1

Creation and characterization of color centers in hexagonal Boron Nitride — •Dennis Heinz Bruno Mors[1,2], Iris Niehues[1], and Daniel Wigger[3] — [1]Institute of Physics, University of Münster, 48149 Münster, Germany — [2]Faculty of Science and Technology, University of Twente, 7522 NB Enschede, Netherlands — [3]Department of Physics, University of Münster, 48149 Münster, Germany

Color centers (CCs) in hexagonal boron nitride (hBN) are promising candidates for stable and bright quantum light sources, despite their unknown origin due to their single-photon emission properties even at room temperature. To explore their potential, we investigate various material sources for their ability to host CCs. We employ mechanical exfoliation to reduce the thickness of bulk crystals to a few layers, resulting in thin hBN flakes that are then transferred onto Si or SiO_2 samples. To enhance the yield of CCs, we thermally anneal the hBN. We then examine our samples using confocal photoluminescence to identify the CCs in the host crystal. Additionally, we utilize a scattering-type scanning near-field optical microscope (sSNOM) to study the photoluminescence (PL) emission characteristics of these quantum emitters. By using a sharp metallic tip, we concentrate the illuminating light field into a nanofocus, enabling us to achieve nanoscale resolution beyond the diffraction limit.[1]

[1] I. Niehues et al., Nanophotonics 2025, 14(3), 335-342.

HL 20.59 Tue 18:00 P1

Spectral wandering of single-photon emitters in the van der Waals material hBN — •Akhilesh Dubey, Robert Schmidt, Johannes Kern, Steffen Michaelis de Vasconcellos, and Rudolf Bratschitsch — Institute of Physics and Center for Nanotechnology, University of Münster, 48149 Münster, Germany

Single-photon emitters in hexagonal boron nitride (hBN) exhibit favorable photophysical optical properties at both room and cryogenic temperatures. However, their performance is limited by various line broadening mechanisms. Here, we present a low-temperature study of the photoluminescence of hBN emitters, investigating linewidth reduction and spectral diffusion at cryogenic temperatures. We believe that the spectral wandering is due to migrating charges in the vicinity of the nanoscale emitter, which could be mitigated by applying an external electric field. Our results essential for developing nanoscale quantum photonic devices based on robust hBN emitters.

HL 20.60 Tue 18:00 P1

2D Lattices of Rb Quantum Emitters on Isolating Substrates — •David Bergmann, Katharina Lorena Franzke, Wolf Gero Schmidt, and Uwe Gerstmann — Paderborn University, Paderborn, Germany

Entanglement plays a decisive role in modern application of quantum information, such as memory atoms and quantum emitters. The central challenge in this context is to address, control and protect systems of many qubits against decoherence.[1] Recently, efficient generation of entangled multiphoton graphs from single ^{87}Rb atoms was reported, overcoming the limitations encountered by probabilistic schemes.[2]

In this theoretical work, we investigate the applicability of different isolating materials to be used as substrate for a 2D lattice or clusters of ^{87}Rb atoms. In contrast to MgO, frequently used in previous investigations [3], NaCl was found to be a substrate that minimizes substrate-mediated interaction between neighboring Rb atoms. It is thus expected to allow entanglement of several individ-

ual atoms as single emitters in the same cavity. Therefore, the system Rb/NaCl promises improved scalability and opens new possibilities for quantum computation and communications.

[1] J. Preskill et al., Quantum 2, 79 (2018).
[2] P. Thomas et al., Nature 608, 677–681 (2022).
[3] R. Broekhoven et al., npj Quantum Information 10, 92 (2024)

HL 20.61 Tue 18:00 P1

Dry transfer of 2D van der Waals heterostructures for quantum sensing — •Timo Strobl, Korbinian Felber, Paul Konrad, Andreas Sperlich, and Vladimir Dyakonov — Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

A highly dynamic research area is dedicated to the development of quantum sensors based on solid-state spin defects. This field was previously focused on three-dimensional (3D) material systems, which posed challenges in positioning spin centers close to the sample surface. The recent discovery of V_B^- spin defects in the 2D van der Waals (vdW) material hexagonal boron nitride (hBN) provided a new approach to overcome this inherent positioning limitation. These defects are suitable for sensing local magnetic fields, temperature, and lattice strain when utilizing the method of optically detected magnetic resonance (ODMR). Hence, these functional hBN layers constitute a powerful tool for investigating fundamental 2D material properties.

To apply the potential in this area, the fabrication of a van der Waals heterostructure is necessary, combining the spin-active hBN with another 2D material. The precise fabrication by stacking these multilayer 2D materials via established dry-transfer polymer techniques is an essential prerequisite for such quantum sensor structures. The preparation procedures presented here provide essential insights required to implement in situ quantum sensing of 2D materials utilizing hBN.

HL 20.62 Tue 18:00 P1

Development of open-source DRC scripts for physical verification of integrated circuits with FinFET technology. — •Lev Churkin — Moscow, Russia

The development of open-source DRC scripts for FinFET technologies necessitates a fundamental shift from planar-based verification. It must encapsulate the three-dimensional nature of the transistor, enforcing complex rules for fin formation, cut patterning, and their strict alignment. Furthermore, rules must integrate with multi-patterning lithography, addressing color decomposition and spacing constraints to prevent printability errors. This requires checking more than simple geometrics. Consequently, a modern DRC script is a complex software model, which needs to manage the interdependencies of density, stress engineering, and manufacturing variability at a more advanced level.

HL 20.63 Tue 18:00 P1

Exciton dressing by extreme nonlinear magnons in a layered semiconductor — •Geoffrey M. Diederich — University of Maryland Baltimore County, 1000 Hilltop Circle, Baltimore MD, USA

Collective excitations presenting nonlinear dynamics are fundamental phenomena with broad applications. A prime example is nonlinear optics, where diverse frequency-mixing processes are central to communication and attosecond science, and extreme (>sixth-order) harmonic generation provides broad wavelength conversion. Leveraging recent progress in van der Waals magnetic semiconductors, we demonstrate nonlinear optomagnonic coupling. In the layered antiferromagnetic semiconductor CrSBr, we observe exciton states dressed by up to 20 harmonics of magnons, resulting from their extreme nonlinearities. We also create tunable optical sidebands via sum- and difference-frequency generation between two optically bright magnon modes under symmetry-breaking magnetic fields. Moreover, we can tune the observed difference-frequency generation mode into resonance with one of the fundamental magnons, which results in parametric amplification of magnons. Our findings realize the modulation of the optical-frequency exciton with the extreme nonlinearity of magnons at microwave frequencies, which could find applications in magnonics and hybrid quantum systems, and provide a method for optomagnonic neuromorphic computing devices.

HL 20.64 Tue 18:00 P1

Synthesis and characterization of new materials from the Sb-Ag-Te system — •Trayana Dolchinkova, Vladislava Ivanova, and Yordanka Trifonova — University of Chemical Technology and Metallurgy, Department of Physics, 8 Kl. Ohridski Blvd., 1797 Sofia, Bulgaria

New bulk chalcogenide materials from the Sb-Ag-Te system were synthesized by single-temperature synthesis in a closed volume. The density of the bulk samples was estimated using the pycnometer technique. Some physicochemical properties such as compactness, the molar volume and the free volume percentage of the materials were calculated, and their dependences on composition were determined. XRD analysis was performed to determine the structure and phase composition of the synthesized samples. A scanning electron microscope were used to study the surface morphology and EDS determined the chemical composition of the bulk samples.

Conclusions were drawn based on the results obtained regarding the influence of Ag content on the properties of the bulk samples.

HL 20.65 Tue 18:00 P1

Investigation of the Thermoelectric Properties of Single-Crystalline and Polycrystalline Bi1-xSbx (x =0, 0.1, 0.15) Alloys — •Fangyi Hu, Yuan Yu, and Matthias Wuttig — I. Physikalisches Institut (IA), RWTH Aachen University, 52074 Aachen, Germany

Thermoelectric (TE) materials can directly convert heat into electricity and vice versa, providing a sustainable and clean energy solution. Bi1-xSbx, a low-temperature n-type TE alloy with great potential between 20-200 K, has drawn increasing attention in cooling applications. Single crystals and polycrystals exhibit different performance and application prospects. In most cases, particularly below 200 K, single-crystal Bi-Sb shows much higher TE performance than polycrystals. However, polycrystalline Bi-Sb offers lower fabrication cost, better mechanical strength, and easier processing, making it attractive for large-scale use. This study compares the TE properties of Bi-Sb alloys in these two forms and clarifies their intrinsic relationship. Single-crystalline and polycrystalline Bi1-xSbx (x = 0, 0.1, 0.15) were prepared by Bridgman and melt-air-cooling methods, respectively. TE properties, with and without magnetic fields, were measured using Thermal Transport Option in a physical property measurement system (PPMS). Microstructures and bonding mechanisms were analyzed via atom probe tomography. By establishing the bonding-structure-property connection, we aim to reveal the origin of the performance difference between the two forms. These results provide insights into improving ZT in polycrystalline Bi-Sb alloys, which are more suitable for practical deployment.

HL 20.66 Tue 18:00 P1

Oxygen Vacancy-Mediated Non-Volatile Memory in RF-Sputtered Ga_2O_3 films — •Aman Baunthiyal, Jon-Olaf Krisponeit, Marco Schowalter, Alexander Karg, Andreas Rosenauer, Martin Eickhoff, and Jens Falta — Institute of Solid State Physics, University of Bremen, Bremen, Germany

To address the memory bottleneck in conventional electronics, resistive switching (RS) has emerged as a promising route for next-generation memory technologies. Among various materials used in RS devices, β-Ga_2O_3 offers advantages such as high breakdown strength and defect-mediated conductivity. However, its direct growth on metal electrodes with controlled microstructure, crucial for scalable vertical devices, remains largely unexplored. Here, we investigate RF-sputtered Ga_2O_3 deposited on smooth Ru(0001) films for non-volatile RS applications.

XRD and TEM confirm the temperature-dependent structural evolution of Ga_2O_3 and its correlation with the I–V response. Devices grown at intermediate temperatures (~400°C) show the best switching window (up to 10^4), with thinner films enabling low set voltages (~1.5 V) [1] but poorer stability. In contrast, thicker layers require higher voltages (~4 V) yet offer better reliability [2]. This behaviour arises from temperature-driven grain growth and the $\gamma \rightarrow \beta$ phase transition [3], which creates mixed phases and grain boundaries that govern oxygen-vacancy-mediated filament dynamics.

[1] A. Baunthiyal *et al.*, *Appl. Phys. Lett.* **123**, 213504 (2023). [2] A. Baunthiyal *et al.*, *2023 IEEE NMDC*, pp. 536-540. [3] A. Baunthiyal *et al.*, *APL Mater.* **13**, 041130 (2025).

HL 21: Focus Session: Quantum Sensing with Solid State Spin defects II (joint session TT/HL/MA)

Time: Wednesday 9:30–10:30 Location: HSZ/0101

See TT 40 for details of this session.

HL 22: Biocompatible Organic Semiconductors

Time: Wednesday 9:30–11:00 Location: POT/0006

HL 22.1 Wed 9:30 POT/0006

Stable n-Type OECTs with BBL: Unlocking Complementary Circuits — •Clemens Rössler[1,2], Laura Teurle[1,2], Hans Kleemann[1,2], and Karl Leo[1,2] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials — [2]TU Dresden

Organic mixed ionic-electronic conductors (OMIECs) have emerged as a key materials platform for next-generation bioelectronics, energy-efficient signal processing, and neuromorphic computing. Among the most versatile OMIEC devices is the organic electrochemical transistor (OECT), whose ability to couple ionic and electronic transport enables low-voltage operation and is particularly advantageous for solid-state electrolyte systems that enable densely integrated circuitry. While p-type materials such as PEDOT:PSS have driven much of the field's progress, the lack of stable and high-performance n-type counterparts remains a critical bottleneck - limiting the realization of complementary circuits, low-power logic, and more complex bioelectronic architectures. In this talk, I present recent progress on n-type OECTs based on the ladder polymer poly(benzimidazobenzophenanthroline) (BBL). I will discuss how we have developed and optimized n-type OECTs that exhibit remarkable stability and a unique electrochemical conditioning behaviour. Spectroscopic, AFM, and transfer curve analyses show that BBL combines excellent optical and morphological stability with a high mobility capacitance product, indicating efficient ion penetration and intrinsically high electronic mobility.

HL 22.2 Wed 9:45 POT/0006

A Nonlinear Organic Infrasound Sensor — •Maarten Mittmann[1], Carsten Habenicht[1], Andreas Hofacker[1], Richard Kantelberg[1], Stefan Jacob[2], Hans Kleemann[1], and Karl Leo[1] — [1]Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute for Applied Physics, Dresden University of Technology, 01062 Dresden, Germany — [2]National Metrology Institute (PTB), 38116 Braunschweig, Germany

Most works on speech recognition using reservoir computing focus on the nonlinear transformation of the data, which is fed electronically from a conventional sensor to the device. However, this approach necessitates two separate devices, consuming power and possibly requiring additional signal processing steps. In this work, we demonstrate that an efficient interface between acoustic stimulation and nonlinear, electronic output can be established using a free-standing viscoelastic film containing a poly(3,4-ethylenedioxythiophene) hexafluorophosphate ($PEDOT:PF_6$) fiber organic electrochemical transistor (OECT). Upon application of a constant drain-source and gate-source voltage, the system shows a time-dependent, nonlinear modulation of the drain current when excited acoustically. This nonlinearity opens possibilities of combining the existing system with a reservoir computing approach to perform complex tasks like infrasound source discrimination and anomaly detection. The devices show great sensitivity within the order of magnitude of $10^2\ mV\ Pa^{-1}$ in the infrasound frequency regime thanks to the amplification via the gate electrode.

HL 22.3 Wed 10:00 POT/0006

Is Printed Electronics a Sustainable Technology? A Framework to Efficiently Implement an Early-Stage Life-Cycle-Analysis — •Laura Teuerle, Tommy Meier, Klara Hänisch, Finn Jaekel, Yeohoon Yoon, Andreas Wendel, and Hans Kleemann — Dresden Integrated Center for Applied Physics and Photonic Materials, TU Dresden, Germany

The rise of microelectronic system has been the major driving focus of the global economy for the last couple of decades. As we are now transitioning to the era of the internet-of-things, with an increasing number of small autonomous electronic circuits, e.g, for sensing, we need to urgently consider the environmental impact of this development due to the unsustainable use of natural resources. Thus, to ensure the environmental sustainability of the development, future electronics must prioritize both performance and environmental impact, explaining the interest in flexible and printed electronics. However, the sustainability claims often connected to the field of flexible and printed electronics must be substantiated using analytic methods, providing the motivation for quantitative Life-Cycle Assessment (LCA). Here we demonstrate our approach to implement an LCA for an early-state research topic such as Organic Electrochemical Transistors (OECTs). Using hands-on examples, we will show how to set up an inventory database (the core of the LCA) using a process-of-record (PoR). By making LCA a standard tool in printed electronics, the community can move beyond sustainability claims to measurable environmental impact, driving truly responsible innovation in electronics.

HL 22.4 Wed 10:15 POT/0006

Obtaining In-Vivo Data for AI Applications Using Implantable Biocompatible Materials — •Finn Jaekel[1], Richard Kantelberg[1], Hans Kleemann[1], Daniel Freund[2], Julia Henne[2], Dennis Wahl[2], Eberhard Grambow[3], Sebastian Hinz[2], Clemens Schafmayer[2], Jochen Hampe[4], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, Dresden, Germany — [2]Klinik und Poliklinik für Allgemeine Chirurgie, Thorax, Gefäß- und Transplantationschirurgie, Universitätsmedizin Rostock, Rostock, Germany — [3]Klinik für Herz-, Thorax- und Gefäßchirurgie (HTG), Universitätsmedizin Göttingen, Göttingen, Germany — [4]Universitätsklinikum Carl Gustav Carus Dresden, Dresden, Germany

Artificial intelligence can be of great use in biomedical applications, especially when implemented in implantable hardware solutions. However, robust, biomedical AI applications crucially depend on real, high-quality, physiological training and input datasets, which are scarce in practice. In this presentation, we provide a prototypical use-case scenario by demonstrating in-vivo impedance measurements in a porcine small-intestinal anastomosis using printed, fully biocompatible organic sensors. Ischemia was induced locally, and manual evaluation shows a characteristic signature in the recorded impedance spectra, confirming that the system captures physiologically relevant data. This positions the technology in a realistic sensor to AI analysis pipeline, where automated detection of ischemia can be used to create an early warning system of anastomotic failure.

HL 22.5 Wed 10:30 POT/0006

Towards Fully Biodegradable and Sustainable Organic Electrochemical Transistors Printed on Leaf-Derived Substrates — •Bilge Kahraman, Rakesh R. Nair, Hans Kleemann, and Karl Leo — Dresden Integrated Center for Applied Physics and Photonic Materials, Technische Universität Dresden, 01187 Dresden, Germany.

The rapid proliferation of disposable electronics has exacerbated electronic waste and its associated environmental burden. Here, we demonstrate fully screen-printed organic electrochemical transistors (OECTs) fabricated on robust biodegradable leaf-derived substrates using non-toxic carbon and PEDOT:PSS-based inks. Magnolia grandiflora leaves were skeletonized to function as sequestering matrices for hydroxypropylcellulose (HPC) based resin, which was subsequently crosslinked to create robust flexible, compostable substrates. Life-cycle assessment (LCA) reveals that the combination of leaf-skeleton-based substrates and carbon gate electrodes for electronic device fabrication reduces CO_2-equivalent emissions by up to four orders of magnitude compared to conventional glass substrates and gold electrodes (19,400 times lower for substrates; 680 times lower for electrodes). The printed OECTs exhibit steady-state performance comparable to devices made on glass using commercial PEDOT:PSS formulations, with on/off ratios > 10^4 and transconductance values exceeding 1 mS. This work presents a viable path toward truly green bioelectronic devices that can be manufactured for disposability and safely returned to the environment after use.

HL 22.6 Wed 10:45 POT/0006

Flexible Organic Photodiodes Based on Advanced Encapsulation Strategies — •Rabiul Islam[1,2], Siddhartha Saggar[1,2], Jakob Wolansky[3], Darius Pohl[4], Markus Löffler[4], Bernd Rellinghaus[4], Johannes Benduhn[3], and Caroline Murawski[1,2] — [1]Institute of Solid-State Electronics, Technische Universität Dresden, Dresden, Germany — [2]Kurt Schwabe Institute for Sensor Technologies, Waldheim, Germany — [3]Dresden Integrated Center for Applied Physics and Photonic Materials, Technische Universität Dresden, Dresden, Germany — [4]Dresden Center for Nanoanalysis (DCN), Technische Universität Dresden, Dresden, Germany

Organic photodiodes (OPDs) are promising for biomedical applications due to their flexibility, spectral tunability, and biocompatibility, yet their moisture sensitivity demands robust encapsulation for long-term operation. Conventional flexible substrates offer limited device protection in humid conditions; to overcome this, we employed a parylene-C/ALD-deposited Al2O3/ZrO2 hybrid substrate, providing flexibility and strong barrier properties. We fabricated flexible OPDs with an ultrathin (7 nm) silver electrode on a hybrid substrate, which remained stable after 10,000 bending cycles and demonstrated high mechanical robustness. Using PM6:PC71BM as the active layer, the OPDs achieved responsivity of 0.26 A/W at -0.1 V under 639 nm illumination, retained 86% of their initial performance after 12 days in deionized water, and remained functional after one hour of machine washing, showing that parylene/nanolaminate-based ultra-flexible OPDs enable long-term operation in aqueous environments.

HL 23: Transport Properties

Time: Wednesday 9:30–12:15 Location: POT/0051

HL 23.1 Wed 9:30 POT/0051

Nonlinear charge transport in single crystalline slabs of Bi2Se3 — •Igor Veremchuk[1], Pavlo Makushko[1], Anita Guarino[2], Muhammad Waqee Ur Rehman[2], Rosalba Tatiana Fittipaldi[2], Tobias Kosub[1], Alexej Pashkin[1], Fabian Ganss[1], Proloy T. Das[1], Rui Xu[1], Rhonald Burgos Atencia[3], Debottam Mandal[3], Antonio Vecchione[2], Carmine Ortix[3,2], and Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., 01328 Dresden, Germany — [2]CNR-Institute for SuPerconductors, Innovative materials, and devices, Salerno, Italy — [3]Dipartimento di Fisica "E. R. Caianiello", Universita di Salerno, IT-84084 Fisciano (SA), Italy

Nonlinear charge transport is central to next-generation high-frequency electronics, enabling efficient rectification and frequency conversion up to the THz range. Nonlinear responses are observed in various material systems often focusing on thin films including Bi [1], Te [2], and Bi2Se3 [3]. In this study, we will report experimental observations of nonlinear charge transport in Bi2Se3 single crystals, which is explained based on peculiarities of the structural properties of layered Bi2Se3 materials. Our findings can be applied to a broad range of van der Waals centrosymmetric compounds.

[1] P. Makushko, I. Veremchuk et al., Nat. Electron. 7, 207 (2024).
[2] B. Cheng et al., Nat. Commun. 15, 5513 (2024).
[3] P. He et al., Nat. Commun. 12, 698 (2021).

HL 23.2 Wed 9:45 POT/0051

Comparing thermal conductivity predictions from open source phonon transport solvers — •Sally Issa, Martí Raya-Moreno, and Nakib H. Protik — Humboldt-Universität zu Berlin, Germany

Phonon transport continues to be an active field of research, both for probing materials physics and developing applications for thermoelectricity and thermal management. Due to their parameter-free nature, ab initio approaches are one of the preferred means for solving the phonon transport problem, offering excellent predictive capabilities, especially for novel materials. Over the last decade, the workflow combining density functional theory (DFT) and the Peierls Boltzmann transport equation (BTE) has gained popularity. Indeed, practitioners in the field have several publicly available BTE code packages to choose from, for example, ShengBTE, AlmaBTE, phonop3py, elphbolt, Phoebe, etc., that use this workflow. Nevertheless, the doubt regarding the comparability of these different codes still remains. At present, a detailed comparative study is missing in the literature. In this work, we fill this gap and carry out a comparison of the phonon thermal conductivity predicted by various codes. For a fair comparison, we use the same DFT generated interatomic force constants from the Alma database [1] for all considered codes. We carefully check the convergence of the thermal conductivity with respect to the wave vector mesh density and compare the results over a range of temperature points.

[1] ALMA database: https://almabte.bitbucket.io/database/

HL 23.3 Wed 10:00 POT/0051

Influence of Thermal Annealing on CMOS-Integrated Graphene Field-Effect Transistors — •Daniel Nickel[1], Daniele Capista[1], Rasuole Lukose[1], Christian Wenger[1,2], and Mindaugas Lukosius[1] — [1]IHP - Leibniz Institute for High Performance Microelectronics, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany — [2]BTU Cottbus Senftenberg, Platz der Deutschen Einheit 1, 03046 Cottbus, Germany

This work investigates the influence of consecutive annealing on CMOS-integrated graphene field-effect transistors (GFETs) with annealing temperatures (T_a) from 150 °C up to 300 °C. The GFETs were fabricated on 200 mm SiO_2/Si wafers with Pd/Au and Ni edge contacts, tungsten backgate and Si_3N_4 passivation. Annealing was carried out in 150 sccm nitrogen flow for 1 h using a 10 °C/min ramp. Electrical transfer measurements show that maximum p- and n-type field-effect mobilities occur at T_a = 200 °C for Pd/Au ($\mu_p \approx 950$ cm^2/Vs, $\mu_n \approx 1650$ cm^2/Vs) and at T_a = 150 °C for Ni ($\mu_p \approx 450$ cm^2/Vs, $\mu_n \approx 890$ cm^2/Vs). Raman analysis indicates an improved graphene quality with increasing T_a. Raman mapping reveals that for Pd/Au, the FWHM of the 2D peak reaches a minimum at T_a = 200 °C, followed by a slight increase in compressive strain at higher T_a. For Ni, broader 2D and G peak distributions and a reduction in p-doping with increased T_a is observed. Raman data measured near the Ni contacts reveal reduced p-doping, whereas doping near the Pd/Au contacts remains largely unaffected. Funding was provided by EU Horizon 2020 Graphene Flagship grants 101189797 and 101120938.

HL 23.4 Wed 10:15 POT/0051

Elucidating mobile charge carriers in granular matter by transient surface photovoltage analysis — •Christoph Merschjann[1], Albert These[2], Christoph Brabec[2,3], Thomas Dittrich[1], and Pablo Jimenéz-Calvo[2,4] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen — [3]Helmholtz-Institute Erlangen-Nürnberg, Erlangen — [4]Max-Planck-Institute of Colloids and Interfaces, Potsdam

Among the most important properties of novel functional materials are their charge transport characteristics, including *n* vs. *p* type conductivity, carrier concentrations, and respective mobilities. However, new solid-state materials are typically first synthesized in granular form, and often this is also the intended morphology for applications (batteries, photocatalysts, etc.). This makes most electrical characterization techniques (e.g. impedance, Hall, time-of-flight photocurrent) extremely challenging, as they rely on current measurements throughout the bulk of the sample. To overcome this drawback, we use contactless transient surface photovoltage (TR-SPV) to detect charge-density shifts on the nanometer scale and in a time range from nanoseconds to seconds. Comparing the results with diffusive charge-transport models of moderate complexity, we are able to deduce the type and mobility of photoinduced charge carriers in a prominent example material, graphitic polymeric carbon nitride (PCN). We encourage transferability of this SPV analysis to other 2D layered systems like metal- or covalent-organic frameworks (MOF / COF).

HL 23.5 Wed 10:30 POT/0051

Deep-learning Hamiltonian Acceleration of Electrical Transport Predictions using the Non-Perturbative *ab initio* Kubo-Greenwood Method for Strongly Anharmonic Materials — •Juan Zhang[1,2], Kisung Kang[3], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at the FHI of the Max Planck Society, Berlin — [2]Department of Optical Science and Engineering, Fudan University, Shanghai — [3]School of Materials Sciences and Engineering, Chonnam National University, Gwangju

Thermal insulators, e.g., needed for efficient thermoelectric materials, feature strong anharmonicity. As a consequence, a perturbative approach of electron-phonon interactions and even the phonon concept for describing vibrations may become invalid. The non-perturbative *ab initio* Kubo-Greenwood (aiKG) method provides an approach for evaluating electron and hole mobilities [1]. However, it requires substantial computational costs due to its high requirements with respect to statistical averages, large supercells, and extrapolation strategies to the zero-frequency limit. This work introduces an AI-assisted aiKG framework for the FHI-aims code, which incorporates the neural-network model, DeepH [2], trained to predict the Kohn-Sham Hamiltonian. Using the thermal insulator KI, we demonstrate the capabilities and predictive power of the approach, which substantially accelerates the calculation of large supercell electronic band structures, temperature-dependent spectral functions, and carrier mobilities with high accuracy.

[1] J. Quan *et al.* Phys. Rev. B 110, 235202 (2024).
[2] X. Gong, *et al.* Nat Commun 14, 2848 (2023).

HL 23.6 Wed 10:45 POT/0051

Quantum oscillations in the correlated metal $CaVO_3$ — Olivio Chiatti[1], Mahni Müller[1], Maria Espinosa[1], Tatiana Kuznetsova[2], Roman Engel-Herbert[2,3], and •Saskia F. Fischer[1,4] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802, USA — [3]Paul-Drude-Institut für Festkörperelektronik, 10117 Berlin, Germany — [4]Center for the Science of Materials Berlin, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

Transparent conductive materials are in great demand in the optoelectronic industry for their high-performance and cost-effectiveness. Strong electron-electron interactions in correlated metals can enhance the carrier effective mass and allow to achieve both high-optical transparency and high-electrical conductivity [1].

Here, we study the electric transport properties of thin $CaVO_3$ epitaxial films grown on $LaAlO_3$ substrates by hybrid molecular beam epitaxy, with residual a high resistivity ratio (RRR) up to 98 [2]. Magnetortransport measurements were performed between 2 and 200 K in magnetic fields up to 64 T. Films with high RRR show quantum oscillations below 10 K. The analysis of the Shubnikov-de Haas oscillations provides parameters within a multi-carrier model and the implications for the complex Fermi surface of $CaVO_3$ are discussed.

[1] Zhang *et al.*, Nature Materials **15**, 204 (2016)
[2] Kuznetsova *et al.*, APL Materials **11**, 041120 (2023)

15 min. break

HL 23.7 Wed 11:15 POT/0051

Modeling the impact of dynamic disorder on optical conductivity of semiconductors using a Kubo approach — •Frederik Vonhoff[1], Michel Panhans[2], David R. Reichman[3], Frank Ortmann[2], and David A. Egger[1] — [1]Physics Dep., TUM School of Natural Sciences, Technical University of Munich, 85748

Garching, Germany — [2]Dep. of Chemistry, TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany — [3]Dep. of Chemistry, Columbia University, New York, NY 10027, USA

Semiconductor devices rely critically on efficient charge-carrier transport, making it essential to understand the underlying transport mechanisms. The optical conductivity is a key transport observable, both experimentally and theoretically, for identifying the scattering mechanisms and transport regimes. However, modeling the transport properties of semiconductors with strong nuclear vibrations is challenging due to the resulting dynamic disorder in the electronic structure [1, 2]. Addressing these challenges, we develop a dynamic-disorder-driven microscopic method to compute optical conductivities in one- and three-dimensional semiconductor model systems by integrating time-dependent electronic Hamiltonians in Kubo transport theory. By systematically varying the static and dynamic disorder strength, we investigate the transition from localization to transient localization to and diffusive behavior, providing insights into scattering mechanisms active in emerging semiconductor materials such as halide perovskites.

[1] J. Fetherolf, et al, Physical Review X 10, 021062 (2020)
[2] F. Vonhoff, et al, Physical Review Materials 9, 094601 (2025)

HL 23.8 Wed 11:30 POT/0051

Self-Trapped Exciton Diffusion in a Lead-Free Two- Dimensional Hybrid Perovskite — •Jan-Heinrich Littmann[1], Lukas Gümbel[1], Philip Klement[1], Meng Yang[2], Markus Stein[1], Johanna Heine[2,3], and Sangam Chatterjee[1] — [1]Institute of Experimental Physics I and Center for Materials Research (ZfM), Justus Liebig University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany — [2]Department of Chemistry and Material Sciences Center, Philipps-Universität Marburg, Hans-Meerwein- Straße, 35043 Marburg, Germany — [3]Institute of Chemistry, Carl von Ossietzky Universität Oldenburg, Ammerländer Heerstraße 114-118, 26129 Oldenburg, Germany

Self-trapped excitons (STEs) in low-dimensional metal-halide perovskites arise from lattice distortions. The mobility of such excitations is expected to be limited, however, remains vastly unexplored experimentally.

Here, we directly image STE transport in a lead-free perovskite using spatially and temporally resolved photoluminescence microscopy. The STEs exhibit measurable mobility and propagate over micrometer distances despite their strongly-localized nature. At low temperatures, their motion is limited and nearly temperature independent. Transport becomes thermally activated above 150k and overcomes local energy barriers. Together this infers trap-limited diffusion. These results establish that STEs are mobile under suitable conditions and provide a quantitative framework for STE transport in lead-free perovskite materials.

HL 23.9 Wed 11:45 POT/0051

Electron-phonon interactions in VASP — •Manuel Engel[1], Henrique Miranda[1], Atsushi Togo[2], Laurent Chaput[3], Martijn Marsman[1], and Georg Kresse[1,4] — [1]VASP Software GmbH, Vienna, Austria — [2]National Institute for Materials Science, Tsukuba, Japan — [3]Lorraine University, Nancy, France — [4]University of Vienna, Vienna, Austria

Understanding electron-phonon interactions with first-principles accuracy is essential for predicting temperature-dependent electronic properties in semiconductors and complex materials. In this work, we present new capabilities implemented in VASP that enable a fully ab initio treatment of electron-phonon coupling using the projector-augmented wave (PAW) method. These developments provide a consistent framework for evaluating band-gap renormalization, phonon-induced linewidths, and finite-temperature electronic transport properties within density functional theory.

Our approach combines perturbative electron-phonon matrix elements with dense Brillouin-zone sampling achieved through interpolation techniques compatible with PAW-based orbitals and higher-level density functionals. We demonstrate accurate predictions of zero-point and thermal band-gap shifts across a range of materials. In addition, we incorporate the electron-phonon scattering rates directly into Boltzmann transport calculations under relaxation-time approximations. This enables temperature-dependent mobilities and conductivities to be computed from first principles.

HL 23.10 Wed 12:00 POT/0051

Investigation of exciton diffusion in GaAs nanowires via cathodoluminescence spectroscopy — •Mikel Gómez Ruiz, Vladimir Kaganer, Jesús Herranz, Lutz Geelhaar, Oliver Brandt, and Jonas Lähnemann — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117 Berlin, Germany

Semiconductor nanowire (NW) structures emitting at tailored wavelengths have attracted notable interest for integration with silicon-on-insulator waveguides. For many of these applications, the efficiency with which carriers are injected into the active region of the sample is relevant.

In this context, carrier transport in phase-pure GaAs nanowires is investigated by spatially-resolved cathodoluminescence spectroscopy. Emission intensity profiles along the nanowire axis are measured to study carrier transfer from the GaAs segment to the axial interfaces at both ends of the nanowire. These interfaces are formed at the top with the axially grown (Al,Ga)As shell and at the bottom with the Si substrate. The recorded intensity profiles are predominantly asymmetric, indicating that carrier recombination at the two interfaces occurs in a different fashion.

These profiles are analyzed using a mathematical model that accounts for carrier generation, diffusion, and recombination. Fitting this model to the experimental profiles reveals a diffusion length exceeding one micron at 10 K, an unprecedented value for GaAs nanowires. This reflects the high crystal quality of our nanowires.

HL 24: 2D Materials IV – Emerging materials and properties

Time: Wednesday 9:30–12:45 Location: POT/0081

HL 24.1 Wed 9:30 POT/0081

Atomic layer deposition of few-layer 1T-TiS_2 and ternary $MoTiS_2$ — •Christian Petersen[1,2], Christian Tessarek[1,2], Marco Schowalter[1,2], Andreas Rosenauer[1,2], and Martin Eickhoff[1,2] — [1]Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany — [2]MAPEX Center for Materials and Processes, University of Bremen, Bibliothekstraße 1, 28359 Bremen, Germany

Theoretical calculations and experimental data concerning electronic and structural properties of 1T-TiS_2 are sparse in comparison to other transition metal dichalcogenides (TMD) such as MoS_2. The available data is contradicting and attributes 1T-TiS_2 a plethora of different properties ranging from a semi-metal like behaviour to different charge density wave phases (2×2 and $\sqrt{7} \times \sqrt{3}$) and even a band gap of up to 2.5 eV. In general, there is a lack of experimental data due to difficulties in synthesis and stabilization of 1T-TiS_2 which rapidly oxidizes in ambient conditions.

In this study, plasma-enhanced sub-atomic layer deposition (ALD) [1] in combination with in situ X-ray photoelectron spectroscopy (XPS) is employed to directly study the effects of the growth conditions on the chemical composition of 1T-TiS_2 while circumventing the problem of oxidation in ambient. To further characterize the 1T-TiS_2 film ex situ, Raman spectroscopy and atomic force microscopy (AFM) is utilized. Additionally, $MoTiS_2$ was synthesized by substitution of ALD cycles of the Ti precursor (TDMAT) by the Mo precursor (BTBMMo).

[1] C. Tessarek et al., 2D Mater. 11, 025031 (2024)

HL 24.2 Wed 9:45 POT/0081

The effect of Lithium intercalation on line defects in the MoS2 monolayer — •Asghar Ali Jan and Peter Kratzer — University of Duisburg-Essen, Duisburg, Germany

MoS2 can be an effective anode material in lithium-ion batteries, as it is scalable at room temperature and has weak van der Waals forces, allowing lithium ions to intercalate between the sheets. Additionally, when using MoS2 as an anode in a lithium-rich environment, the phase transition from the most stable H phase to the T' phase must also be considered. Certain defects, such as sulfur vacancies and grain boundaries, are often present in experimentally synthesized MoS2 layers. These grain boundaries introduce metallic states within the bulk band gap. As a result, the conductivity of MoS2 is reduced. Up to now, the H-to-T' phase transition in MoS2 has been extensively studied, but generally without considering the possible presence of defects such as grain boundaries. Therefore, we have investigated the interaction of lithium intercalation with the grain boundaries present in a MoS2 monolayer. For example, we examine how the presence of lithium near a mirror twin boundary (MTB) affects the one-dimensional line of charge trapped in the MTB. It is also important to consider the grain boundary formed when a T' phase created from the H phase due to lithium intercalation directly meets the remaining H phase that does not interact with lithium. Our density functional theory calculations provided insights about the stability and electronic properties of these line defects in the presence of lithiation.

HL 24.3 Wed 10:00 POT/0081

Wafer-scale growth of hexagonal boron nitride thin films using pulsed laser deposition — •Daniel Klenkert[1,2], Benedikt Winter[1], Paul Konrad[2], Andreas Sperlich[2], Vladimir Dyakonov[2], and Jens Ebbecke[1] — [1]Technology Campus Teisnach Sensor Technology, Deggendorf Institute of Technology, 94244 Teisnach — [2]Experimental Physics 6, Julius-Maximilians-University Würzburg, 97074 Würzburg

Hexagonal boron nitride (hBN) has attracted significant attention due to its wide bandgap, high thermal conductivity and its ability to host optically active defects, which are promising as single photon emitters and for quantum sensing applications. Thus far the sample preparation of hBN usually relies on tape exfoliation or high temperature chemical vapor deposition. Here we report on our progress using an alternative approach to prepare thin films of hBN on different substrates: pulsed laser deposition. This enabled the preparation of microcrystalline hBN layers on large scale wafer substrates at temperatures below 850°C. The stoichiometry preserving properties of pulsed laser deposition also allows for the preparation of carbon doped thin films. These are especially interesting for research on carbon related, optically active defects, which are noted for their high brightness and single photon purity.

HL 24.4 Wed 10:15 POT/0081

Doping-Induced Modulation of Structural and Electronic Properties in Transition Metal Dichalcogenides — •Cem Sanga[1,3], Nadire Nayir[1,3], Yusuf Kerem Bostan[2], Fahrettin Sarcan[2], Diwakar Singh[4], and Tanushree Choudhury[4] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117 Berlin, Germany — [2]Department of Physics, Faculty of Science, Istanbul University, Vezneciler, Istanbul, 34134, Turkey — [3]Department of Physics Engineering, Istanbul Technical University, Maslak, Istanbul, 34467, Turkey — [4]Department of Metallurgical Engineering and Materials Science, Indian Institute of Technology Bombay, Mumbai, Maharashtra 400076, India

Transition metal dichalcogenides (TMDCs) hold promise for electronic applications, yet their performance is limited by inadequate doping strategies. This density functional theory investigation examines substitutional and interstitial doping in MoS_2 and WS_2 using chlorine and oxygen dopants. Formation energy calculations reveal chlorine preferentially occupies sulfur vacancy sites in MoS_2. Electronic structure analysis demonstrates that strategic doping enables bandgap engineering in TMDC systems.

HL 24.5 Wed 10:30 POT/0081

Opposite In-Plane Electrical Anisotropy in $ZrSe_3$ and ZrS_3 Flakes — •Davin Höllmann[1], Lars Thole[1], Sonja Locmelis[2], and Rolf J. Haug[1,3] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, 30167 Hannover, Germany — [3]Laboratorium für Nano- und Quantenengineering, Leibniz Universität Hannover, 30167 Hannover, Germany

The anisotropy in form of quasi one-dimensional (1D) chains in transition metal trichalcogenides (TMTCs) makes them stand out compared to other more conventional two-dimensional (2D) materials [1]. Through width-dependent [2] and direct measurements, we investigated the electrical properties of $ZrSe_3$ and ZrS_3 flakes, in particular, the influence of the anisotropic effective electron masses [3] in the 2D plane. Flakes with a height of 26 nm were exfoliated from the respective bulk materials grown by a chemical vapour transport method.

Despite their identical quasi 1D layered crystal structure, $ZrSe_3$ and ZrS_3 exhibit inverted in-plane electrical anisotropy. While $ZrSe_3$ exhibits the highest conductivity across the 1D chains with an anisotropy ratio of 0.60, ZrS_3 is shown to favour electron transport along the 1D chains with a ratio of 1.69. Using DFT, we attribute this to the different chalcogen contributions at the conduction band minimum.

[1] J. O. Island et al., 2D Materials 4, 0220033 (2017)
[2] D. Höllmann et al., ACS Appl. Electron. Mater. 7, 9, 4049-4054 (2025)
[3] Y. Jin et al., Phys. Chem. Chem. Phys. 17, 18665-18669 (2015)

HL 24.6 Wed 10:45 POT/0081

Observation of Bernal Stacking in Few-Layer Graphene on C face Silicon Carbide — •Jonas Rose, Oliver Brandt, Michael Hanke, Joao Marcelo Lopes, Philipp John, and Hans Tornatzky — Paul-Drude-Institut, Berlin

Epitaxial growth of few-layer graphene (FLG) on SiC(000$\bar{1}$) (C face) is widely assumed to yield films with rotational disorder, in contrast to the well-ordered Bernal (AB) stacking typically associated with SiC(0001) (Si face) growth. In this work, we show that surface graphitization on the C face of SiC can, under appropriate conditions, produce FLG with genuine AB stacking and remarkably low mosaic spread. Using detailed Raman spectroscopy, supported by complementary structural characterization, we identify clear spectral signatures of Bernal ordering, including a well-defined 2D-band lineshape. These findings demonstrate that ordered stacking is achievable on the C face under controlled sublimation conditions. We will present our full spectroscopic analysis and discuss its implications for the structural and electronic properties of the grown FLG.

15 min. break

HL 24.7 Wed 11:15 POT/0081

Influence of Defects, Doping and Layer Twisting on Phonon Dispersions in Bilayer Graphene and MoS_2 from Machine-Learned Force Fields — •Sabuhi Badalov and Harald Oberhofer — Chair for Theoretical Physics VII and Bavarian Center for Battery Technologies, University of Bayreuth

In two-dimensional (2D) layered materials, phonon dispersion plays a central role in determining transport and electronic properties. In bilayer systems, phonon dispersion is highly sensitive to the stacking configuration, twist angle, defects, and doping types. Using *state-of-the-art* machine learning force fields trained on the *first-principles* data, we perform large-scale phonon calculations for bilayer graphene and MoS_2 to investigate how layer twist and defect density alter phonon spectra and interlayer vibrational modes. We also analyze the influence of p- and n-type doping on phonon dispersions and their interactions with the underlying electronic structure. Our results reveal characteristic shifts in low-energy acoustic and optical branches that are directly linked to microscopic structural motifs, including *Moiré*-induced phonon properties. These findings provide microscopic input for future calculations of electron-phonon coupling and possible phonon-mediated superconducting states in twisted and doped 2D materials and establish machine learning force fields as a powerful framework for exploring phonon-electron interaction in quantum materials.

HL 24.8 Wed 11:30 POT/0081

Efficient GW band structure calculations using Gaussian basis functions and application to atomically thin transition-metal dichalcogenides — •Rémi Pasquier[1], María Camarasa-Gómez[2,3], Anna-Sophia Hehn[4], Daniel Hernangómez-Pérez[5], and Jan Wilhelm[1] — [1]Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, 93053 Regensburg, Germany — [2]Centro de Física de Materiales (CFM-MPC), CSIC-UPV/EHU, Paseo Manuel de Lardizabal 5, 20018 Donostia-San Sebastián, Spain — [3]Departamento de Polímeros y Materiales Avanzados: Física, Química y Tecnología, Facultad de Química, UPV/EHU, 20018 Donostia-San Sebastián, Spain — [4]Institute of Physical Chemistry, Christian-Albrechts-University Kiel, Max-Eyth-Strasse 1, 24118 Kiel, Germany — [5]CIC nanoGUNE BRTA, Tolosa Hiribidea 76, 20018 San Sebastián, Spain

The GW approximation is widely used to compute self-energies and related electronic properties but remains computationally demanding, motivating the development of more efficient approaches. We present a space-time GW algorithm for periodic systems in a Gaussian basis with spin-orbit coupling, enabling accurate and efficient quasiparticle band-structure calculations for atomically thin materials. For monolayer MoS_2, $MoSe_2$, WS_2, and WSe_2, the resulting GW band gaps agree on average within 50 meV with plane-wave reference values. Full G_0W_0 band structures can be computed in less than two days on a laptop (Intel i5, 192 GB RAM) or under 30 minutes using 1024 cores.

HL 24.9 Wed 11:45 POT/0081

Investigating the Ferroelectric Potential Landscape of 3R-MoS_2 through Optical Measurements — •Jan-Niklas Heidkamp[1], Johannes Schwandt-Krause[1], Swarup Deb[1,2,3], Takashi Taniguchi[4], Kenji Watanabe[4], Rico Schwartz[1], and Tobias Korn[1] — [1]Institute of Physics, University of Rostock, Rostock, Germany — [2]Homi Bhabha National Institute, Mumbai, India — [3]Saha Institute of Nuclear Physics, Kolkata, India — [4]National Institute for Material Science, Tsukuba, Japan

In recent years, sliding ferroelectricity has emerged as a topic of significant interest due to its possible application in non-volatile, reconfigurable storage devices. This phenomenon is unique to two-dimensional van der Waals materials, where out-of-plane ferroelectric polarization switching is induced by relative in-plane sliding of adjacent layers. The intrinsic stacking order influences the resulting polarization, creating distinct polarization regions separated by domain walls. These can be manipulated using an applied vertical electric field, enabling a switchable system that retains the environmental robustness of van der Waals materials. This study investigates 3R-MoS_2 using various optical measurement techniques at room temperature and reveals apparent signal changes corresponding to different ferroelectric stacking orders and variations in layer count. Our findings demonstrate that fast optical mapping at room temperature is a reliable method for probing ferroelectric potential steps in 3R-stacked MoS_2 samples, thereby facilitating the identification of the ferroelectric configuration.

HL 24.10 Wed 12:00 POT/0081

Robust Orbital-Selective Flat Bands in Transition-Metal Oxychlorides — Xiangyu Luo[1], •Ludovica Zullo[2], Sahaj Patel[1], Dongjin Oh[1], Qian Song[1], Asish K. Kundu[3], Anil Rajapitamahuni[3], Elio Vescovo[3], Natalia Olszowska[4], Rafal Kurleto[4], Dawid Wutke[4], Giorgio Sangiovanni[2], and Riccardo Comin[1] — [1]Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139, USA — [2]Universität Würzburg, 97074 Würzburg, Germany, ct.qmat — [3]National Synchrotron Light Source II, Brookhaven National Laboratory, Upton, NY, USA — [4]Solaris National Synchrotron Radiation Centre, Jagiellonian University, Czerwone Maki 98, 30-392 Krakow, Poland

Flat electronic bands, which amplify electron correlations by quenching kinetic energy, provide an ideal foundation for exotic quantum phases. Here, we unveil an intrinsic orbital-selective flat-band mechanism in the van der Waals materials $NbOCl_2$ and $TaOCl_2$, directly observed by angle-resolved photoemission spectroscopy (ARPES) and understood through density functional theory (DFT) and Wannier analysis. Crucially, we experimentally demonstrate that this momentum-independent flat band exhibits remarkable robustness, surviving from the bulk crystal down to the few-layer limit at room temperature. Our theoretical analysis traces its origin to the hybridization between Nb-dz^2 orbital chains and the Lieb-like dx^2-y^2 sublattice, which is further reinforced by Peierls dimerization. Our findings uncover a new orbital-selective design principle for realizing flat bands in quantum materials.

HL 24.11 Wed 12:15 POT/0081

Tuning the Metal-to-Semiconductor Transition in Bilayer PtTe2 via Electric Field Control — •Sharieh Jamalzadeh Kheirabadi, Farzan Gity, Paul K.Hurley, and Lida Ansari — Tyndall National Institute, University College Cork, Cork, Ireland

Abstract: One effective method to induce a bandgap in graphene is applying a perpendicular electric field to its bilayer structure [1]. This process works by breaking the inversion symmetry of BL gra-phene with an external electric field, leading to electrostatic screening between the two layers and splitting the π and π^* bands that intersect at the Fermi level [2]. Platinum ditelluride (PtTe2) has garnered significant interest due to its unique physical and chemical properties [3,4]. PtTe2 retains its semi-metallic properties for thicknesses down to BL but transits to a semiconductor when re-duced to a monolayer due to the quantum confinement effect [5]. We demonstrate that a bandgap emerges in BL-PtTe2 when an electric field is applied perpendicular to the layers, ultimately transforming the system into a semiconductor. We have identified reliable critical electric fields within the range of 2-3 MV/cm to achieve a bandgap comparable to conventional semiconductors in BL-PtTe2. Further, we have investigated the effect of a vertical electric field on a BL-PtTe2 based field effect transistor using density functional theory (DFT) and non-equilibrium Green*s function (NEGF) methods. The results demonstrate device performance compatible with low-power require-ments for ION and IOFF, as projected in the IRDS 2028 roadmap [6].

HL 24.12 Wed 12:30 POT/0081

Circular Dichroism ARPES Reveals Orbital Chirality in Single-Layer TMDs — •Shubham Patel, Luke Pimlott, and Habib Rostami — Department of Physics, University of Bath, Claverton Down BA2 7AY, United Kingdom

The electron wavefunctions in momentum space are fundamental to understanding the microscopic physical properties of solids. Circular dichroism (CD), a key feature observable in angle-resolved photoemission spectroscopy (ARPES) [1]. Recent experimental investigations have indicated a direct relationship between CD-ARPES and the Berry curvature of electronic bands [2], motivating theoretical efforts to interpret CD within this framework. The Berry curvature-based approach fails to capture certain critical sign-reversal features near the time-reversal-invariant K(K') points. Moreover, this method lacks dependence on the photon energy of the incident light, as it is derived purely from the momentum-space wavefunction characteristics. In the present work, we adopt this plane wave approximation to compute CD-ARPES spectra and find excellent agreement with experimental observations. We solve tight-binding Hamiltonian for single-layer TMDs, and generalize the dipole matrix elements. This formalism successfully captures the sign-changing behavior of CD near the K(K') points, a feature absent in the Berry curvature approach, and provide a control on tunability of the dichroic response with the photon energy. Notably, our theoretical approach offers an alternative explanation that differs from the Berry curvature-based framework.

[1] PRL 110, 216801 (2013) [2] PRL 121, 186401 (2018)

HL 25: Focus Session: Young Semiconductor Forum

The young semiconductor forum gives a platform for post-docs at all career stages to present themselves and their scientific ideas. It consists of an oral session with invited talks about their work and/or scientific vita. With this format, we hope to attract both postdocs and senior researchers and decision makers to join this forum: for postdocs, to give them a platform to present themselves, and for professors, to meet the next generation of scientists.

Organized by Rudolf Bratschitsch, Alexander Holleitner, and the AGyouLeaP (Lucas Kreuzer and Aisha Aqeel)

Time: Wednesday 9:30–12:15 Location: POT/0251

Invited Talk HL 25.1 Wed 9:30 POT/0251

Quantum dots for single-electron current sources — •Johannes C. Bayer, Thomas Gerster, Dario Maradan, Niels Ubbelohde, Klaus Pierz, Hans W. Schumacher, and Frank Hohls — Physikalisch-Technische Bundesanstalt, 38116 Braunschweig, Germany

Generating accurate currents can be achieved in an elegant and direct way by applying a periodic signal to a tunable barrier quantum dot. Such devices are called single-electron pumps (SEPs) due to their capability of emitting a well defined number of n electrons per cycle of an external drive. With driving frequency f and elementary charge e this leads to a controlled and clocked current of $I = nef$, thereby providing a suitable basis for a quantum current standard. While individual SEPs can already achieve errors in the sub-ppm range for currents of the order $I \approx 100$ pA [1], implementing larger systems consisting of multiple well-performing SEPs remains a challenging task. We here present DC transport as well as pumping characteristics of multiple SEP devices toward scaling to higher currents.

[1] F. Stein, et. al., Metrologia 54, S1-S8 (2017)

Invited Talk HL 25.2 Wed 10:00 POT/0251

Optical readout of reconfigurable in-plane magnetic domains in CrSBr — •Aleksandra Łopion[1], Pierre-Maurice Piel[1], Manuel Terbeck[1], Jan-Hendrik Larusch[1], Jakob Henz[1], Marie-Christin Heissenbüttel[2], Thorsten Deilmann[2], Michael Rohlfing[2], Zdenek Sofer[3], and Ursula Wurstbauer[1] — [1]Physikalisches Institut and Center for Soft Nanoscience (SoN), University of Münster, Wilhelm Klemm Str. 10, Münster, 48149, Germany — [2]Institut für Festkörpertheorie, University of Münster, Wilhelm Klemm Str. 10, Münster, 48149, Germany — [3]Department of Inorganic Chemistry, University of Chemistry and Technology, Prague Technická 5, Prague, 616628, Czech Republic

Two-dimensional van der Waals (vdW) magnets have overcome the Mermin-Wagner expectation by hosting long-range order while remaining tunable through stacking, strain, gating, and external fields. Their reconfigurability and hysteresis are attractive for information technologies, particularly when antiferromagnetic (AFM) multistability is accessed and read optically. We discover a reconfigurable multilayer magnetic domain structure in the A-type antiferromagnetic semiconductor. The layered out-of-plane domain structure can be tuned by external stimuli and read out via domain-modulated optical contrast. This coupled magnetic-optical functionality demonstrates the possibility of encoding, processing, and storage of information in magnetic textures with a photonic-compatible readout. The domain landscape highlights CrSBr as a platform for "intelligent matter" and a building block for ultracompact opto-spintronic memories and neuromorphic hardware.

Invited Talk HL 25.3 Wed 10:30 POT/0251

Ferroelectric switching in Mn-doped epitaxial $BaTiO_3$ films and superlattices on silicon — •Alfredo Blázquez Martínez[1], Valentin Väinö Hevelke[1,2], Ibukun Olaniyan[1,2], Minh-Anh Luong[1,3], Ines Häusler[1], Sven Wiesner[1], Christoph T. Koch[4], Dong-Jik Kim[1], and Catherine Dubourdieu[1,2] — [1]Helmholtz-Zentrum Berlin fur Materialien und Energie, 14109 Berlin, Germany — [2]Freie Universität Berlin, 14195 Berlin, Germany — [3]CEMES-CNRS and Université de Toulouse, F-31055 Toulouse, France — [4]Humboldt-Universität zu Berlin, 12489 Berlin, Germany

The integration of epitaxial ferroelectric oxides on silicon remains a key challenge for realizing energy-efficient and CMOS-compatible nanoelectronic devices. Among these materials, barium titanate ($BaTiO_3$) is a prototypical perovskite ferroelectric with a high remanent polarization and a low coercive field. Molecular beam epitaxy (MBE) enables the growth of high-quality epitaxial $BaTiO_3$ on Si, yet these films typically show high leakage currents, which preclude polarization measurements and the realization of functional devices on Si. Here, we demonstrate robust ferroelectric hysteresis in epitaxial $BaTiO_3$ films grown on p-type Si using Mn doping. The introduction of a suitable amount of Mn suppresses leakage currents by up to seven orders of magnitude. We will then discuss the properties of (Mn-doped $BaTiO_3/SrTiO_3)_n$ superlattices hosting vortex polar textures of a few nanometers in diameter. This work highlights Mn-doping as an effective path to reduce leakage currents in epitaxial $BaTiO_3$ heterostructures to enable future topotronic devices integrated monolithically on semiconductors.

15 min. break

Invited Talk HL 25.4 Wed 11:15 POT/0251

Tunability of quantized Hall plateaus — •Serkan Sirt[1], Vladimir Umansky[2], and Stefan Ludwig[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [2]Weizmann Institut of Science, Rehovot, Israel

The textbook single-particle description of the quantum Hall effect based on the Landauer-Büttiker picture explains the extent of quantized Hall plateaus as a function of magnetic field in terms of disorder-broadened Landau levels. In contrast, the screening theory includes electron-electron interactions and predicts the formation of extended Hall plateaus based on the confinement potential, without the need for disorder [1].

To test these contrasting models, we investigate the tunability of the plateaus in gate-defined Hall bars. We employ a global top gate to deplete the two-dimensional electron system and an additional screen gate on the sample surface, separated by an insulating layer, to define the Hall bar. Varying the gate voltages allows us to tune the edges of the Hall bar continuously from hard to soft confinement. We find that, for softer confinement, the plateaus become wider by extending to lower magnetic fields. These results support the screening theory and are inconsistent with the Landauer-Büttiker picture.

This work establishes a new method for controlling and manipulating quantized Hall plateaus, which may become relevant for quantum Hall metrology and quantum technology applications.

[1] R. R. Gerhardts, Phys. Status Solidi B 245, 378 (2008)

Invited Talk HL 25.5 Wed 11:45 POT/0251

How to achieve high gain in organic photodetectors? — •Johannes Benduhn — Institute of Applied Physics, TU Dresden, Germany — German Centre for Astrophysics, Görlitz, Germany

Organic photodetectors (OPDs) match their inorganic counterparts in performance, with additional features like semitransparency, flexibility, and narrowband detection, opening new sensing applications. However, high-gain OPDs are challenging due to disorder. This work discusses two alternative principles to achieve gain.

The first approach uses unbalanced charge-carrier transport. Photo-generated charges accumulated near one of the contacts generate a local field that triggers charge injection of charges from the external circuit into the active layer. Under dark conditions, this injection is absent; therefore, these devices reach impressive EQE values of 1,000-10,000 %. However, the underlying microscopic mechanisms remain unclear. Here, we precisely tune the interface layers via vacuum deposition, enabling us to reveal the injection mechanism.

Another solution is photoactive transistors. We introduce vertical organic-permeable base transistors (OPBTs) that operate at low driving voltages and achieve high switching speeds. We report, for the first time, a photogating effect in OPBTs. By leveraging the unique structure of OPBTs and conducting a detailed investigation into the underlying charge-storing mechanism, we have achieved record responsivity values reaching 10^9 A/W, specific detectivities of 10^{15} Jones (based on noise measurements), and retention times exceeding 10^5 s. [1]

[1] Schröder, Benduhn *et al.* Nature Photonics 19, 1088-1098 (2025).

HL 26: Poster II

Time: Wednesday 9:30–11:30 Location: P1

HL 26.1 Wed 9:30 P1

Quantum Dots in Nonlinear Mechanical Resonators — •Jona Richter, Noah Spitzner, Emeline Nysten, Matthias Weiss, and Hubert Krenner — Universität Münster, Münster, Germany

Surface acoustic waves are employed in a broad range of technologies, including radio-frequency filters in wireless communication systems and life-science applications. In the presented work, SAWs are utilized to drive mechanical modes in a quantum-dot membrane patterned into rings on a lithium niobate substrate. Generation of the SAWs is achieved by fabricating a comb-shaped interdigital transducer on the substrate. When an RF signal is applied, the piezoelectric response of the lithium niobate converts the electrical excitation into coherent acoustic waves propagating on the surface of the substrate. The propagating SAW induces a periodic modulation of the QD lattice constant, resulting in a corresponding modulation of the emission energy at the driving frequency. This mechanism enables the use of individual QDs as point-like nanoscale sensors, which can be probed through photoluminescence spectroscopy using ultrafast optical detection. When sweeping the RF frequency over a range of 200-900 MHz, pronounced resonances in the emission-energy modulation are observed, but only for QDs located within the ring structures. Both time-integrated as well as time-resolved measurements exhibit clear signatures of nonlinear mechanical behavior for example a hysteresis.

HL 26.2 Wed 9:30 P1

Gallium Nitride arrays for proton imaging — •Nico Frédéric Brosda[1], Matilde Siviero[2], Maxime Hugues[2], Stéphane Higueret[3], Nicolas Arbor[3], Andreas Wieck[1], and Jean-Yves Duboz[2] — [1]Ruhr University Bochum, Faculty of Physics and Astronomy, Experimental Physics VI, D-44780 Bochum, Germany — [2]Université Côte d'Azur, CNRS, CRHEA, 06560, Valbonne, France — [3]Université de Strasbourg, CNRS, IPHC UMR 7178, F-67000 Strasbourg, France

The MATRIX project is advancing proton therapy for cancer treatment by developing novel, highly durable detectors designed to improve real-time control of irradiation doses. Proton detection is performed by measuring the charge generated within the active regions of PIN GaN diodes. These GaN-based devices are fabricated as linear arrays containing 128 diode elements, as well as two-dimensional imaging arrays with up to 11 × 11 elements, covering an area of 1 cm^2 and achieving spatial resolutions of up to 500 μm. Owing to microelectronic fabrication techniques, even higher resolutions can be realized when required. The spatial performance of these detectors was validated through proton radiography of test objects using a 24 MeV beam, benchmarked against non-pixelated Gafchromic film. Measurements with phantoms of varying thickness further demonstrated the detector's capability for energy-resolved proton imaging. With achieved frame times of 1 ms, the MATRIX detector also provides a first proof of concept for real-time proton beam monitoring.

HL 26.3 Wed 9:30 P1

Impact of Ge-doping on the photoelectrochemical response of cubic (Ga,In)N photoelectrodes — •Sundas Hamid[1,2], Marius Wasem[1,2], Mario F. Zscherp[1,2], Silas A. Jentsch[1,2], Jörg Schörmann[1,2], Sangam Chatterjee[1,2], and Matthias T. Elm[1,2] — [1]Center for Materials Research, Heinrich-Buff-Ring 16, 35392 Giessen — [2]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Giessen

(Ga,In)N is a promising electrode material for electrochemical water splitting as the amount of indium determines the band gap of the semiconductor alloy. In this study we focus on the influence of germanium doping on the photoelectrochemical response of cubic (In,Ga)N photoanodes, which were grown by molecular beam epitaxy (MBE). Different methods like open circuit potential, cyclic voltammetry and electrochemical impedance spectroscopy were used to analyse charge carrier transport and the properties of the electrode electrolyte interface, such as flat band potential. The non-intentionally doped samples show a high photocurrent, indicating less recombination and efficient charge separation, while doping decreases the photoelectrochemical response. Despite the lower photocurrent, the doped samples show higher electrochemical stability displaying structural strength and chemical resistance at the interface. The results show that a trade-off between stability and activity needs to be achieved by controlling doping and indium concentration to develop durable and efficient III-nitride photoanodes for solar water splitting.

HL 26.4 Wed 9:30 P1

First Principle Calculations of Scandium-Aluminium-Nitrides — Max Grossmann, Malte Grunert, and •Wichard beenken — Technische Universität Ilmenau, Institut für Physik, Theoretische Physik I, Ilmenau, Germany

We have calculated the crystal structures and optical spectra of $Sc_xAl_{1-x}N$ compounds in trigonal/hexagonal and tetragonal/cubic lattices. For increasing Scandium content, we could confirm the experimentally found first order phase transition from Wurtzit to Rock-Salt structure. Furthermore we found a second order phase transition to the theoretically predicted metastable hexagonal-MgO-structure. Thereby, we studied various possible superstructures for rational Scandium to Aluminium proportions in detail. Using LDA, *GW*, and BSE methods, we calculated band structures and optical dielectric functions for selected $Sc_xAl_{1-x}N$ compounds with high precision.

HL 26.5 Wed 9:30 P1

Tracing Charge Carrier Transport in Freestanding Core-Shell GaN Nanowires on n-Si(111) Substrates — •Juliane Koch[1], Patrick Häuser[2], Peter Kleinschmidt[1], Lisa Liborius[2], Nils Weimann[2], and Thomas Hannappel[1] — [1]Technische Universität Ilmenau, Fundamentals of Energy Materials, Ilmenau, Germany — [2]University of Duisburg-Essen, Components for High Frequency Electronics (BHE) and CENIDE, Duisburg, Germany

Precisely engineered heterojunctions are essential for advancing nanoscale systems with superior electrical performance. The structure and electrical behavior of nanostructured devices must be examined with high spatial resolution.

This study investigates the charge carrier transport in freestanding core-shell GaN nanowires (NW) grown via polarity- and site-controlled metal-organic vapor phase epitaxy with a site-dependent AlN interlayer on pre-structured n-type Si(111) substrates. Multi-tip scanning tunnelling microscopy and electron beam-induced current mapping were utilized to probe local transport phenomena with high precision. Transport pathways of charge carriers within the NWs and across key interfaces were resolved. Distinct I-V characteristics appeared for different facets, while scanning transmission electron microscopy revealed no direct shell-core contact. Consequently, current transport is governed by three serially connected diodes: shell-shell, shell-core, and NW-substrate junctions. These results reveal mechanisms shaped by geometry and interfaces, advancing understanding of charge carrier dynamics in III-N nanostructures.

HL 26.6 Wed 9:30 P1

Optical loss characterization in UV multimode AlGaN waveguides with and without a backside absorbing layer — •Leonardo Wildenburg[1], Verena Kowallik[1], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Berlin, Germany — [2]Ferdinand-Braun-Institut (FBH), Berlin, Germany

Photonic integrated circuits (PICs) in the UV range enable complex optical functions on a chip-scale platform, e.g. for the detection of gases and biomolecules by absorption or Raman spectroscopy. The implementation of UV PICs requires wide-bandgap materials to ensure optical transparency. Among the available material systems, one promising candidate is AlGaN due to its application in UV-LEDs and laser diodes. In this work, the optical losses near 265 nm of n-$Al_{0.76}Ga_{0.24}N$ waveguides with a width of 200 μm are investigated using a monolithically integrated UV-LED and UV-photodetector. The influence of straylight from the substrate backside was investigated with and without an absorbing 200 nm thin SiN layer. When operating the LEDs at a constant output power of 0.2 mW, the photocurrent decreases exponentially with increasing waveguide length according to Beer-Lambert-law. The reduction of scattered light was confirmed by measurements of photodetectors of the same wafer, but not connected to the emitting LED by a waveguide. Thus, optical losses of (40 ± 5) cm^{-1} with an absorbing layer and (33 ± 5) cm^{-1} without were measured for the n-$Al_{0.76}Ga_{0.24}N$ waveguides. It was also determined that the optical losses strongly depend on the amount of scattered light from the UV-LED signal.

HL 26.7 Wed 9:30 P1

Optimization of etching processes for quantum well structures to enhance IR emission — •Daniel Janzen[1], Peter Zajac[1], Sascha R. Valentin[2], Arne Ludwig[1], and Andreas D. Wieck[1] — [1]Ruhr-Universität Bochum, Bochum, Germany — [2]Gesellschaft für Gerätebau mbH, Klönnestr. 99, 44143 Dortmund

The precise control of etching processes is crucial for the properties of quantum well structures, especially in terms of IR emitter efficiency. This study examines how different etching techniques affect surface quality, defect formation, and electrical properties of the epitaxially grown GaSb layers. A critical aspect is the formation of oxides and metallic antimony, which can lead to leakage currents and short circuits. Through Atomic Force Microscopy (AFM) the influence of etching parameters are investigated. Reducing defect states and optimizing material passivation could contribute to the long-term improvement of emission efficiency. This research bridges materials science and semiconductor physics by discussing strategies to optimize surface states for IR emitters. The findings are relevant not only for quantum optics but also for sensor applications and industrial semiconductor fabrication.

HL 26.8 Wed 9:30 P1

Hydrogen Annealing of Silicon Micro- and Nanostructures through Rapid Thermal Processing — •Kyra Malcherek, Thomas Grap, and Markus Kaiser — Helmholtz Nano Facility, Forschungszentrum Jülich, Germany

As semiconductor devices continue to scale into the lower nanometer range, achieving smooth surfaces becomes increasingly important for device performance. In particular, silicon nanowires used in Gate-All-Around Metal-Oxide-Semiconductor Field-Effect Transistors (GAA-MOSFETs) require these characteristics to ensure uniform electrostatic control over the channel. Therefore, Hydrogen Annealing of silicon is a promising process to enable shape transformation and surface smoothing.

In this study, we characterized the effects of Hydrogen Annealing. Silicon microstructures showed a significant reduction in surface roughness and rounded corners after the process. In addition, stable crystal facets were formed and identified as (111) and (113) planes. The influence of the relevant process parameters - temperature, annealing time, hydrogen flow and pressure - were investigated. The radius of curvature increases with both temperature and annealing time, whereas hydrogen flow and pressure show no significant influence.

The process was further applied to silicon-on-insulator nanostructures, creating free-floating silicon nanowires after oxide etching. Subsequent hydrogen annealing effectively smoothed and rounded the structures, demonstrating its potential for the fabrication of GAA-MOSFETs.

HL 26.9 Wed 9:30 P1

Processing and Characterization of Mid Infrared Emitters from III-V Epitaxy — •Peter Zajac[1], Sascha R. Valentin[1], Timo A. Kurschat[1], Rainer Krage[1], Arne Ludwig[2], and Andreas D. Wieck[3] — [1]Gesellschaft für Gerätebau mbH, Klönnestr. 99, 44143 Dortmund, Germany — [2]Arbeitsbereich Epitaxie, Experimentalphysik VI, Ruhr-Universität Bochum, 44801 Bochum, Germany — [3]ehem. Lehrstuhl für Angewandte Festköperphysik, Ruhr-Universität Bochum, 44801 Bochum, Germany

A layer structure optimized for mid-infrared emission, containing W-type quantum wells has been realized with III-V epitaxy on GaSb. The processing workflow presented here, from the MBE-grown wafer sample to an emitting device, includes mesa etching, photolithography and electrical contacting. The contribution outlines the challenges faced in progressing towards the first prototype, including the optimization of the wet-etching process with respect to the observed trench formation and surface roughness. The electrical characterization includes contact resistance and I-V measurements. Electroluminescence spectroscopy is performed for optical characterization.

HL 26.10 Wed 9:30 P1

GaAs nanowire networks by electrochemical etching as a universal platform for oxide and nitride architectures — •Eduard Monaico[1], Sebastian Lehmann[2], Elena Monaico[1], Xinzhi Li[2], Veaceslav Ursaki[1], Ion Tiginyanu[1], and Kornelius Nielsch[2] — [1]Technical University of Moldova, Chisinau, Moldova — [2]Leibniz Institute of Solid State and Materials Research, Dresden, Germany

GaAs nanowire networks obtained by electrochemical etching provide a versatile platform for semiconductor-oxide-nitride architectures with controlled geometry and crystallinity. Depending on the orientation of the GaAs substrate ((100), (111)B, (001)), the resulting nanowires can be tilted, vertical, or oriented parallel to the surface. Formed by selective electrochemical dissolution rather than epitaxial growth, they retain the structural quality of the bulk crystal, offering a low-defect scaffold suitable for subsequent transformations.

In this work, we explore their conversion into oxides and nitrides. Thermal treatment in argon with 3% oxygen led to selective formation of Ga2O3 on the nanowires while preserving the GaAs substrate, confirmed by SEM, EDX, XRD, and Raman analysis. Preliminary nitridation tests also show the feasibility of forming GaN-based architectures. These findings highlight the potential of electrochemically derived GaAs nanowire networks as a universal platform for oxide and nitride structures relevant to optoelectronics, photonics, and sensing technologies.

We thank the BMFTR and NARD for the funding of ProMoMo project DEHYCONA.

HL 26.11 Wed 9:30 P1

Influence of AlInP(100) Surface Reconstruction on TiO_2/III–V Interface Chemistry and Band Alignment — Mohammad Amin Zare Pour[1,2], Christian Höhn[3], Negin Mogharehabed[1], Roel van de Krol[3], Thomas Hannappel[2], and •Agnieszka Paszuk[1] — [1]BMFTR Junior Research Group PARASOL, Technische Universität Ilmenau, Germany — [2]Fundamentals of Energy Materials, Technische Universität Ilmenau, Germany — [3]Institute for Solar Fuels, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Germany

TiO_2/III–V heterointerfaces are crucial for photoelectrochemical devices, as their chemistry and band alignment govern photogenerated charge-carrier transfer. The TiO_2/InP(100) heterointerface was recently studied using XPS/UPS and *ab initio* molecular dynamics simulations [Adv. Funct. Mater. 2025, 2506105]. ALD-grown TiO_2 on phosphorus-terminated (P-rich) InP(100) shows strong interface-induced band bending, $InPO_x$ formation related to the P-rich surface, and Cl incorporation from $TiCl_4$, reflecting precursor-dependent chemistry. Here, we relate these findings to AlInP(100) surfaces prepared with either P-rich or indium-rich termination, as well as with a thin oxide layer. By comparing oxide states and valence-band positions with those of InP, we analyze how surface reconstruction governs the formation and energetic alignment of TiO_2/III–V heterointerfaces. These insights highlight how AlInP surface preparation controls the formation and electronic structure of TiO_2/III–V interfaces.

HL 26.12 Wed 9:30 P1

Measuring the Temperature Distribution of GaSb Wafers during MBE Growth — •Timo A. Kurschat[1], Sascha R. Valentin[1], Peter Zajac[1], Rainer Krage[1], Arne Ludwig[2], and Andreas D. Wieck[3] — [1]Gesellschaft für Gerätebau mbH, Klönnestr. 99, 44143 Dortmund — [2]Arbeitsbereich Epitaxie, Experimentalphysik VI, Ruhr-Universität Bochum, 44801 Bochum — [3]ehem. Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44801 Bochum

During epitaxial growth the substrate temperature is one of the essential parameters. To obtain high-resolution temperature maps we use a single-lens reflex (SLR) camera with the infrared filter removed. The sensor is sensitive up to a wavelength of about 1 μm and can therefore be used as a pyrometer. With wafer rotation disabled, temperatures down to T_S = 400 °C can be measured. With rotation and a reduced exposure time of 0.25 s images can still be obtained at the growth temperature of T_S = 680 °C.

To optimize the temperature distribution, so called washers are used during growth that cover parts of the wafer. With the original washers, the center of our quarter 2" wafers is more than 20 K hotter than the corners. Without a washer the profile inverts. Therefore we designed a new washer which greatly improves the homogeneity.

On the other hand an inhomogeneous temperature profile can be used to optimize growth parameters, which we show with photoluminescence measurements of quantum wells and atomic force microscope images.

HL 26.13 Wed 9:30 P1

Impact of Al containing nucleation layers on Si(100)/GaP heterointerface — •Kai Daniel Hanke[1], Angieszka Paszuk[1,2], Peter Kleinschmidt[1], and Thomas Hannappel[1] — [1]Technische Universität Ilmenau, Fundamentals of Energy Materials, Ilmenau, Germany — [2]Technische Universität Ilmenau, BMFTR Junior Research Group PARASOL, Ilmenau, Germany

Monolithically grown III-V-on-silicon (100) tandem solar cells show great promise for applications such as direct solar water splitting. A critical interface in these devices is the Si/GaP heterointerface, at which defects originate and subsequently propagate through the entire III-V epitaxial stack. Minimizing defect formation at this initial interface is therefore essential for achieving high-efficiency water-splitting performance. The use of TMAl during the pulsed nucleation of the GaP layer has previously been shown to lower defect densities, particularly stacking faults, stacking-fault pyramids (SF/SFP), and threading dislocations (TDs). In this study, we investigate the effect of TMAl on the formation of SF/SFP and on the density of TDs. We further analyze how TMAl modifies the interfacial energetic band alignment using X-ray photoelectron spectroscopy, and study its impact on surface anisotropy and interface-related optical transitions by low-temperature reflection anisotropy spectroscopy. Defect densities are quantified by electron channeling contrast imaging, a scanning electron microscopy technique that exploits electron channeling at an acceleration voltage of 30 kV.

HL 26.14 Wed 9:30 P1

Enhanced Field Emission Current Density in Chemically Engineered Multiwall Carbon Nanotube Neodymium Oxide Heterostructures — •Anima Mahajan[1], Menaka Jha[2], and Santanu Ghosh[1] — [1]Department of Physics, Indian Institute of Technology, Hauz Khas, New Delhi -110016, India. — [2]Institute of Nano Science & Technology, Knowledge City, Sector-81, Mohali, Punjab- 160062, India.

The MWCNT, neodymium oxide (Nd*O*), and MWCNT-Nd*O* heterostructure were successfully fabricated through a facile three-step synthesis process: the synthesis of MWCNT rods by the chemical vapor deposition technique, the synthesis of the Nd*O* nanoparticles by using the micellar-assisted solid-state route, and the fabrication of the MWCNT-Nd*O* heterostructure. Moreover, the MWCNT-Nd*O* heterostructure exhibits enhanced field emission properties, with a lower turn-on field of 2.4 V/*m compared to pure MWCNT and Nd*O*, which have turn-on fields of 3.6 and 3.8 V/*m, respectively. The MWCNT*Nd*O* heterostructure exhibits an enhancement in current density of approximately 6365% compared to pure Nd*O* and around 172% relative to pristine MWCNT. The emission current stability at a preset value of 6 V/*m over an 8-hour duration is found to be fairly good, characterized by current fluctuations within * 3% of the average value. The enhanced field emission (FE) performance of the MWCNT-Nd*O* heterostructure is attributed to its high enhancement factor (β) of ~3.3*10*.

HL 26.15 Wed 9:30 P1

Low temperature photoluminescence excitation spectroscopy on thin film zinc phthalocyanine — •Josephine Braun, Sebastian Hammer, and Jens Pflaum — Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

The optical properties of molecular semiconductors are determined by the electronic properties of the molecular constituents and their respective intermolecular (IM) interaction [1]. To disclose the IM interaction, polymorphic materials like Zinc-phthalocyanine (ZnPc) provide perfect prototypical systems [2]. Its luminescence in the α-phase is dominated by excimer emission [3], wheras the β-phase luminescence is governed by a highly temperature sensitive Frenkel exciton emission. While temperature dependent luminescence studies provide insight into the IM interaction potential, the excitation spectrum does the same without being prone to effects of excitonic relaxation. In this contribution we investigate the excitonic system of ZnPc thin films in the α- and β-phase via temperature dependent photoluminescence excitation (PLE) and photoluminescence (PL) spectroscopy between 4 K and 300 K. We show, that while the PL spectra exhibits strong variability with temperature, the PLE spectra show only minor changes. This suggests that rather than a large modulation of the IM interaction with temperature, exitonic relaxation processes are at the heart of ZnPc's pronounced spectral luminescence changes.

[1] Hestand and Spano, *Chem. Rev.* **118** (2018), p. 7069–7163
[2] Hammer et al., *Appl. Phys. Lett.* **115** (2019), p. 263303
[3] Hammer et al., *Mater. Horiz.* **10** (2023), p. 221–234

HL 26.16 Wed 9:30 P1

Host-Emitter Interactions in Single-Gaussian Deep-Blue Europium(II) OLED Emitters — •Mahmoud Soleimani[1,2], Paulius Imbrasas[2], Jan-Michael Mewes[2], Felix Kaden[2], Sebastian Schellhammer[1], Toni Bärschneider[2], Carsten Rothe[2], and Sebastian Reineke[1] — [1]Institute of Applied Physics (IAP), Technische Universität Dresden, Germany — [2]beeOLED GmbH, Dresden, Germany

Lanthanide-based emitters offer a promising approach to stable and efficient deep-blue organic light-emitting diodes (OLEDs). While divalent europium [Eu(II)] and trivalent cerium [Ce(III)] can provide ideal emission colors with near-unity exciton utilization, their integration into thin-film architectures remains insufficiently understood. In particular, the compatibility of lanthanide complexes with organic host materials and possible lanthanide-specific interactions are open questions. To shed light on and gain a deeper understanding of these aspects, we combine photoluminescence spectroscopy and density functional theory to evaluate the behavior of a literature-reported Eu(II) emitter and to introduce two new carborate-based Eu(II) complexes. These novel materials exhibit deep-blue single-Gaussian 4f-5d emission. Our experimental and theoretical analysis provides a framework for understanding electron confinement and shielding in Eu-based emitters, establishing design principles for a new class of stable, efficient deep-blue OLED materials.

HL 26.17 Wed 9:30 P1

Flexible OLED-OPD System in a Rolled Geometry for Angle-Resolved Optical Sensing — •Shujun Pei, Jan Schardt, Markus Köpke, and Martina Gerken — Chair for Integrated Systems and Photonics, Faculty of Engineering, Kiel University, Kiel, Germany

We investigate an integrated sensing platform combining an organic light-emitting diode (OLED) and multiple organic photodetector (OPD) pixels fabricated on a single flexible PET substrate. After fabrication, the substrate is rolled manually such that the OLED and OPDs face each other across the inner circumference of a cylindrical channel. This geometry enables angle-dependent optical paths through fluids flowing inside the tube, providing a basis for reconstructing absorption and scattering profiles relevant for chemical and biomedical sensing.

To independently assess OLED-OPD performance, devices were characterized on separate flat substrates. OPD responsivity was quantified using a calibrated LED solar simulator and direct OLED illumination. Distance-dependent photocurrent measurements reveal the expected decay consistent with Lambertian emission and simple geometric coupling between the OLED and OPD pixels. Numerical modeling, including finite emitter and detector areas as well as realistic alignment offsets, closely reproduces the measured photocurrent trends.

These results demonstrate the feasibility of compact, flexible OLED-OPD assemblies for multi-angle optical sensing and provide a foundation for future device refinement.

HL 26.18 Wed 9:30 P1

Organic Narrowband Near-infrared Photodiodes for Breath Monitoring — •Sudhi Mahadevan[1,2], Siddhartha Saggar[1,2], Rabiul Islam[1,2], and Caroline Murawski[1,2] — [1]Institute of Solid-State Electronics, Technische Universität Dresden, 01062 Dresden, Germany — [2]Kurt Schwabe Institute for Sensor Technologies, Kurt-Schwabe-Straße 4, 04736 Waldheim, Germany

For clinical diagnosis of various diseases, breath analysis has become a powerful non-invasive tool, which demands the development of reliable and efficient sensing technologies. However, conventional respiratory monitors hinder users' mobility, provide discomfort, and affect natural breathing patterns. Recent progress in organic and wearable optoelectronics presents an opportunity to develop thin, flexible, and imperceptible sensors. In this work, we report high-performance near-infrared (NIR) organic photodiodes (OPD), using a PM6:Y6 blend combining a polymer donor with an NIR-absorbing small molecule processed from the green solvent o-xylene. In this simplified device architecture, the hole-blocking functionality is incorporated directly into the active layer, reducing fabrication complexity and enabling cost-effective production. A narrow-band optical response at 800 nm is achieved via an organic photo-filtering layer that allows only long-wavelength photons into the active layer. The optical breath sensor will integrate organic light-emitting diodes (OLEDs) to emit light onto the chest, while an OPD will capture changes in diffusely scattered light from the skin during breathing. This work aims to advance organic electronic devices into the NIR spectrum for non-invasive medical diagnosis applications.

HL 26.19 Wed 9:30 P1

Wavelength-selective, ultraviolet (Mg,Zn)O photodiodes — •Jonas Elz, Holger von Wenckstern, and Marius Grundmann — Leipzig University, Felix Bloch Institute for Solid State Physics, Semiconductor Physics Group, Leipzig, Germany

Ninety-five percent of the UV radiation that reaches the Earth's surface is in the UVA band (315-400 nm). In order to assess the potential harmful effects of UVA radiation on the human epidermis with compact, wearable devices, semiconductor technology can be used. Magnesium zinc oxide is a suitable material for detectors in such devices because it exhibits a bandgap between 3.3 and 4.8 eV.

One photodiode design uses a filter and an active layer with different material compositions to achieve sensitivity in different optical bands [2].

In this study, we use combinatorial pulsed laser deposition to fabricate metal-semiconductor-metal photodiodes that are sensitive to different wavelength ranges. With the same mask system and similar targets as in [3], we achieve multiple compositions of filter and active layers on a single substrate.

[1] von Wenkstern et al. "The (Mg, Zn)O Alloy" in "Handbook of zinc oxide and related materials" pp 257-320
[2] Zhang et al. Appl. Phys. Lett. 108, 243503 (2016)
[3] Thyen et al. J. Vac. Sci. Technol. A 41, 020801 (2023)

HL 26.20 Wed 9:30 P1

Determination of activation energies in vertical co-doped κ-Ga_2O_3 Schottky barrier diodes — •Elise Morawe, Sofie Vogt, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix-Bloch-Institut für Festkörperphysik Halbleiterphysik, Leipzig, Germany

The predicted spontaneous polarization of κ-Ga_2O_3 renders this polymorph of Ga_2O_3 highly interesting for, e.g., high electron mobility transistor devices [1]. As shown by Kneiß et al., vertical Schottky barrier diodes can be realized on pulsed laser deposition (PLD) grown κ-Ga_2O_3 thin films [2]. For that, the addition of tin in the process is mandatory to induce the surfactant-mediated growth of the κ phase [3]. We present κ-Ga_2O_3 thin films grown by PLD on indium tin oxide (ITO) layer on different substrates: c-sapphire and yttria-stabilized zirconia (YSZ). We discuss the influence of co-doping of the κ-Ga_2O_3 thin films with ZrO_2 or SiO_2 in addition to SnO_2 on the performance of Schottky barrier diodes. Furthermore, the activation energies of Sn, Zr and Si in the κ-Ga_2O_3 are determined by thermal admittance spectroscopy.

[1] Juyeong Kim et al, Appl. Phys. Express, 11, 061101 (2018)
[2] M. Kneiß et al, J. Appl. Phys. 130, 084502 (2021)
[3] M. Kneiß et al, APL Mater. 7, 022516 (2019)

HL 26.21 Wed 9:30 P1

How To Tame Your Iodine in Reactive Sputtering and Similar UHV Thin Film Deposition Processes — •Christiane Dethloff, Sebastian Köpp, Sofie Vogt, Lukas Trefflich, Holger von Wenckstern, and Marius Grundmann — Felix-Bloch-Institute for Solid State Physics, Universität Leipzig, Germany

Sputtering in reactive atmospheres involves several challenging conditions, like target poisoning, or a hysteresis of the reactive gas partial pressure, leading to an unstable operation regime [1]. In order to investigate and control these process conditions, and therefore tune the properties of the resulting thin film, a controlled flux of the reactive species is crucial. Commonly, this is achieved by mass flow controllers, when O and N are the reactive gases [2]. However, in the case of an iodine enriched atmosphere this is hardly feasible, due to the corrosive effect and low inlet pressures.

We present an optical measurement setup, enabling real-time measurements of the iodine content in an iodine enriched Ar flow from an iodine vaporizer into a deposition chamber. Our investigations comprise the growth and characterization of functional p-type copper iodide (CuI) thin films by reactive magnetron sputtering under a well defined iodine flux.

[1] D. Güttler *et al.*, Applied Physics Letters 85.25 (2004): 6134 – 6136 DOI:10.1063/1.1835002.
[2] A. Welk, M. Grundmann *et al.*, Physical Review Applied 17.2 (2022): 024007 DOI: 10.1103/PhysRevApplied.17.024007

HL 26.22 Wed 9:30 P1

Investigation of vertical α-Ga_2O_3/$(Al_xGa_{1-x})_2O_3$ diodes grown by pulsed laser deposition — •Veronika Lunova, Sofie Vogt, Paul Bokemeyer, Holger von Wenckstern, and Marius Grundmann — Universität Leipzig, Felix Bloch Institute for Solid State Physics, Semiconductor Physics Group, Leipzig, Germany

With a bandgap of 5.3 eV and a dielectric breakdown field of 10 MV/cm, α-phase gallium oxide is a promising ultra-wide bandgap semiconductor for high-power electronics [1]. Furthermore, alloying with isostructural α-Al_2O_3 is possible without a miscibility gap and allows for even higher band gaps and electrical breakdown fields [2]. In this work, we present a systematic investigation of vertical Schottky diode structures based on α-$(Al_xGa_{1-x})_2O_3$ thin films grown by pulsed laser deposition (PLD). The heterostructures consist of an undoped α-Ga_2O_3 buffer layer, highly doped intermediate layers, and an $(Al_xGa_{1-x})_2O_3$ layer. Achieving sufficient conductivity in $(Al_xGa_{1-x})_2O_3$ remains a major challenge; thus, we investigate donor activation as a function of aluminum content [3]. The structural quality and electrical properties of the resulting heterostructures were investigated, with focus on the influence of Al incorporation on crystal structure, carrier activation, and vertical transport behavior.

[1] Higashiwaki *et al.*, Appl. Phys. Lett. **100**, 013504 (2012).
[2] Hassa *et al.*, J. Phys. D: Appl. Phys. **54** 223001 (2021).
[3] Varley *et al.*, Appl. Phys. Lett. **120**, 262104 (2022).

HL 26.23 Wed 9:30 P1

Titania-based aerodynamic nanomaterials produced by atomic layer deposition — •Tudor Braniste[1], Vladimir Ciobanu[1], Sebastian Lehmann[2], Phil Goldberg[2], Kornelius Nielsch[2], Niklas Wolff[3], Lorenz Kienle[3], Rainer Adelung[3], and Ion Tiginyanu[1] — [1]Technical University of Moldova, Chisinau, Moldova — [2]Leibniz Institute for Solid State and Materials Research, Dresden — [3]Institute for Materials Science, Kiel University, Germany

In this work, we report on a technology for the production of TiO2, Zn2TiO4, and Mg2TiO4 aero-nanomaterials. Titanium and magnesium oxides were deposited using atomic layer deposition (ALD) onto a sacrificial network of ZnO microtetrapods. After deposition, the sacrificial ZnO layer was removed using two different technological routes. The first route involves removing the zinc oxide in a citric acid solution at room temperature, followed by critical-point drying of the titania-based material. The second route consists of removing the ZnO substrate in a hydrogen atmosphere at high temperature. At temperatures as high as 850 °C in an atmosphere of H2 + Ar (2% + 98%), the ZnO core decomposes, and the resulting aero-nanomaterial consists of hollow microtetrapods with porous microtubular arms composed of Zn2TiO4 or (ZnMg)TiO2. Scanning and transmission electron microscopy, as well as X-ray analysis, were used to elucidate the morphology, composition, and crystal structure of the produced aeromaterials. The investigations revealed the influence of annealing temperature and the sequence of technological steps on the morphology and properties of the resulting materials.

HL 26.24 Wed 9:30 P1

Band-Gap Trends in Halide Double Perovskites from Quasiparticle Self-Consistent GW — •Louis Meier[1], Timur Biktagirov[1], Volodymyr Vasylkovskyi[2], Anastasiia Kultaeva[2], and Wolf Gero Schmidt[1] — [1]Physics Department, Paderborn University, 33098 Paderborn, Germany — [2]Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

Halide double perovskites represent a chemically versatile class of optoelectronic materials with tunable band gaps dependent on their cation and halide composition. Their diversity requires a first-principles framework that can predict these trends consistently. Semilocal density functional theory (DFT) underestimates band gaps, while many-body GW results depend sensitively on the DFT starting point. In this contribution, we assess the quasiparticle self-consistent GW (QSGW) method as a unified, starting-point-independent approach for predicting the electronic structure of the $Cs_2MM'X_6$ family (M = Bi, Tl; M' = Ag, Cu; X = Cl, Br), focusing on trends with composition and spin-orbit coupling.

HL 26.25 Wed 9:30 P1

Atomistic Modeling of A- and X-Site Mixing in Halide Perovskites using Cluster Expansion — •Hilde Bellersen[1], Ana M. Valencia[2], and Caterina Cocchi[1] — [1]Friedrich-Schiller-Universität Jena, Germany — [2]Carl von Ossietzky Universität Oldenburg, Germany

Designing stable and efficient halide perovskites involves navigating a vast space of possible chemical substitutions. To address this challenge, we combine density-functional theory calculations with a machine-learning-based cluster expansion framework [1] to efficiently explore multi-component perovskite alloys. Our training structures systematically sample A-site mixing (FA, MA, Cs), X-site mixing (I, Br, Cl), as well as simultaneous A- and X-site co-mixing, with the lattice parameters adjusted according to Vegard's law. These configurations provide the basis for constructing cluster expansion models capable of capturing key energetic trends across the full compositional space. Such models can be used to identify stability landscapes and quantify the influence of configurational effects. We present the methodology, dataset construction, and first insights from the ongoing model development, highlighting the importance appropriate settings to ensure model accuracy, as well as the potential of this approach to guide the design of complex halide perovskite alloys.

[1] M. Ångqvist et al., Advcd Theory and Sims 2, (2019).

HL 26.26 Wed 9:30 P1

Cavity-enhanced microscopy: absorption measurements of single perovskite nanocubes and photo-switchable lipids — •Ayesha Khan[1], Ines Amersdorffer[1,2], David Hunger[3], and Thomas Hümmer[1,2] — [1]Qlibri GmbH, Munich, Germany — [2]Ludwig Maximilian University of Munich, Munich, Germany — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany

Optical studies of nano-scale systems through spectroscopy and imaging can reveal intrinsic optical properties of materials including resolving the exitonic fine structure of systems. However, due to diminutive absorption of nano-scale systems, it is challenging to perform absorption spectroscopy.

For a nano-scale system placed inside an optical resonator, the light passes through the sample thousands of times, enhancing the absorption and thus, allowing measurements.

Here we demonstrate the use of a fiber-based, open-access microcavity to perform direct measurements of the absorption of single perovskite nanocubes. We further image and obtain hyperspectral maps of perovskite nanocubes.

We also present the use of the cavity microscope to image label-free Azo-PC phospholipid bilayers in both cis and trans state and show the diffusion of the two states.

The successful measurements of different nano-scale systems promise that fiber-based microcavities can become standard tools for absorption measurements of these systems.

HL 26.27 Wed 9:30 P1

Excitonic Reststrahlen Effect in $(PEA)_2PbI_4$ — •Michael Pfeufer, Patrick Grenzer, Friedrich Schöppler, and Tobias Hertel — Institute of Physical and Theoretical Chemistry, Julius-Maximilains-University Würzburg, Germany

Layered Ruddlesden-Popper perovskites with their natural quantum well structure allow for strongly confined excitons with very high oscillator strengths. In this work, evidence of an excitonic Reststrahlen effect, a phenomenon in which strong exciton resonances push the real permittivity below zero, was identified and characterized in phenethylammonium lead iodide $(PEA)_2PbI_4$. Transfer-matrix method simulations of the thin film were employed to fit temperature-dependent transmission measurements to an isotropic Lorentz oscillator model and to extract the dielectric function of the material. Additionally, we show that the behaviour of the Reststrahlen band in thickness-dependent transmission spectra is consistent with that found in other materials featuring a Reststrahlen-like response. Electric field calculations inside the material slab suggest natural exciton-polaritonic formation in the material, as well as longitudinal modes near the zero crossing of the real permittivity.

HL 26.28 Wed 9:30 P1

Optical Composition-Property Relationships in a Lead-Free Isostructural 2D Hybrid Metal-Halide Series — •Nils Kasten[1], Jan-H. Littmann[1], Meng Yang[2], Natalie Dehnhardt-Fehst[2], Lukas Gümbel[1], Ralph Kusche[2,3], Markus Stein[1], Johanna Heine[2,3], and Sangam Chatterjee[1] — [1]Institute of Experimental Physics I and Center for Materials Research (ZfM), Justus Liebig University Giessen, Heinrich-Buff-Ring 16, 35392 Giessen, Germany. — [2]Department of Chemistry and Material Sciences Center, Philipps-Universität Marburg, Hans-Meerwein-Straße, 35043 Marburg, Germany. — [3]Insitute of Chemistry, Carl von Ossietzky Universität Oldenburg, Ammerländer Heerstraße 114-118, 26129 Oldenburg, Germany.

Organic–inorganic metal halides have achieved notable success in photovoltaics. Among these, metal-halide perovskites represent a versatile class of compounds, exhibiting diverse optoelectronic behaviour, ranging from narrow-band emission to broadband white-light photoluminescence (PL), typically arising from self-trapped excitons (STEs). These characteristics render them relevant for optoelectronic applications. In this study, we investigate a lead-free isostructural series of two-dimensional hybrid metal halides, $[(R)\text{-1-(4-F)PEA}]_4[E_2X_{10}]$; (R)-1-(4-F)PEA = (R)-1-(4-fluoro) phenylethylammonium, where E = Sb, Bi and X = Cl, Br, I. All compounds share a common structural framework, which allows us to isolate the effects of metal-cation and halide-anion substitution on the optical response. We employ PL and Raman spectroscopy to characterize these compounds.

HL 26.29 Wed 9:30 P1

Stokes, Anti-Stokes and selective excitation of Si-vacancies in SiC — •Emilian Eisermann, Vladimir Dyakonov, and Andreas Sperlich — Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

Our group has demonstrated a room temperature continuous-wave maser that uses the silicon vacancy (V2) in silicon carbide (4H-SiC) (arXiv:2312.08251). Stimulated emission arises from an optically pumped population inversion in these spin defects. However, only a low output power could be achieved and laser heating caused instabilities. To enhance the maser characteristics, we investigate the fundamental pumping behavior of V2 (zero phonon line at 916.2 nm). Hereby, we distinguish between common Stokes excitation (CSE) (<916.2 nm), Anti-Stokes excitation (ASE) (>916.2 nm) and selective excitation (=916.2 nm). Using electron paramagnetic resonance spectroscopy, we resolve microwave absorption and emission signals due to the optical polarization of Zeeman split states. By analyzing these features, we calculate the population inversion and hence the pump efficiency. At low temperatures selective excitation is particular efficient and CSE outcompetes ASE, which requires thermally driven phonons. At room temperature, the increased phonon activity and the shortened T_1 lifetime cause ASE (λ=950 nm) to have an efficiency of around 50 % compared to CSE. ASE however allows for a very targeted excitation of V2 and we identify an optical pumping sweet spot that is promising for future maser implementations.

HL 26.30 Wed 9:30 P1

Double Gaussian Defect Cavity Design for Semiconductor Based Entangled Photon Sources — •Xian Zheng, Fei Ding, and MIchael Zopf — Institute of Solid State Physics, Leibniz University of Hannover, Appelstr. 2, 30167 Hannover, Germany

Polarization-entangled photon pairs are essential resources for quantum communication and quantum networks, enabling protocols such as quantum key distribution, teleportation, and entanglement swapping. However, simultaneously controlling cavity spectrum, field profile, and balanced coupling to multiple radiative transitions in a solid-state emitter remains challenging. In this work, we design a double-Gaussian defect cavity as a flexible platform to engineer semiconductor quantum-dot entangled photon sources. Two Gaussian-shaped, microsphere-like thickness modulations are embedded inside a DBR cavity and sculpt the axial and lateral field distributions, providing independent knobs, such as cavity height and defect width, to simultaneously tune the cavity resonance close to emission lines, such as biexciton and exciton emission and optimize the emission wavelength. Using FDTD simulations and time-domain exponential decay fitting, we extract the quality factor, mode volume, and Purcell enhancement, and quantify their dependence on the geometric parameters. The resulting design framework provides practical guidelines for tailoring cavity*quantum-dot coupling in double-Gaussian defect geometries and supports the development of bright, on-demand entangled photon sources suitable for future integrated quantum-network architectures.

HL 26.31 Wed 9:30 P1

Low-density InAs quantum dots for telecom O-band single-photon emission — •Elias Kersting, Nikolai Spitzer, Hans Georg Babin, Severin Krüger, Phil Julien Badura, and Arne Ludwig — Ruhr-Universität Bochum, EP6 , Bochum, Germany

InAs quantum dots (QDs) grown by molecular beam epitaxy (MBE) are promising candidates for single-photon sources (SPS), particularly for quantum communication. Emission in the telecom O-band (1260 - 1360 nm) is especially desirable due to the low transmission loss in optical fibers. However, conventional Stranski-Krastanov (SK) InAs QDs face challenges in achieving low and well-controlled densities in the range of 0.1- 10 QDs/um^2, as well as in precisely tuning the emission wavelength. We present an alternative approach to address this issue based on local droplet etching (LDE), in which nanoholes in a GaAs matrix are filled with InAs to form QDs. The quantum dot density is defined by the nanohole pattern, enabling precise and scalable control. A strain-reducing layer (SRL) shifts the emission wavelength into the telecom O-band. Homogeneous low-density (~2 QDs/um^2) growth is achieved through shutter-synchronized deposition, making this approach well suited for scalable SPS fabrication. We detail the fabrication method and present structural and optical characterization results.

HL 26.32 Wed 9:30 P1

Effect of TiO_2 thin films on shallow NV centers in co-doped diamond. — •Arthur Witte, Dominic Reinhardt, Peter Schlupp, Holger von Wenckstern, Jan Meijer, and Marius Grundmann — Universität Leipzig, Felix-Bloch Institute for Solid State Physics, Germany

The nitrogen vacancy (NV) center is a color center in diamond, that was proposed as a platform for solid state quantum computing. Essential for this idea is the spin-dependent photoluminescence of the negatively charged NV center, through which an optical spin polarization can be achieved and its relatively long spin coherence time at room temperature. Much research has been done in this direction: to engineer the required negative charge of the NV centers, co-doping of the diamond with donors was developed [1]. Shallow NV centers are subject to surface effects that cause charge instabilities, as well as magnetic and electronic noise. Various surface treatments have been explored to mitigate these effects, including the deposition of a passivation layer on the diamond surface. We combine surface engineering and charge engineering by co-doping and study the effects of these methods on the charge state and T_2 time of shallow NV centers. This is done by sputtering transparent titanium dioxide layers of varying thickness onto a diamond with shallow NV centers in differently co-doped environments. Additionally, effects of annealing of the layer on both the layer itself and the NV properties are discussed.

[1] T. Lühmann, et al. *Phys. Status Solidi a* **8**(1), 1671-1703. (2021)

HL 26.33 Wed 9:30 P1

High-Resolution Lift-Off Process for Sub-100-nm Metal Features using a PMMA Bilayer Stack — •Melina Sporkett[1], Lina Trippelsdorf[1,2], Thomas Grap[1], Florian Lentz[1], and Markus Kaiser[1] — [1]Helmholtz Nano Facility, Forschungszentrum Jülich, Germany — [2]Peter Grünberg Institute, Forschungszentrum Jülich, Germany

A reliable and reproducible lift-off process is essential for the fabrication of high-resolution metal structures in micro- and nanotechnology. This has become increasingly important due to recent advances in quantum computing. In quantum devices, these nanoscale electrodes and interconnects are needed to realize the electrical connections to qubits.

In this study, we present a PMMA bilayer lift-off process that enables the reliable fabrication of structures below 100 nm, including fine lines and spaces. The resist stack consists of a copolymer bottom layer that creates a defined undercut and a thin PMMA/CSAR top layer. Through specifically optimized electron-beam lithography and development using a methoxypropanol-based developer, a clearly defined resist profile was achieved. Subsequent metal deposition using Ti/Au electron beam evaporation enabled the fabrication of lines with a width of only 30 nm.

These results demonstrate a robust and practical process for fabricating ultra-fine metallic interconnects for nanoelectronic applications.

HL 26.34 Wed 9:30 P1

Diamond devices for high contrast electrical readout of NV centers — •Melina F. V. Pees[1], Lina M. Todenhagen[1], Joachim P. Leibold[2], Dominik B. Bucher[2], and Martin S. Brandt[1] — [1]Walter Schottky Institut, TU Munich, Am Coulombwall 4, 85748 Garching — [2]Department of Chemistry, TU Munich, Lichtenbergstr. 4, 85748 Garching

Nitrogen-vacancy (NV^-) centers in diamond enable optically and electrically detected magnetic resonance (ODMR and EDMR/PDMR, respectively) and are a promising semiconductor platform for spin-based sensing. Metal contacts often influence the NV^- charge state, change current flow near the surface and worsen the spin contrast in resonance measurements. In this work we investigate shallow, implanted NV ensembles under Ti/Pt/Au contacts using combined photoluminescence, photocurrent and ODMR/EDMR measurements as a function of applied bias voltage, nitrogen implantation depth and position relative to the metallized surface. We have recently shown that Pt, just as other metals, strongly influences the charge state of the NV centers underneath the contacts, leading to mostly neutral or positively charged centers. Here, we show that via application of bias voltages, the negative charge state can be partially recovered, leading to an increase in the spin contrast. This approach allows to stabilize the NV^- charge state and improves the suitability of such diamond devices for quantum sensing applications.

HL 26.35 Wed 9:30 P1

Fabrication of SNSPDs on TF-LNoI for measurement device independent QKD — •Simon Palitza[1,2,3], Bilal Malik[1,2,3], and Carsten Schuck[1,2,3] — [1]Department for Quantum Technology, University of Münster — [2]Center for NanoTechnology - CeNTech, Münster — [3]Center for Soft Nanoscience - SoN, Münster

Thin-Film Lithium Niobate on Insulator (TF-LNoI) has been recognized as a promising platform for realizing low-loss propagation and high-speed modulation of optical signals in photonic integrated circuits. However, quantum technology applications, such as quantum key distribution (QKD) also require integrating single photon detection capabilities with nanophotonic functionalities. Here we show how crucial optical circuit components of a QKD-receiver can be co-integrated with Nb-based Superconducting Nanowire Single Photon Detectors (SNSPDs) on the TF-LNoI-platform. We specifically assess the influence of ubiquitous lithium diffusion on SNSPD performance and explore mitigation strategies in the design and nanofabrication process flow, such as introducing diffusion barrier layers. Combining efficient measurement capabilities with the stability and low loss routing of optical signals in monolithic LNoI-circuits provides a viable way towards realizing quantum communication protocols, such as measurement device independent QKD.

HL 26.36 Wed 9:30 P1

Role of a Quarter-Wave Plate in Resonant Laser Spectroscopy: Signature of Spin-Orbit Interactions of Light — •Wenze Lan, Anton Lögl, and Bernhard Urbaszek — Institute for Condensed Matter Physics, Technische Universität Darmstadt, 64289 Darmstadt, Germany

Resonant laser spectroscopy is a powerful technique for probing the intrinsic optical transitions, coherence properties, and spin dynamics of single quantum emitters. Although polarization-based dark-field confocal microscopy enables nearly background-free detection of resonant fluorescence [1], the role of an additional quarter-wave plate in further improving extinction has remained unclear. Here, we elucidate the mechanism by which a commercial quarter-wave plate enhances polarization extinction in a simple confocal geometry. Under cross-polarization conditions, the transmitted beam exhibits a robust first-order Hermite-Gaussian mode, which explains the improved background suppression and we identify it as a direct signature of spin-orbit interactions of light [2-3]. Our findings inspire applications in polarization optics, nanophotonics, and quantum photonics. [1] Rev. Sci. Instrum. 84, 073905 (2013); [2] J. Opt. 15, 014001 (2013); [3] Nat. Photon. 9, 796-808 (2015).

HL 26.37 Wed 9:30 P1

Phonon-Polaritons in MOVPE-grown hexagonal Boron Nitride — •Oskar Schröer[1], Maximilian Scharpey[1], Lena Miler[2], Johannes Binder[2], Andrzej Wysmołek[2], Daniel Wigger[3], and Iris Niehues[1] — [1]Institute of Physics, University of Münster, Germany — [2]Faculty of Physics, University of Warsaw, Poland — [3]Department of Physics, University of Münster, Germany

Two-dimensional materials composed of atomically thin layers have attracted great interest due to their unique optical and electronic properties. Using a scattering-type scanning near-field optical microscope (s-SNOM), surface phonon polaritons (SPhPs) are observable in the insulating polar van-der-Waals material hexagonal boron nitride (hBN) [1]. While most works focus on exfoliated single-crystalline layers of hBN, we show that SPhPs can also be excited in hBN grown by metalorganic vapor phase epitaxy (MOVPE). Here, grain boundaries and defects play a major role for the propagation properties of the polaritons. By evaluating the real-space interference patterns, we extract dispersion relations and compare propagation characteristics for the two sample types. The results contribute to a deeper understanding of light-matter interactions in polar van der Waals materials and may pave the way towards improved control and manipulation of light-matter excitations on the nanometer scale.

[1] Caldwell et al., Nat. Commun. **5**, 5221 (2014).

HL 26.38 Wed 9:30 P1

Predicting nonlinear optical properties from the linear response: Generalized Miller Formulae — •Maximilian Tim Meyer and Arno Schindlmayr — Universität Paderborn, Department Physik, 33095 Paderborn, Germany

Predicting the nonlinear optical response of real materials from first principles remains a major challenge, since quantitative calculations require strong simplifications and large computational resources. As a shortcut, Miller's rule provides an empirical relation between the linear and second-harmonic coefficients. It can be extended to higher-order nonlinearities and is now accepted as a useful tool for guiding experiments and computational materials discovery. However, its theoretical foundation had long been limited to a simple derivation for the classical Lorentz model with a weak anharmonic perturbation, whose properties differ from those of real quantum-mechanical electrons. We have developed a mathematical framework which enabled us to prove that Miller's rule is nevertheless equally valid for weakly anharmonic quantum-mechanical oscillators [1]. For three-dimensional anharmonic oscillators, we further derived generalized Miller formulae that express all orders of the nonlinear response to an arbitrary multi-frequency field exactly in terms of the linear optical susceptibility [2]. These generalized formulae are applicable to a much broader range of nonlinear optical processes and systems. The practical implementation is illustrated by means of a numerical example. [1] Meyer and Schindlmayr, J. Phys. B **57**, 095001 (2024). [2] Meyer and Schindlmayr, Dynamics **5**, 34 (2025).

HL 26.39 Wed 9:30 P1

Revisiting Cross-Polarized Resonant Excitation: Spin-Orbit Interaction in Confocal Dark-Field Microscopy — •Anton Lögl, Wenze Lan, and Bernhard Urbaszek — Institute for Condensed Matter Physics, Technische Universität Darmstadt, 64289 Darmstadt, Germany

Resonant excitation is a key experiment for accessing and probing the optical properties of semiconductor quantum emitters. The typical epifluorescence geometry of the cryostat environment presents an experimental challenge: separating the much weaker emission of the sample from the much stronger excitation, typically addressed using a cross-polarization scheme [1]. It is well known that confocal microscopy in combination with a dark-field technique can surpass the intrinsic extinction limit of commercial polarizers [1, 2]. In this work, we investigate the spin-orbit interaction of light observed when a polarized Gaussian beam is reflected from a mirror surface within such a microscope arrangement. We revisit the model from [2] and demonstrate that slight modifications allow us to phenomenologically model all of our results within the linear and circular polarization basis. Our results pave the way for improved characterization and optimization of optical setups used to measure the optical properties of various quantum emitters. Simultaneously, our results highlight how poorly understood the physical principles of one of the most common characterization techniques in resonant spectroscopy are.

[1] A. V. Kuhlmann, et al. Rev. Sci. Instrum. 84, 073905 (2013)
[2] Benelajla, M. et al. Phys. Rev. X 11, 021007 (2021)

HL 26.40 Wed 9:30 P1

Optical properties of $(Ti_xGa_{1-x})_2O_3$ — •Leonard Käferstein, Clemens Petersen, Daniel Splith, Holger von Wenckstern, Chris Sturm, and Marius Grundmann — Felix Bloch Institute for Solid State Physics, Leipzig University, Leipzig, Germany

The high bandgap energy in the order of 5.3 eV and its high predicted electrical breakdown field of about 10 MV cm^{-1} make α-Ga_2O_3 a quite promising material for transparent electronic devices and high power applications [1]. Alloying αGa_2O_3 with Ti leads to a decrease of the band gap. Here we report on the optical properties, especially the dielectric function, of $(Ti_xGa_{1-x})_2O_3$ determined by spectroscopic ellipsometry as a function of the cation composition.

A $(Ti_xGa_{1-x})_2O_3$ thin film with a lateral composition gradient was deposited by combinatorial pulsed laser deposition [2]. X-ray diffraction indicates a transformation from the tetragonal rutile phase for large Ti concentration ($x > 0.55$) toward a rhombohedral phase for $x < 0.4$. As $(Ti_xGa_{1-x})_2O_3$ is optically uniaxial and the optic axis is within the surface plane, generalized spectroscopic ellipsometry was applied. In the transparent spectral range, we determined a decrease from positive birefringence for high x towards negative birefringence for $x \approx 0$. As expected, we observe a redshift of the bandgap energy with increasing Ti-content from 5.1 eV for $x \approx 0$ down to 4.3 eV for $x \approx 0.85$.

[1] M. Higashiwaki *et al.*, Appl. Phys. Lett. **100**, 013504 (2012).
[2] H. v. Wenckstern *et al.*, Ph. Status Solidi B **257**, 1900626 (2020).

HL 26.41 Wed 9:30 P1

***In situ* investigation of PEC devices by time-resolved photoluminescence** — •Peter Kleinschmidt, Ali Omar, Sahar Shekarabi, David Ostheimer, and Thomas Hannappel — TU Ilmenau, Institute of Physics, Fundamentals of Energy Materials, 98693 Ilmenau

Direct, unassisted photoelectrochemical (PEC) water splitting is a promising approach for the generation of solar hydrogen. At present, PEC devices still suffer from rapid degradation during operation in the electrolyte. In PEC devices, the control of the dynamics of minority charge carriers is crucial for efficient operation. *In situ* time-resolved photoluminescence (TRPL) measurement provides a direct access to charge carrier lifetimes in the PEC environment. We demonstrate that *in situ* TRPL reveals early-stage, localized degradation in PEC devices under operating conditions long before any decline in conventional performance metrics, such as a reduction in hydrogen evolution current density, becomes detectable. With this method, we investigate the effect of different surface treatments of dual junction PEC devices, in particular the functionalization with passivation layers and catalysts, on the stability and overall performance.

HL 26.42 Wed 9:30 P1

Propagation of Bloch surface polaritons in ZnO — Sebastian Henn, •Dmitry Sayenko, Marius Grundmann, and Chris Sturm — Felix Bloch Institute for Solid State Physics, Leipzig University, Leipzig, Germany

Here we present the long-range propagation of Bloch surface polaritons (BSP) in ZnO, which are formed through the strong interaction between light and excitons. Of special interest are BSP particles as they are bosonic quasi-particles and inherit the long-range propagating properties of the involved photons. In contrast to typically used microcavities, BSPs are formed at the surface of a photonic crystal, and thus the fabrication of these structures requires less technical effort and the properties of the BSP are surface-sensitive. In our studies, we realized BSPs in a photonic crystal made of distributed Bragg reflector made of yttria-stabilized zirconia (YSZ) and Al_2O_3. As an active medium, we used a ZnO surface layer, allowing strong coupling up to 430 K [1]. For the coupling of the BSPs to the vacuum modes, a 1D grating was etched onto the surface. By employing non-resonant excitation and varying the distance of the excitation with respect to the grating, the propagation length of BSPs was determined. We found that the propagation length of the BSP is about five times larger than would be expected for a pure photonic mode traveling through the ZnO layer [2]. We attribute this enhancement of the propagation lenght to the extended field distribution within the structure.

[1] S. Henn *et al.*, New J. Phys. **23**, 093031 (2021).
[2] S. Henn *et al.*, Appl. Phys. Lett. **125**, 211104 (2024).

HL 26.43 Wed 9:30 P1

Comparative *ab initio* characterization of $LiNbO_3$, Li_3NbO_4 and $LiNb_3O_8$ — •Frederik Schmidt and Arno Schindlmayr — Universität Paderborn, Department Physik, 33095 Paderborn, Germany

Ferroelectric lithium niobate ($LiNbO_3$) is an important material for nonlinear optical technologies. It is part of the Li_2O–Nb_2O_5 system, whose two components can not only form $LiNbO_3$ but also other phases with different Li:Nb ratios, such as Li_3NbO_4 or $LiNb_3O_8$. Both are studied as possible materials for lithium-ion batteries on their own, but they may also occur as unwanted secondary phases during the growth of lithium niobate crystals when pure $LiNbO_3$ is preferred. As a consequence, it is important to detect and identify the different phases. In this work, we employ *ab initio* methods including density-functional theory, the *GW* approximation and the Bethe-Salpeter equation in order to characterize the three compounds with identical computational techniques and convergence parameters. In particular, we compare the density of states, electronic band structure and optical absorption spectrum of Li_3NbO_4 and $LiNb_3O_8$ to $LiNbO_3$. Despite qualitative similarities, our results reveal quantitative differences in the electronic and optical properties that should be clearly measurable in experiments. Compared to $LiNbO_3$, the electronic band gap of Li_3NbO_4 is 1.0 eV larger and that of $LiNb_3O_8$ is 0.4 eV smaller. The optical absorption edges also vary correspondingly.

HL 26.44 Wed 9:30 P1

Improving the optical readout of NV-centers in diamond by oxide surface coating — •Klemens Wurl, Michael Bar, Holger von Wenchstern, and Marius Grundmann — Universität Leipzig, Felix-Bloch Institute, Germany

Successful quantum computing has many advantages compared to regular computing, especially in simulations. It is proposed that nitrogen-vacancy (NV) centers in diamond could be used as qubits at room temperature, which would make everyday applications of quantum computing easier compared to solutions that rely on superconductivity.[1] The quantum states of the NV-centers can be controlled by optical excitation via laser and spin-state manipulation by microwave radiation.[2] The main objective of this research is to improve the optical readout of the NV-center by the use of solid immersion lenses (SIL). For this purpose, transition metal oxides are used, which are optically transparent and do not exhibit photoluminescence for the given wavelength. PLD is used for the surface coating, but the optical properties are limited by particle density. Therefore, peripheral target ablation was used to decrease the particle density as it allows for higher control of the plasma plume deflection. The influence of O_2 partial pressure and fluence will be investigated in order to record the corresponding growth window for decreased particle expulsion as well as increased optical transparency and refractive index.

[1] S.Pezzagna *et al.*, Appl. Phys. Rev. **8**(1), 011308, (2021).
[2] F. Jelezko *et al.*, Phys. Stat. Sol.(a) , **203**(13), 3207-3225, (2006).

HL 26.45 Wed 9:30 P1

Two-color sensitive II-VI wide-bandgap diodes with PbTe quantum dots for visible and infrared detection and emission — •Jakub Gluch[1], Sergij Chusnutdinow[1], Michal Szot[1,2], Piotr Wojnar[1], and Grzegorz Karczewski[1] — [1]Institute of Physics, Polish Academy of Sciences, 02-668 Warsaw, Poland — [2]International Research Center MagTop, 02-668 Warszawa, Poland

We present the results of research on p-n diode working as two-color photodetector, made from combined narrow- and wide-bandgap semiconductors. With the use of molecular beam epitaxy (MBE) we managed to create diode structures (p-ZnTe/(Active Layers - AL)/n-CdTe) with lead telluride (PbTe, 0.32 eV in 300K) quantum dots embedded in cadmium telluride matrix (CdTe, 1.49 eV in 300K). To create quantum dots we first grown 20 alternating layers of PbTe and CdTe on top of p-type layer, which followed by thermal annealing which break down PbTe layers in to dots. We performed current-voltage measurements for the basic characteristics followed by an optical measurements to obtain diode spectral response curves with respect to different temperatures in the visible and infrared ranges (350 - 3500nm in 300K). In photoluminescence measurement we observe emission from PbTe quantum dots. We confirmed junction formation in the diode by electron beam induced current (EBIC) measurements. On cross sections of this structures, we observed formation of double p-n junction at the interface of p-type layer and AL, and AL and n-type layer. Measurements show promising possibilities for creating infrared LED and at the same time photodetector with wide spectrum of detectivity.

HL 26.46 Wed 9:30 P1

Microscopic reverse-bias electroluminescence spectra and spectral images of 850 nm oxide-confined VCSELs during burn-in — •Arndt Jaeger[1], Nikolay Ledentsov Jr.[2], Sebastian Haberkern[1], Helmut Meinert[1], Alexander Moll[1], Dominik Ölke[1], Ilya E. Titkov[2], Oleg Yu. Makarov[2], and Nikolay Ledentsov[2] — [1]Esslingen University of Applied Sciences, Flandernstrasse 101, 73732 Esslingen, Germany — [2]VI Systems GmbH, Hardenbergstrasse 7, 10623 Berlin, Germany

850 nm vertical-cavity surface-emitting lasers (VCSELs) are studied during high-current burn-in operation utilizing both reverse-bias electroluminescence (ReBEL) spectra and spectral images. High-resolution spectral images are generated by means of a confocal scanning optical microscope using interference filters whereas microscopic spectra are obtained with a fiber-coupled sensitive USB spectrometer. Recently unfiltered ReBEL images have proven to be sensitive to operation-induced changes of VCSELs because defect states evolved during high-current stress trigger avalanche breakdown and give rise to ReBEL emission. In particular, local current crowding during high current burn-in leads to spatial distributions of ReBEL emission being characteristic to the aging status and contain spectral portions due to quantum well as well as AlGaAs barrier emissions. In contrast, electroluminescence spectra measured under near flat-band conditions exhibit only quantum well emission at 848 nm.

HL 26.47 Wed 9:30 P1

Optical Properties of a Transition-metal Dichalcogenide - ZnO Nanowire Field-effect Transistor — •Yashvi Bulsara[1], Maximilian Tomoscheit[1], Omid Ghaebi[1], Edwin Eobaldt[1], Carsten Ronning[1], and Giancarlo Soavi[1,2] — [1]Institute of Solid State Physics, University of Jena — [2]Abbe Center of Photonics, University of Jena

Transition-metal dichalcogenide (TMD) monolayers combined with zinc-oxide (ZnO) nanowires (NW) represent a promising platform for electrically tunable nanophotonic devices. ZnO NWs are naturally nanoscale lasers, supporting waveguiding, field amplification and being the gain medium at the same time. A further major step towards the success and broad applicability of NW lasers is the possibility to actively tune their laser properties via external stimuli, such as the piezo-electric effect[2]. Recently, we have demonstrated that coupling of ZnO NWs to monolayer TMDs leads to an increase of the lasing intensity threshold[3]. Building on this approach. in this poster I will propose a device where the laser emission of a ZnO NW can be electrically tuned by coupling it to a TMD based field-effect transistor. Besides the main idea and device architecture, I will present preliminary results of device fabrication and characterization. [1] M. Zapf, Nano Lett., 2017, 17 (11), 6637-6643 [2] E. Eobaldt, Nanoscale, 2022,14, 6822-6829.

HL 26.48 Wed 9:30 P1

PT-Symmetry in Excitonic Spectra of TMDC Monolayers under Influence of Magnetic Fields — •Michiel Snoeken, Andreas Knorr, and Henry Mittenzwey — Nichtlineare Optik und Quantenelektronik, Institut für Physik und Astronomie (IFPA), Technische Universität Berlin, D-10623 Berlin, Germany

Excitons in TMDC monolayers under the influence of an in-plane magnetic field are theoretically studied. We demonstrate that in-plane magnetic fields induce a hybridization between spin-bright and spin-dark exciton transitions, resulting in

a brightening of spin-dark excitons in optical experiments. We provide a thorough analytical characterization of the spectrum and demonstrate that, upon including dissipation, such a system can be interpreted as a gain-loss system as described in PT-symmetric quantum mechanics.

HL 26.49 Wed 9:30 P1

Calculation of thermodynamic potentials and heat capacities of ScN , YN and Au_2InYb — •Clemens Vogel and Jens Kortus — TU Bergakademie Freiberg, Institut für Theoretische Physik

ScN and YN can be incorporated in AlN to improve piezoelectric pro-perties and electromechanical coupling. The Heusler phase Au_2InYb is of interest due to its potential for thermoelectric properties. In this work we computed the thermodynamic potentials, the entropy, the specific heat capacities C_p and C_V, and the thermal expansion coefficient. The calculations were performed using DFT/DFPT in Quantum ESPRESSO (PBE-XC) using the quasi-harmonic approximation for phonons. C_p and C_V were determined over the range of 3-600 K, as well as entropy and thermal expansion coefficient; C_p exceeds the Dulong-Petit limit. For Au_2InYb, the projected density of states was also calculated, which reveals a strong $4f$ density of states near the Fermi level and indicating valence fluctuation (in agreement with experimental findings); the calculated heat capacities agree very well with the experimental measurements.

HL 26.50 Wed 9:30 P1

Super-Resolution Terahertz Spectroscopy via Near-Field Electro-Optic Sampling — •Kevin Berwagner, Moritz Heindl, Fabian Brütting, and Georg Herink — Universität Bayreuth

Electro-optic sampling of THz radiation transmitted through a specimen provides a non-invasive way to analyze materials, however, the spatial resolution is typically constrained by the diffraction limit of the THz beam to a few hundred microns.

In this contribution, we will present our progress in developing a novel method for sampling pulsed terahertz fields with potentially sub-micron spatial resolution. Specifically, the approach is based on local imaging of THz nearfields via an electro-optic material in close contact with the specimen. In contrast to established near-field approaches, the method does not require the scanning of local probes such as SNOM or micro-antennas. We analyze phase-matching conditions and effective resolutions, and we demonstrate the super-resolution capabilities.

HL 26.51 Wed 9:30 P1

Highspeed ultrafast spectroscopy via active synchronization of dual-comb lasers — •Simeon Schmitt, Julia Lang, and Georg Herink — University of Bayreuth, Germany

Dual-comb lasers enable ultrafast spectroscopic measurements at high speeds by generating optical delays without the motion of mechanical elements. According to the asynchronous optical sampling (ASOPS) scheme, pulses from two mode-locked lasers with detuned repetition rates are combined to automatically scan relative delays throughout the pulse period. In contrast, here, we present a novel approach which features flexible active synchronization of both lasers: Employing precisely timed electrical signals and fast electro-optical modulators, we achieve full control over the overall scanning process. This concentrates the scanning range to the region of interest by limiting it to several picoseconds, resulting in record fast scanning rates. Furthermore, the scanning resolution can be arbitrarily adjusted up to tens of THz by varying the repetition rate difference. We adopt this process to realize ultrafast acquisition speeds for rapid THz time domain spectroscopy and present first measurements.

HL 26.52 Wed 9:30 P1

Ultrafast negative thermal expansion in NbO_2 — •Florian Baltrusch[1], Marc Herzog[1], Florin Boariu[2], Matthias Rössle[2], Jutta Schwarzkopf[3], and Matias Bargheer[1,2] — [1]Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Germany — [2]Helmholtz-Zentrum Berlin, Berlin, Germany — [3]Leibniz-Institut für Kristallzüchtung, Berlin, Germany

Niobium dioxide (NbO_2) exhibits negative thermal expansion (NTE), meaning it contracts upon heating rather than expanding like most materials. Below 200 K, bulk NbO_2 shows a monotonic contraction of the tetragonal c-axis, while the a/b-axes expand. This behaviour not only enables zero-expansion composites but also provides an unconventional elastic driving mechanism for magneto-elastic materials on picosecond timescales.

In epitaxial thin films, however, the lattice response is modified by substrate constraints via the Poisson effect. Temperature-dependent XRD measurements show that the film response depends strongly on the thermal-expansion mismatch between film and substrate during equilibrium heating.

Using ultrafast X-ray diffraction (UXRD), we directly observe ultrafast NTE in NbO_2 thin films. On picosecond timescales, the substrate remains effectively "frozen", allowing us to isolate the intrinsic response of the NbO_2 layer. This enables us to determine the timescale of contraction, which provides crucial insights about its driving mechanism.

HL 26.53 Wed 9:30 P1

Development of single-shot spectral referencing to increase signal-to-noise ratio in broadband 2D electronic spectroscopy — •Lotte Polling, Anton Trenczek, Pavel Trofimov, Trideep Kawde, and Hélène Seiler — FU Berlin

Two-dimensional optical spectroscopy is a powerful technique for resolving couplings between electronic states. Its implementation relies on the availability of a broadband light source in the visible range, typically generated using non-collinear optical parametric amplifiers or gas-filled hollow-core fibers. These sources exhibit shot-to-shot spectral fluctuations which can be as high as 10-15% depending on the laser source. Here, we introduce a setup for single-shot spectral referencing with the end goal of significantly increasing the signal-to-noise ratio in broadband 2D electronic spectroscopy measurements.

HL 26.54 Wed 9:30 P1

Ultrafast Lattice Dynamics in Gold Beyond the Kinematic Approximation — •Helena Hollstein[1,2], Sebastian Hammer[2], and Heinrich Schwoerer[1] — [1]Max-Planck-Institut für Struktur und Dynamik der Materie, 22761 Hamburg, Germany — [2]Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany

In the interpretation of electron diffraction experiments, the kinematic scattering approximation and simple phonon models are often used to reduce computational cost when modeling structural dynamics [1]. However, even for well-studied benchmark systems such as polycrystalline gold thin films, it often remains unquestioned how reliably these assumptions hold under strong nonequilibrium excitation [2].

In this work, we investigate a 20 nm gold thin film under optical excitation using ultrafast electron diffraction (UED) and static temperature dependent electron diffraction to extract transient atomic displacements and determine phonon excitation by analyzing the Debye-Waller effect. We compare our experimental findings of lattice heating dynamics with simulated diffraction patterns that rely on kinematic scattering and harmonic phonon models. We hereby assess to what extent the commonly used theoretical frameworks cease to describe the structural response accurately. Our findings demonstrate that neglecting possible anharmonic potentials, phonon-phonon coupling and multiple scattering-effects can lead to systematic misinterpretations of ultrafast lattice dynamics and thermophysical material properties.

[1] Schäfer et al. *Chem. Phys. Lett.* **515** (2011)
[2] Durham et al. *Struct. Dyn.* **9** 064302 (2022)

HL 26.55 Wed 9:30 P1

Ultrafast dynamics of exciton–exciton interaction in monolayer MoS_2 investigated by high-order pump–probe micro-spectroscopy — •Ruidan Zhu, Patrick Grenzer, Simon Büttner, Matthias Hensen, Tobias Hertel, and Tobias Brixner — Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Exciton–exciton interaction (EEI), as a many-body effect, sets a fundamental limit to optimizing the photoluminescence efficiency of light-emitting devices based on 2D materials under high exciton densities [1]. A detailed understanding of the underlying EEI mechanisms provides crucial insight for the optimization of the device performance. However, EEI dynamics are challenging to probe directly as their signatures are mixed with the dominant single-exciton background in conventional ultrafast measurements. Here, we apply our recently developed high-order pump–probe spectroscopy [2] in a cryo-microscope to study exciton interaction in freestanding and supported MoS_2 monolayers. We aim to separate different EEI-related processes (fifth and higher orders of the system's nonlinear response) from the single-exciton dynamics (third order) and further investigate how the dielectric environment influences EEI dynamics. We present our current progress toward isolating EEI dynamics.

[1] Y. Yu et al., Phys. Rev. B 2016, 93, 201111.
[2] P. Malý et al., Nature 2023, 616, 280.

HL 26.56 Wed 9:30 P1

Impulsive Stimulated Raman Scattering: Highspeed Detection Strategies — •Laura Hüllmandel, Julia A. Lang, and Georg Herink — Universität Bayreuth

Pulse interaction of femtosecond pulses inside Ti:Sapphire lasers is mediated by Raman-active modes with terahertz beats causing bound states of solitons at fixed time delays [1]. In this contribution, we employ extra-cavity impulsive stimulated Raman scattering (ISRS) to quantitatively determine the phase-shifts involved to further our understanding of the intra-cavity formation of so-called "soliton molecules". We compare spectral-shift and interferometric methods for phase-sensitive detection and achieve efficient noise reduction of multiplicative $1/f$ noise sources – where lock-in amplification is ineffective – through rapid scan-averaging and balanced detection.

[1] A. Völkel et al., "Intracavity Raman Scattering Couples Soliton Molecules with Terahertz Phonons.", Nature Communications 13.1 (2022).

HL 27: 2D Materials: Electronic structure, excitations, etc. II (joint session O/HL/TT)

Time: Wednesday 10:30–12:30 Location: TRE/MATH

See O 59 for details of this session.

HL 28: Topology and symmetry protected materials & Topological insulators (joint session O/HL/TT)

Time: Wednesday 15:00–17:45 Location: HSZ/0401

See O 63 for details of this session.

HL 29: Quantum Transport and Quantum Hall effects (joint session HL/TT)

Time: Wednesday 15:00–16:15 Location: POT/0006

HL 29.1 Wed 15:00 POT/0006

High Harmonic Hall Currents Driven by Curved Conducting Nanoarchitecture — •Ching-Hao Chang[1,2], Botsz Huang[1,2], Wei-Xiang Yin[1,2], and Xiao Zhang[3] — [1]Department of Physics, National Cheng Kung University Tainan, Taiwan — [2]Center for Quantum Frontiers of Research and Technology (QFort), National Cheng Kung University Tainan 70101, Taiwan — [3]Institute for Theoretical Solid State Physics Leibniz Institute for Solid State and Materials Research Dresden Helmholtzstr. 20, D-01069 Dresden, Germany

We theoretically establish a realizable non-perturbative mechanism for generating high harmon- ics (up to 6th order) in Hall currents within curved two-dimensional nanoarchitectures. Unlike previously explored perturbative mechanisms based on inversion symmetry breaking or Berry curvature, the high-harmonic generation demonstrated here is driven by magnetic-field dipoles induced purely by nanoscale curvature under an applied uniform magnetic field. We develop a theory showing that these harmonics originate from unique snake orbits induced by the interplay between an alternating electric field and curvature-induced magnetic-field dipole. Moreover, we establish quantitative control over harmonic suppression and enhancement by tuning the amplitude and orientation of the magnetic field, uncovering distinct symmetry-based even/odd harmonic selection rules. These findings provide a tunable platform for engineering nonlinear currents in curved electronics, with potential applications in developing high-frequency Hall sensors and THz devices.

HL 29.2 Wed 15:15 POT/0006

Gate-tunable isospin switching in graphene Mach-Zehnder electronic interferometers — •Antonio Lacerda-Santos, Lilian Seyve, Yassine Setti, Bikash Barik, Leo Pugliese, Preden Roulleau, and Cosimo Gorini — SPEC, CEA, CNRS, Université Paris-Saclay, 91191 Gif-sur-Yvette, France

Graphene has become an exciting platform for electron (quantum) optics experiments [1]. Compact electronic interferometers can be realised via p-n interfaces, which in quantizing magnetic fields host counter-propagating chiral edge states. In a paradigmatic architecture with a single junction, such quantum Hall states form a Mach-Zehnder interferometer [2, 3]. The precise position of such edge states is set by the electrostatics of a given device [4], which can be determined to great accuracy with the self-consistent Schrödinger-Poisson solver Pescado [5].

We perform electrostatic and quantum transport simulations accompanying conductance measurements in a graphene Mach-Zehnder interferometer, and show that remote gates can be used to control the position of the p-n junction on sub-nanometer scales. Such a fine control does not meaningfully affect the edge state positions and lengths, but induces valley-isospin oscillations. The interferometer thus behaves as a tunable valley-isospin transistor.

[1] H. Chakraborti et al., J.Phys.:Condens.Matter 36 (2024) 393001 [2] D.S.Wei et al, Science Advances 3, e1700600 (2017) [3] M. Jo et al, PRL 126, 146803 (2021) [4] I.M. Flor et al, PRB 105, L241409 (2022) [5] A. Lacerda-Santos, arXiv:2507.03131v1

HL 29.3 Wed 15:30 POT/0006

Phase-coherent autonomous nonequilibrium demon — •José Balduque[1,2] and Rafael Sánchez[1,2,3] — [1]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain. — [2]Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, Spain — [3]Instituto Nicolás Cabrera (INC), Universidad Autónoma de Madrid, Madrid, Spain.

Mesoscopic conductors enable the efficient management and useful conversion of not only thermal resources but also nonequilibrium electron distributions. The latter scenario makes it possible to define demonic modes of operation, in which the entropy of a subsystem is autonomously reduced without extracting net particles or energy from the subsystem that provides the nonequilibrium resource [1]. We propose an implementation of such a nonequilibrium demon, or N-demon, in a multiterminal system that exploits carrier coherence. This is achieved by directly coupling the demonic subsystem to an isothermal two-terminal conductor via a scanning tip, enabling the local injection of electrons in a nonthermal distribution that participates in the phase-coherent interference processes governing the system's transport response [2]. In this way, we uncover an extrinsic, nonlocal, and phase-tunable transport response induced by the demon [3].

[1] R. Sánchez, et al., Phys. Rev. Lett. 123, 216801 (2019).
[2] R. Sánchez, et al., Phys. Rev. B, 105, 239903 (2022).
[3] J. Balduque and R. Sánchez, in preparation.

HL 29.4 Wed 15:45 POT/0006

Exploring the Influence of Electron Density on the Giant Negative Magnetoresistance — •Lina Bockhorn[1], Christian Reichl[2], Werner Wegscheider[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Germany — [2]Laboratorium für Festkörperphysik, ETH Zürich, Switzerland

Ultra-high mobility two-dimensional electron gases exhibit a robust negative magnetoresistance at zero magnetic fields, characterized by a temperature-independent peak around $B = 0$ T and a temperature-dependent giant negative magnetoresistance (GNMR) at higher fields [1-4]. By varying the electron density in situ, we gain valuable insights into the nature of GNMR. Our study shows a significant dependence of GNMR on electron density, suggesting that scattering potential variations [5] may not be fully addressed in current theoretical models. By examining these dependencies for different temperatures, we enhance the understanding of unresolved aspects of GNMR theory, potentially bridging the gap between experimental observations and theoretical predictions.

[1] L. Bockhorn et al., Phys. Rev. B 83, 113301 (2011).
[2] L. Bockhorn et al., Phys. Rev. B 90, 165434 (2014).
[3] L. Bockhorn et al., Appl. Phys. Lett. 108, 092103 (2016).
[4] L. Bockhorn et al., Phys. Rev. B 109, 205416 (2024).
[5] Y. Huang et al., Phys. Rev. Materials 6, L061001 (2022).

HL 29.5 Wed 16:00 POT/0006

A topological field-effect memristor — •Fabian Hartmann[1], Manuel Meyer[1], Selena Barragan[1], Sergey Krishtopenko[1,2], Jean-Baptiste Rodriguez[3], Eric Tournie[3], Benoit Jouault[2], Gerald Bastard[1], Frederic Teppe[2], Lukas Worschech[1], Victor Lopez-Richard[4], and Sven Höfling[1] — [1]Lehrstuhl für Technische Physik, Julius-Maximilians-Universität Würzburg — [2]L2C, CNRS-Université de Montpellier, France — [3]IES, Université de Montpellier, France — [4]Departamento de Fisica, Universidade Federal de Sao Carlos, Brazil

Quantum and neuromorphic computing rely on unconventional materials and device functionalities, yet achieving resilience to imperfections and reliable operation remains a major challenge. This has motivated growing interest in topological materials that provide robust and low-power operation while preserving coherence. However, integrating topological transport with memory functionality into a reconfigurable device has remained elusive. Here, we realize a topological field-effect memristor in which topological protection preserves edge state coherence, enabling the coexistence of coherent transport and non-volatile memory functionality. Utilizing inverted InAs/GaInSb/InAs trilayer quantum wells, we realize a quantum spin Hall insulator that exploits its intrinsic floating-gate behavior. This feature allows one to reconfigure the conventional field-effect transistor operation into memristive functionality with broad electric-field tunability. One resistance state is entirely governed by dissipationless, coherent transport.

HL 30: 2D Materials V – Magnetic, spintronic, and topological properties (joint session HL/TT)

Time: Wednesday 15:00–17:15 Location: POT/0081

Invited Talk HL 30.1 Wed 15:00 POT/0081

Dual proximity engineering of spin-orbit and magnetic effects in graphene heterostructures — •Christoph Kastl — Walter Schottky Institute, School of Natural Sciences, Technical University of Munich — Munich Center for Quantum and Technology (MCQST)

The coexistence of induced spin-orbit coupling (SOC) and magnetic exchange fields is predicted to drive graphene into topological phases, such as the quantum anomalous Hall state. Here, I will discuss the prospect of using monolayer graphene proximitized by WSe_2 (SOC) and $Cr_2Ge_2Te_6$ (magnetic exchange) for such dual proximity control. To determine the type and strength of the induced SOC, I will compare Landau fan analysis, where level anticrossings can serve as direct signatures of spin-orbit splittings, to optoelectronic measurements on graphene/WSe_2 heterostructures, where the photogalvanic effect can provide an indirect fingerprint of SOC. Low-temperature magnetotransport measurements of the heterostructures with combined magnetic and SOC proximity reveal a large and gate-tunable anomalous Hall effect persisting at zero magnetic field, signaling an intrinsic Berry curvature arising from the interplay of SOC and magnetism. These results highlight the coexistence of spin-orbit and magnetic proximity effects in graphene-based van der Waals heterostructures and establish a route toward topological graphene phases.

HL 30.2 Wed 15:30 POT/0081

Twist angle and pressure tuning of proximity-induced spin-orbit coupling in graphene/WSe_2 heterostructures — Tobias Rockinger[1], Bálint Szentpéteri[2], Szabolcs Csonka[2], Marina Marocko[1], Julia Amann[1], Ziyang Gan[3], Antony George[3], Andrey Turchanin[3], Kenji Watanabe[4], Takashi Taniguchi[4], Dieter Weiss[1], Péter Makk[2], and •Jonathan Eroms[1] — [1]Department of Physics, University of Regensburg, Germany — [2]Department of Physics, Budapest University of Technology and Economics, Budapest, Hungary — [3]Institute of Physical Chemistry, Friedrich Schiller University Jena, Germany — [4]National Institute for Materials Science, Tsukuba, Japan

Proximity-induced spin-orbit interaction in heterostructures of graphene and transition metal dichalcogenides has been studied intensely in the past few years. However, present experiments still suffer from poor reproducibility, as one key parameter, the twist angle between the crystal axes of both materials, has not been systematically controlled during fabrication. Band structure calculations, on the other hand, have predicted a decisive influence of this parameter. In our experiments, we control the twist angle during fabrication by aligning fractured or CVD grown edges and resolving the ambiguity of zigzag and armchair directions using a crystallographic etching process. We employ weak antilocalization to extract the spin-orbit coupling parameters quantitatively, and report excellent reproducibility and a good match to theoretical predictions. We also confirm the influence of high pressure on the proximity effect.

HL 30.3 Wed 15:45 POT/0081

Nonlinear optical probing of local quantum geometry — •Nele Tornow[1], Paul Herrmann[1], Clemens Schneider[2], Jan Wilhelm[2], and Giancarlo Soavi[1,3] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany — [2]Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy, Regensburg, Germany — [3]Abbe Center of Photonics, Friedrich Schiller University Jena, Jena, Germany

With its direct relation to many phenomena in solid matter, quantum geometry has become a concept of increasing interest in solid state physics. However, measurements of the local quantum geometry, *e.g.,* Berry curvature, has been possible to date only *via* angle-resolved photoemission spectroscopy [1]. On the other hand, in one of our recent theoretical works [2] we have shown that there is a link between linear circular dichroism and derivatives of Berry curvature in 3D crystals with preserved time-reversal symmetry (TRS).

In this presentation I will further demonstrate both, experimentally and with analytical solutions of semiconductor Bloch equations, that in a 2D semiconductor with broken TRS, the emerging second-harmonic circular dichroism can be used as a direct probe of the Berry curvature at the opposite ± K valleys, providing a new all-optical approach to access the local quantum geometry in 2D materials.

[1] Schüler, M. et al., Sci. Adv. 6, eaay2730 (2020)
[2] Soavi, G. and Wilhelm, J., arXiv:2501.03684 (2025)

15 min. break

HL 30.4 Wed 16:15 POT/0081

Proposal for Resolving Quantized Landau Orbits via Elastic XUV Scattering — •Sabrina Meyer[1], Andreas Knorr[1], Stephen Hughes[2], and Lara Greten[1,2] — [1]Institut für Physik und Astronomie, Technische Universität Berlin, Germany — [2]Department of Physics, Queen's University, Kingston, Canada

In a strong perpendicular magnetic field, a two-dimensional electron gas is quantized into discrete Landau levels. We propose a method to extract the spatial structure of Landau orbits via scattering with extreme ultraviolet radiation, whose wavelength naturally matches the Larmor radius. In a microscopic theory, we derive the far-field spectrum emitted by the optically induced current density. Contributions from Landau orbits within this spectrum are suppressed due to scattering effects imposed by the sample geometry. By normalizing against the zero-magnetic-field reference, however, we define a Landau level scattering spectrum that isolates Landau orbit information. This gives access to the probability density distributions of individual Landau level wave functions featuring radial maxima at the quantized Larmor radii.

HL 30.5 Wed 16:30 POT/0081

Berry Phase Shift in Folded Bilayer Graphene — •Hannes Kakuschke, Lina Bockhorn, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

Mono- and bilayer systems of graphene have been extensively researched due to their unique magnetic und electronic transport properties. In more recent works, folded graphene [1-5] has gained interest as a platform for topological phenomena, such as zero-line modes [4]. However, these systems rely on self-assembled folded graphene, found by chance during exfoliation or induced by tearing [1-5]. Our dry-transfer approach allows us to fold graphene around hBN in a controllable manner, decoupling the overlapping graphene regions. In these samples, we observe a Berry phase shift from 2π to π near the edge of folded bilayer graphene, attributed to local strain fields and stacking shifts.

[1] J. C. Rode et al., Ann. Phys. 529, 1700025 (2017).
[2] J. C. Rode et al., 2D Mater. 6, 015021 (2018).
[3] L. Bockhorn et al., Appl. Phys. Lett. 118, 173101 (2021).
[4] S. J. Hong et al., 2D Materials 8, 045009 (2021).
[5] S. J. Hong et al., Phys. Rev. B 105, 205404 (2022).

HL 30.6 Wed 16:45 POT/0081

Probing spin-orbit coupling in graphene/WSe_2 heterostructures by the circular photogalvanic effect — Ernst Knöckl, •Matthias Klein, Alexander Holleitner, and Christoph Kastl — Walter Schottky Institute, School of Natural Sciences, Technical University of Munich

We investigate proximity-induced spin–orbit coupling (SOC) in graphene/WSe_2 heterostructures using the circular photogalvanic effect (CPGE) as a symmetry-selective and experimentally accessible probe of spin–valley-locked band textures [1]. By measuring helicity-dependent photocurrents as a function of gate voltage, excitation energy, and device geometry, we aim to disentangle Rashba and valley-Zeeman SOC contributions and to extract their magnitude and sign as a function of the graphene–WSe_2 twist angle. The observed trends in CPGE sign reversals and scaling behavior provide quantitative indications of interfacial symmetry breaking and moiré-enhanced spin–valley coupling, supported by comparison to microscopic transport models. These results are expected to establish CPGE as a promising metrological probe of proximity SOC in 2D heterostructures and to complement ongoing efforts in twist-angle-dependent spin–orbit engineering in graphene/TMD systems [2,3].

[1] Kiemle, J., et al. ACS nano 16.8, 12338-12344 (2022)
[2] Yang, H., et al. Nat. Mater. 23, 1502-1508 (2024)
[3] Zhang, Y., et al. Natur 641, 625-631 (2025)

HL 30.7 Wed 17:00 POT/0081

Study of the non-trivial spin texture in Tellurium and the consequences in charge-spin interconversion — •Andrés Martínez-García[1], Daniel Gosálvez-Martínez[1], Carlos Sabater[1], and Juan José Palacios[2] — [1]Departamento de Física and Instituto Universitario de Materiales de Alicante (IUMA), Universidad de Alicante, Alicante, Spain. — [2]Departamento de Física de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, Spain.

Tellurium is a chiral semiconducting material with a narrow band gap that can be synthesized with well-defined handedness in nanowires and flakes, making it an excellent platform for studying chirality-related charge-spin interconversion in nanodevices. The coupling between charge and spin degrees of freedom is closely connected to the spin texture in momentum space. In this work, we demonstrate that tellurium exhibits a nontrivial radial spin texture at the top of the valence band, where the spin polarization aligns parallel to the HK direction of the Brillouin zone, while spins in the perpendicular ZHL plane display a nontrivial winding. We investigate the electronic transport and resulting spin

polarization within the Landauer transport formalism using first-principles calculations. This approach allows us to map the transport properties along each crystallographic direction and to identify correlations between the spin polarization of the induced current and the underlying momentum-space spin texture. Our results provide microscopic insight into chirality-driven spin responses in tellurium and highlight its potential for spintronic applications.

HL 31: Materials and Devices for Quantum Technology I

Time: Wednesday 15:00–16:15 Location: POT/0251

HL 31.1 Wed 15:00 POT/0251

Escaping AB caging via Floquet engineering: photo-induced long-range interference in an all-band-flat model — Aamna Ahmed, •Mónica Benito, and Beatriz Perez-Gonzalez — Institute of Physics, University of Augsburg, 86159 Augsburg, Germany

Flat-band lattices hosting compact localized states are highly sensitive to external modulation, and the tailored design of a perturbation to imprint specific features becomes relevant. Here we show that periodic driving in the high-frequency regime transforms the all-flat-band diamond chain into one featuring two tunable quasi-flat bands and a residual flat band pinned at zero quasienergy. The interplay between lattice geometry and the symmetries of the driven system gives rise to drive-induced tunneling processes that redefine the interference conditions and open a controllable route to escaping Aharonov-Bohm (AB) caging. Under driving, the diamond chain effectively acquires the geometry of a dimerized lattice, exhibiting charge oscillations between opposite boundaries. This feature can be exploited to generate two-particle entanglement that is directly accessible experimentally. The resulting drive-engineered quasi-flat bands thus provide a versatile platform for manipulating quantum correlations, revealing a direct link between spectral fine structure and dynamical entanglement.

HL 31.2 Wed 15:15 POT/0251

Floquet theory for the quantum-to-classical crossover of light-matter models — •Beatriz Perez Gonzalez[1], Sigmund Kohler[2], and Mónica Benito[1] — [1]Institute of Physics (University of Augsburg), Augsburg, Germany — [2]Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Madrid, Spain

Rabi-type Hamiltonians, comprising either a time-periodic driving or a quantized electromagnetic field, have become ubiquitous across physics. Despite the well-established physics of both the semi-classical and quantum descriptions, when and how classical Floquet physics emerges from a fully quantum treatment remains the subject of active debate [1] and study [2].

We present a unified framework for the quantum-to-classical mapping, emphasizing the gauge-invariant formulation of the quantum Rabi Hamiltonian. This allows a systematic comparison of quasienergies, spectra, entanglement, and dynamics across high- and low-frequency regimes, and clarifies how Floquet frames correspond to gauge choices once photonic Fock states are interpreted as Fourier harmonics. We further assess the suitability of quantum high-frequency expansions and benchmark them against alternative methods for deriving effective Hamiltonians, including Schrieffer-Wolff transformations and projector-based approaches.

[1] Phys. Rev. Lett. 129, 183603 (2022); Phys. Rev. Research 2, 033033 (2020); [2] B. Perez-Gonzalez et al., Quantum 9, 1633 (2025); Comm. Phys. 7, 419 (2024)

HL 31.3 Wed 15:30 POT/0251

Understanding optically detected magnetic resonance (ODMR) of InSi-Sii-defects — •Kevin Lauer[1,2], Bernd Hähnlein[1], Mario Bähr[1], Kai Kühnlenz[1], Philipp Kellner[1], Dirk Schulze[2], Stefan Krischok[2], Alexander Rolapp[3], Christian Möller[1], and Thomas Ortlepp[1] — [1]CiS Forschungsinstitut für Mikrosensorik GmbH, Konrad-Zuse-Str. 14, 99099 Erfurt, Germany — [2]Technische Universität Ilmenau, Institut für Physik, Weimarer Str. 32, 98693 Ilmenau, Germany — [3]IMMS Institut für Mikroelektronik- und Mechatronik-Systeme gGmbH, Konrad-Zuse-Str. 14, 99099 Erfurt, Germany

Defects from the acceptor-interstitial silicon (ASi-Sii)-defect category were found to be promising candidates for qubits in silicon-based quantum technology [1]. To further explore their qubit properties optically detected magnetic resonance (ODMR) measurements are carried out on quenched indium-doped silicon samples featuring InSi-Sii-defects. Depending on the antenna design (omega or rod) four different ODMR signals are found in the spectra. An approach to understand these spectra in frame of a triplet system formed by two holes at the InSi-Sii-defect will be discussed. On that basis possible electronic level schemes are proposed.

[1] K. Lauer et al., 'Examining the properties of the ASi-Sii-defects for their potential as qubits', presented at the GADEST but unpublished, Bad Schandau: ResearchGate, May 2024. doi: 10.13140/RG.2.2.18793.51048.

HL 31.4 Wed 15:45 POT/0251

Time-bin encoded quantum key distribution over 120 km with a telecom quantum dot source — •Jingzhong Yang[1], Jipeng Wang[1], Joscha Hanel[1], Zenghui Jiang[1], Raphael Joos[2], Michael Jetter[2], Eddy. Patrick Rugeramigabo[1], Simone. Luca Portalupi[2], Peter Michler[2], Xiao-Yu Cao[3], Hua-Lei Yin[3,4], Shan Lei[5], Jingzhong Yang[1], Michael Zopf[1], and Fei Ding[1] — [1]Leibniz University of Hannover, Hannover, Germany — [2]University of Stuttgart, Stuttgart, Germany — [3]Nanjing University, Nanjing, China — [4]Renmin University of China, Beijing, China — [5]Anhui University, Hefei, China

Quantum key distribution (QKD) with deterministic single photon sources has been demonstrated over intercity fiber and free-space channels, but mainly on polarization encoding schemes. In contrast, time-bin encoding offers inherent robustness and has been widely adopted in mature QKD systems using weak coherent laser pulses.

In this work, we presents the first demonstration of the time-bin encoded quantum key distribution (QKD) using the telecom single photons from a quantum dot. A maximum tolerable transmission distance of 127 km is identified as the system error ratio approaches the security threshold. The result demonstrates the feasibility of realizing robust and scalable quantum communication network based on solid-state single-photon technology.

HL 31.5 Wed 16:00 POT/0251

high-efficiency photonic interfaces for VV centres in silicon carbide — •Nien-Hsuan Lee[1,2], Jonas Schmid[1,2], Berke Demiralp[3], Felix David[1], Kevin Menguelti[3], Stephan Kucera[1], Eva Weig[3,4,5], and Florian Kaiser[1,2] — [1]Luxembourg Institute of Science and Technology, Belval, Luxembourg — [2]University of Luxembourg, Belval, Luxembourg — [3]Technical University of Munich, Garching, Germany — [4]Munich Center for Quantum Science and Technology, Munich, Germany — [5]TUM Center for Quantum Engineering, Garching, Germany

In this work, we present a systematic investigation of etching processes aimed at optimising photonic structures for VV centres in bulk SiC. A wide range of fabrication parameters is explored, including metallic and non-metallic etch masks, plasma chemistries, and etching strategies to reduce surface and sidewall roughness while improving reproducibility. Structural and optical characterisation of the resulting waveguides enables identification of key loss mechanisms and the critical parameters governing high-efficiency photon transmission. Building on these process developments, we demonstrate a new generation of free-standing SiC waveguides with high wafer-scale uniformity and excellent reproducibility, enabling very high coupling efficiencies. Furthermore, we introduce a nanocone photonic structure in SiC, which simulations indicate can achieve more than a ten-fold enhancement in photon collection efficiency compared with unstructured bulk SiC. These results provide a scalable and reproducible photonic platform for wafer-scale integration of SiC colour centres for quantum communication.

HL 32: 2D Materials 2 (joint session DS/HL)

Time: Wednesday 15:00–17:30 Location: REC/C213

See DS 14 for details of this session.

HL 33: Nitrides I – Growth and fabrication

Time: Wednesday 16:30–17:45 Location: POT/0006

HL 33.1 Wed 16:30 POT/0006

Homoepitaxial growth of AlN by plasma-assisted molecular beam epitaxy — •Xin Du, Hossein Yazdani, and Yongjin Cho — Paul-Drude-Institut für Festkörperelektronik (PDI), Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5–7, 10117 Berlin, Germany

Wurtzite AlN can be considered an electrical insulator because of its ultrawide bandgap of 6.2 eV. However, it can become electrically active as either *n*-type or *p*-type through direct chemical doping or polarization doping when alloyed with the other group-III cations. This broad tunability in electrical conductivity, combined with its high thermal conductivity of about 340 W/m·K, makes AlN highly attractive for power electronics and deep-UV optoelectronic devices. Interest in AlN has considerably increased with the recent development of high-quality AlN bulk substrates with dislocation densities below 10^4 cm^{-2}. To fully leverage the high structural quality of these substrates in subsequent epitaxial layers, the native oxide must be removed before growth. Although Al-assisted deoxidation of AlN substrates has recently been shown to be effective for MBE growth, achieving consistently complete oxide removal and subsequently high-quality AlN homoepitaxy remains challenging. In this talk, we show how various cleaning methods and MBE growth conditions influence AlN homoepitaxy. This work serves as a seeding study at PDI for future investigations aimed at achieving reliable doping control in AlN with minimized compensating defects.

HL 33.2 Wed 16:45 POT/0006

Phase transition regions of epitaxially sputtered TiAlN layers on TiN and AlN buffer layers — •Emine Kaynar, Florian Hörich, Jürgen Bläsing, Fabian Grossmann, Usha Velpuri, Armin Dadgar, André Strittmatter, and Arne Busse — Institut für Physik, Otto-von-Guericke Universität Magdeburg, Magdeburg, Germany

For manufacturing vertical GaN-based power devices on Si substrates, it is advantageous to replace insulating AlN/AlGaN layers at the Si interface. AlN/AlGaN layers are currently required to ensure high-quality GaN on Si. TiAlN alloys offer a tunable bandgap from metallic conduction up to 6 eV and thermal robustness, making them promising alternatives to insulating Al(Ga)N buffers when epitaxial growth on Si is feasible. In this work, TiAlN layers were epitaxially grown on n-type Si (111) using TiN and AlN buffers prepared by a two-step sputtering process at growth temperatures below 900 °C. Highly crystalline cubic TiN (ω-FWHM ~ 0.3°, RMS < 1 nm) served as a conductive template. By tuning the power ratio between Ti and Al targets, Al content was systematically controlled, enabling direct mapping of the cubic-wurtzite transition. On TiN buffers, cubic TiAlN remained stable up to x ~ 0.4. On wurtzite AlN buffers, the opposite transition from wurtzite to cubic occurred as Ti incorporation increased. For all AlN-buffered samples, ω-FWHM stayed below 1° and RMS roughness remained < 5 nm. These results demonstrate precise phase control and high crystalline quality, positioning TiAlN as a strong candidate for conductive buffer layers in vertical GaN-on-Si device architectures.

HL 33.3 Wed 17:00 POT/0006

Epitaxial Growth of ZrN on Si(111) — •Muthukani Kathiresan, Usha Velpuri, Arne Busse, Florian Hörich, Jürgen Bläsing, Armin Dadgar, and André Strittmatter — Institut für Physik, Otto-von-Guericke Universität Magdeburg, Magdeburg, Germany

Transition metal nitrides can add new functionalities to GaN devices. These range from conducting buffer layers for the growth of vertical GaN devices on Si, as template for the growth of N-polar GaN up to enhanced piezo- and ferroelectric properties when alloyed with AlN. Transition-metal nitrides (TMNs) such as ZrN, HfN, TiN and ScN crystallize in the rock-salt structure and exhibit metallic conductivity except for ScN which is semiconducting. For nitride growth, ZrN is particularly attractive due to its favorable lattice relationship, exhibiting an in-plane mismatch of only 1.35% between ZrN (111) and GaN (0001). Additionally, ZrN layers can be deposited by sputtering, whereas layer growth by MOVPE suffers from the low-vapor pressure of available precursors.In this work, we present recent progress in the sputter epitaxy of ZrN on Si (111). For 100-nm-thick films grown at 900 °C in N2/NH3, we achieved an ω-FWHM of 0.5°. Introducing NH3 promoted a transition from a columnar grain structure to a compact, two-dimensional morphology, with a surface roughness of 1.7 nm. The thermal stability of these layers was assessed through annealing at 1100 °C under NH3, which led to reduced film density by void formations, revealed by X-ray reflectivity (XRR) measurements and scanning electron microscopy (SEM).

HL 33.4 Wed 17:15 POT/0006

In-situ fabrication of $In_{0.3}Ga_{0.7}N$ pseudo-substrates on GaN (0001) templates via a three-step protocol in plasma-assisted molecular beam epitaxy — •Huaide Zhang, Aidan Campbell, Jingxuan Kang, Jonas Lähnemann, Oliver Brandt, and Lutz Geelhaar — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117, Berlin, Germany

The considerable lattice mismatch between GaN and InN introduces significant strain into (In,Ga)N epitaxial layers grown on GaN templates. This strain impedes the incorporation of In and induces a strong piezoelectric field in (In,Ga)N/GaN quantum wells, which diminishes the internal quantum efficiency. Furthermore, the accumulated strain can prompt plastic relaxation of the lattice, generating additional threading dislocations. The high In content required for (In,Ga)N-based light-emitting diodes (LEDs) operating in the amber/red spectral range necessitates, hence, a substrate with an adjusted lattice constant. In this work, we present a three-step growth method for fabricating a highly relaxed $In_{0.3}Ga_{0.7}N$ pseudo-substrate directly on GaN(0001) templates which is conducted entirely within a plasma-assisted molecular beam epitaxy system. In contrast to other approaches, our method does not require any ex-situ patterning, providing thus advantages in terms of scalability and cost. The resulting structure demonstrates superior characteristics in key properties, including In content, degree of strain relaxation, and surface smoothness compared to existing alternatives.

HL 33.5 Wed 17:30 POT/0006

Influence of A-Site Cations on Structure, Defect Density and Photoactivity of Tantalum-Based Perovskite Oxynitride Photoelectrodes — •Gabriel Grötzner[1,2], Aleksandr Kochergov[1,2], Oliver Brune[1,2], Laura I. Wagner[1,2], Saswati Santra[1,2], Verena Streibel[1,2], and Ian D. Sharp[1,2] — [1]Walter Schottky Institute, Technische Universität München, Germany — [2]Physics Department, TUM School of Natural Sciences, Technische Universität München, Germany

Perovskite oxynitrides are emerging materials for photoelectrochemical (PEC) water splitting, yet the influence of the A-site cation on their material properties remains poorly understood. Here, we investigate a series of $ATaON_2$ thin films (A = La, Ce, Pr, Nd, Gd, ordered by decreasing ionic radius) to elucidate the role of the A-site cation on structural, optoelectronic, and PEC properties. X-ray diffraction analysis reveals a systematic lattice contraction with decreasing ionic radius of the A-site cation. This structural change is accompanied by an increase in optical band gap from 1.8 eV to 2.2 eV and a reduction in sub-bandgap absorption, indicating lower defect densities for smaller A-site cations. Electrical measurements show reduced conductivity for $GdTaON_2$ compared to $LaTaON_2$, consistent with defect suppression. By changing the A-site cation from La to Gd, the photocurrent density in PEC measurements doubles, despite an increase in optical band gap, which indicates the beneficial impact of reduced defect-mediated recombination. These insights offer design principles for defect and band-structure engineering in perovskite oxynitride photoanodes.

HL 34: Quantum Dots and Wires: Telecom Wavelength

Time: Wednesday 16:30–17:45 Location: POT/0051

HL 34.1 Wed 16:30 POT/0051

All-photonic quantum teleportation at telecom wavelength with frequency converted photons from remote quantum dots — •Tim Strobel[1], Michal Vyvlecka[1], Ilenia Neureuther[1], Tobias Bauer[2], Marlon Schäfer[2], Stefan Kazmaier[1], Nand Lal Sharma[3], Raphael Joos[1], Jonas H. Weber[1], Cornelius Nawrath[1], Weijie Nie[3], Ghata Bhayani[3], Caspar Hopfmann[3], Christoph Becher[2], Peter Michler[1], and Simone Luca Portalupi[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQ^{ST}) and SCoPE, University of Stuttgart, Stuttgart, Germany — [2]Fachrichtung Physik, Universität des Saarlandes, Saarbrücken, Germany — [3]Institute for Integrative Nanosciences, Leibniz IFW Dresden, Dresden, Germany

A future terrestrial quantum internet relies on distant quantum network nodes connected via optical fiber channels. In this context, semiconductor quantum dots (QDs) are promising sources of quantum light. Here, we report on an all-photonic quantum teleportation experiment with photons from remote QDs emitting at ca. 780 nm. The polarization state of a single photon emitted by one QD is prepared and interfaced with one photon of an entangled pair from a second QD in a Bell state measurement. This process teleports the polarization state onto the second photon of the entangled pair. Polarization-preserving

quantum frequency converters eliminate the frequency mismatch between photons, allowing for interference at telecom wavelengths. Teleportation succeeds with post-selected fidelities up to 0.721(33).

HL 34.2 Wed 16:45 POT/0051

Telecom C-band Quantum Dots Coupled to Gaussian-shaped Microlens Cavities — •Michelle Pfahl[1], Raphael Joos[1], Lena Engel[1], Johannes Michl[2], Katharina Dahler[1], Ponraj Vijayan[1], Tobias Huber-Loyola[2], Michael Jetter[1], Simone L. Portalupi[1], Sven Höfling[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen (IHFG), Center for Integrated Quantum Science and Technology (IQST) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart — [2]Julius-Maximilians-Universität Würzburg, Physikalisches Institut, Lehrstuhl für Technische Physik, Am Hubland, 97074 Würzburg

Single-photon sources emitting in the telecom C-band are a key resource for applications in quantum communication and quantum cryptography, as they enable long-distance quantum networks. Semiconductor quantum dots (QDs) are particularly well suited for this since they have a high quality optical emission and can achieve high efficiency when coupled to microcavities. Here, we investigate telecom C-band InAs QDs, which are embedded in a resonator made of distributed Bragg reflectors (DBRs), with the upper dielectric DBR being shaped into Gaussian lenses using an etching process. This structure promises Purcell enhancement, which reduces the decay time of the QDs and enables efficient collection of the emitted photons. We investigate the optical modes of the resonators by an in-depth characterization of microlenses with different design parameters. Furthermore, the quantum-optical properties of the QDs coupled to cavities are analyzed by means of autocorrelation and decay time measurements.

HL 34.3 Wed 17:00 POT/0051

InGaAs/GaAs preparation at 1.55 micrometer telecom wavelengths — •Juwana Jose, André Strittmatter, Armin Dadgar, Jürgen Bläsing, and Usha Velpuri — Otto von guericke university, Magdeburg, Germany

Quantum key distribution is a secure way of generating and sharing encryption keys using photons. Single photons as qubits for key generation is an efficient method of secure data transmission. It guarantees absolute eavesdropping detection since it is impossible to copy a quantum state. Qubit transmission at telecom wavelengths of 1.55 micrometer using InGaAs quantum dots on GaAs substrates is a challenge. We explore the conventional Stranski-Krastanow growth mode to shift the wavelengths far beyond the spectral 1.3-1.4 *m region. Photoluminescence experiments on high-density QD ensembles show remarkable intensities in a wavelength range of 1.5-1.6 micrometer at room-temperature. This luminescence shifts by xx nm into the blue upon cooling down to 15 K. By tailoring the thickness of the initial InGaAs deposition to the 2D/3D transition region low QD densities of 108 cm-2 and below are achieved. Single photon emission experiments will be conducted after preparation of individual QD emitters.

HL 34.4 Wed 17:15 POT/0051

Integration of telecom C-band quantum dot-based single-photon emitters onto silicon photonic platform using micro-transfer printing — •Simon Oberle[1], Ponraj Vijayan[1], Alessandro Buzzi[2], Hugo Larocque[2], Michael Jetter[1], Simone Luca Portalupi[1], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen (IHFG), University of Stuttgart — [2]Research Laboratory of Electronics (RLE), Massachusetts Institute of Technology

Silicon photonics for telecommunications applications has garnered much attention recently. The optical transparency and the large refractive index contrast of silicon at telecommunication wavelengths allow the implementation of high-density photonic integrated circuits. One disadvantage of silicon photonics is the lack of mature deterministic light sources. One potential solution is the integration of III-V material, which offers outstanding optical emission properties, on a silicon platform. The direct growth of III-V materials on silicon the most scalable and therefore desired approach. However, it is challenging because of the material polarity difference and the lattice mismatch between GaAs and silicon. An alternative approach is the hybrid integration of III-V structures using micro-transfer printing, which enables integration of prefabricated devices onto silicon. Our group has previously developed telecom C-band emitting InAs quantum dots grown on InGaAs. Here, we report our approach to designing and fabricating structures for the hybrid integration of these QDs onto a silicon platform using micro-transfer printing.

HL 34.5 Wed 17:30 POT/0051

Automated optical imaging for telecom Quantum Dot deterministic fabrication — •Eden Arbel[1], Lukas Wagner[1], Peter Gierss[1,2], Ponraj Vijayan[1], Michal Vyvlecka[1], Michael Jetter[1], Simone L. Portalupi[1], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQ^{ST}) and SCoPE, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]Physikalisch Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig

Semiconductor quantum dots (QDs) are promising sources of single- and entangled-photon pairs. Due to its low absorption in silica fibers, operation in the telecom C-band (1530-1565nm) is desired. Integrating these QDs into Circular Bragg Grating cavities (CBGs) enhances extraction efficiency and enables Purcell enhancement. Our method employs wide-field imaging for deterministic preselection of QDs for subsequent CBG fabrication. The QD positions are referenced using e-beam-written markers. Smart preselection of suitable candidates, embedded in an automated setup, promises higher yield and efficiency, with the potential for AI integration. We demonstrate that deterministically processed CBGs exhibit significant improvements in brightness and enhance the decay time of the two-level state. With higher throughput and continually improving quality of telecom QD samples, this approach will enable to provide single-photon sources tailored to specific needs of various applications, such as quantum memories or long-distance quantum communication.

HL 35: Optical Properties II

Time: Wednesday 16:30–19:00 Location: POT/0251

HL 35.1 Wed 16:30 POT/0251

Polarization-Angle-Resolved Raman Spectroscopy for Reliable Raman Tensor Analysis — •Hans Tornatzky[1], Jonas Rose[1], Luca Choi[2], Moritz Meissner[1], Zbigniew Galazka[3], and Markus R. Wagner[1,2] — [1]Paul Drude Institut — [2]Technische Universität Berlin — [3]Institut für Kristallzüchtung

Phonons are fundamental to materials, shaping the physical properties that underlie device functionality. Accurate knowledge of their quantitative description, specifically the Raman tensor, is essential for a detailed understanding of materials and for reliable modeling and optimization of structures and devices.

This talk presents state-of-the-art approaches for determining relative Raman tensor elements using polarization-angle-resolved Raman (PARRS) spectroscopy, alongside discussion of major challenges and sources of error encountered in the process. We also introduce a newly developed fitting procedure that enables robust disentanglement of strongly overlapping signals arising from different modes, permitting precise extraction of their characteristics – energy, FWHM, symmetry, and tensor elements – with enhanced reproducibility.

These techniques are demonstrated across several materials recently studied by our group, including rutile GeO_2, Ga_2O_3, and $LaInO_3$.

HL 35.2 Wed 16:45 POT/0251

Characterization of Exciton-exciton entanglement in different phases: A many-body investigation in low dimensions — •Fangzhou Zhao[1], Carlos Mejuto-Zaera[2], Vojtech Vlcek[3], and Angel Rubio[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Laboratoire de Physique Théorique, LPT, CNRS, Toulouse, France — [3]UCSB, Santa Barbara, USA

There have been emerging experimental investigations on exciton-exciton correlations, especially in moiré superlattices. However, theoretical understanding of exciton-exciton interactions - which requires an accurate treatment of four-point Green's functions and the validity of a bosonic description of excitons- remains relatively underdeveloped. We construct an exactly solvable one-dimensional model to investigate exciton-exciton correlations and entanglement using many-body exact techniques. We identify phase boundaries separating excitonic phases with different degrees of binding, and extrapolate the data to the thermodynamic limit to infer properties in large systems. We also apply a wavefunction projection technique to characterize the strength of entanglement between excitons, as well as the strength of entanglement between the electron and hole inside an exciton. Our results show that, over a broad parameter range, excitonic correlations remain weak, validating the applicability of many-body perturbation theory in most cases. We also explored the quantum confinement effect of multi-exciton state in 1D systems and uncovered the conditions under which the confinement effects emerge.

HL 35.3 Wed 17:00 POT/0251

Excited-state trions in a quantum well — Sourabh Jain[1], Mikhail Glazov[2], and •Ashish Arora[1] — [1]Indian Institute of Science Education and Research, Pune 411008 India — [2]St. Petersburg, Russia

Recently, excited-states of trions were discovered in a layered semiconductor raising strong interest in many-body physics of Coulomb-bound quasiparticles in solids [1]. Here, we report on the observation of an excited 2s state of a trion in a GaAs quantum well (QW) using magneto-optical Kerr effect (MOKE) spectroscopy under out-of-plane magnetic fields up to 6 T [2]. This resonance ap-

pears slightly below the 2s exciton in energy. Strikingly, the 2s trion is found to be bound only for magnetic fields larger than 1 T. The signature of the 2s trion is absent in the magneto-reflectance spectra, while it is detectable in the MOKE spectra signifying the importance of the powerful technique. Similar to the 1s states, the 2s trion shows an opposite degree of magnetic-field-induced polarization compared to its exciton counterpart, in agreement with our theoretical calculations. This transfer of oscillator strength between the complexes establishes an optical fingerprint of the 2s excited trion. Our work addresses a four-decade old problem of excited-state trions in a quantum well, and opens scope for further investigations of many-body physics in solids. [1] Phys. Rev. Lett. 123, 167401 (2019) [2] Phys. Rev. Lett. 134, 246902 (2025)

HL 35.4 Wed 17:15 POT/0251

Directional lasing and optical coupling in indium phosphide nanowires — •Lukas Raam Jäger[1], Wei Wen Wong[2], Hark Hoe Tan[2], and Carsten Ronning[1] — [1]Friedrich-Schiller-Universität Jena, Fürstengraben 1, 07743 Jena, Germany — [2]The Australian National University, Canberra ACT 2600, Australia

Indium phosphide (InP) nanowires (NWs) are promising nanoscale light sources due to their strong optical confinement and compatibility with selective-area epitaxy. We investigate optical coupling in vertically standing lasing InP NWs using finite-difference time-domain simulations and angle-resolved photoluminescence. Single NWs lase in the TE01 mode for diameters above about 250 nm and exhibit far-field patterns shaped by interference of emission from the top and bottom facets. Coupled NW structures enable controlled emission engineering. In NW pairs, coupling splits the TE01 mode into two hybrid modes with orthogonal directional lobes, in good agreement with experiment. Mode selection is highly sensitive to subtle geometric differences, while asymmetric pumping has negligible effect. Extending this concept to arrays of NW pairs shows that array-level interference can further narrow the emission lobes. Triplet NW structures exhibit three distinct hybrid modes with characteristic far-field patterns. These results demonstrate designable directional nanoscale emitters based on coupled NW lasers.

HL 35.5 Wed 17:30 POT/0251

Optical emission of monolayer-hybridized nanowire lasers — •Moritz Willems, Edwin Eobaldt, Alexander Zaunick, Aurelia Eberhard, Lukas Jäger, Xiao Chen, and Carsten Ronning — Friedrich Schiller Universität, Jena, Deutschland

Semiconductor Nanowires have attracted substantial scientific interest as foundation for nanoscale coherent light sources and all-optical circuits, based on to their remarkable waveguide properties and their intrinsic ability to lase. 2D-Materials offer a functional environment that enables influencing the lasing characteristics, including emission wavelength and lasing threshold, of ZnO nanowires. These hybrid structures thus allow for electrical and optical charge and energy transfer. Deterministic nanowire integration is achieved through stage-assisted transfer using PDMS and tip-assisted nanomanipulation. Comparative micro-photoluminescence measurements are used to investigate how the 2D-materials influence and modify the lasing behaviour of individual nanowires.

HL 35.6 Wed 17:45 POT/0251

Bandgap and exciton engineering in two-dimensional transition $Mo_{1-x}W_xSe_2$ alloys for next-generation photonics. — •Muhammad Hussain[1], Omid Ghaebi[1], Mohammad Monfared[2], Marco Gruenewald[1], Umer Ahsan[3], Fedor Lipilin[3], Jan Luxa[3], Zdenek Sofer[3], Ulf Peschel[2,4], and Giancarlo Soavi[1,4] — [1]Institute of Solid-State Physics, Friedrich Schiller University Jena, Germany — [2]Institute of Condensed Matter Theory and Optics, Friedrich Schiller University Jena, Germany. — [3]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Czech Republic — [4]Abbe Center of Photonics, Friedrich Schiller University Jena, Germany

Alloys of 2D transition metal dichalcogenides (TMDs), provide a unique platform for bandgap engineering at the atomic scale. In this work, we investigate the nonlinear optical response of $Mo_{1-x}W_xSe_2$ alloys focusing in particular on second harmonic generation (SHG) and two-photon photoluminescence (TP-PL) [1]. We find that alloyed TMDs exhibit enhanced nonlinearities compared to their pristine counterparts. By combining SHG and TP-PL and the respective optical selection rules, we are able to extract the energy difference between 1s and 2p exciton states in samples of different alloy composition. By doing this, we find that the exciton binding energy in such alloys varies with the W composition (x). This can be used as a knob to tune not only the optical bandgap, but also the exciton binding energy by changing the alloy composition.

[1] M. Hussain, et al. Adv. Opt. Mater. 13, 01000 (2025).

15 min. break

HL 35.7 Wed 18:15 POT/0251

Photoluminescence of single color centers in hBN below the diffraction limit — •Iris Niehues[1], Daniel Wigger[2], Korbinian Kaltenecker[3], Annika Klein-Hitpass[1], Johannes Binder[4], Andrzej Wysmołek[4], and Rainer Hillenbrand[5] — [1]Institute of Physics, University of Münster, Germany — [2]Department of Physics, University of Münster, Germany — [3]Department of Physics, Ludwig-Maximilians-Universität München, Germany — [4]Faculty of Physics, University of Warsaw, Poland — [5]CIC nanoGUNE BRTA, Spain

Color Centers in hexagonal boron nitride (hBN) are promising quantum light sources due to their stable single-photon emission at room temperature. Using a scattering-type near-field optical microscope, we investigate photoluminescence (PL) properties of hBN grown via metalorganic vapor phase epitaxy. Our experiments employ the microscope in tapping mode to detect PL signals influenced by the metallic AFM tip. We demonstrate near-field optical excitation and emission via the tip's nanofocus, creating a sub-diffraction limited tip-enhanced (TE)PL hotspot [1]. Additionally, an "arc" forms around the emitter, explained by constructive interference between direct beams between the optics and the emitter and indirect beams scattered from the tip. This tip-assisted (TA)PL method can be used to map in-plane dipole orientations of hBN color centers at the nanoscale.

[1] I. Niehues et al., Nanophotonics 14(3), 335-342 (2025)

HL 35.8 Wed 18:30 POT/0251

Role of lattice temperature for the optical properties of boron nitride — •Peter Kratzer[1] and Andre Schleife[2] — [1]Faculty of Physics, University Duisburg-Essen, 47057 Duisburg, Germany — [2]Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, USA

We carried out a computational study of boron nitride both in its cubic (c-BN) and hexagonal (h-BN) polytypes as a prototypical system for the renormalization of optical properties in semiconductors by lattice vibrations. While band-gap renormalization due to electron-phonon coupling is a well-explored concept in semiconductor physics, this topic has gained renewed attention in the context of pump-probe spectroscopies where high fluences may lead to local lattice excitation. With this motivation, we performed first-principles calculations of c-BN and h-BN supercells using the DFT+GW method, treating lattice excitation via explicit atomic displacements. Finally, the frequency-dependent dielectric function and the optical absorbance are obtained including many-particle effects on the level of the Bethe-Salpeter equation. The results show that the atomic displacements in the 2x2x2 supercells used in this study have little effect in c-BN but lead to a considerable narrowing of the optical gap in h-BN. In h-BN, the band splitting due to 'frozen' phonons gets even amplified on the GW level of theory. The binding energy of approximately 0.5eV of the exciton derived from the band edges, however, is found to be only weakly affected by the atomic displacements.

Financial support from CRC 1242 is gratefully acknowledged.

HL 35.9 Wed 18:45 POT/0251

Half-saddle excitons in monolayer SnS2: a first-principles study — •Vinicius Alves Bastos[1], Fulvio Paleari[2], Eleonora Luppi[3], Marco Gibertini[1,2], and Alice Ruini[1,2] — [1]Dipartimento di Scienze Fisiche, Informatiche e Matematiche, UNIMORE, Modena (Italy) — [2]CNR-Nano, Modena (Italy) — [3]Laboratoire de Chimie Théorique, Sorbonne Université and CNRS, Paris (France)

Monolayer SnS2 has been demonstrated as a visible-light absorber with promising characteristics for applications in fuel cells and thin film photovoltaics [1]. Motivated by that, we have performed a first-principles study of bound excitons in this system within the GW-BSE formalism [2]. We have gone beyond previous works by analysing the exciton symmetries, electron-hole contributions, and transition dipoles. We find a richer structure of bound excitons than previously reported, e.g., deeply bound dark excitons with binding energies of about 0.9 eV and a very strong bright exciton at 2.9 eV, in good correspondence with the experimental absorption peak. Also, the bound excitons are localized around the direct band gap at the M point, which exhibits a saddle point at the top valence band and a minimum at the bottom conduction band. Consequently, we show that linearly polarized light can be used to completely select two of the three inequivalent M saddles, as previously demonstrated in graphene [3]. PNRR MUR project ECS_00000033_ECOSISTER

[1] Y. Sun et al., Angew. Chem. Int. Ed. 51, 8727 (2012). [2] D. Sangalli et al., J. Phys. Condens. Matter. 31, 325902 (2019). [3] S. Sharma et al., arXiv preprint, arXiv:2503.21376 (2025).

HL 36: 2D Materials VI – Optoelectronic properties

Time: Wednesday 17:30–18:30 Location: POT/0081

HL 36.1 Wed 17:30 POT/0081

Surface acoustic wave-controlled photocurrent in few-layer WSe2 — •Benjamin Mayer, Felix Ehring, Matthias Weiss, Hubert Krenner, Ursula Wurstbauer, and Emeline Nysten — Institute of Physics, University of Münster, Germany

Surface acoustic waves (SAWs) offer a versatile platform for nanoscience applications [1]. Their ability to integrate GHz-frequency control and sensing schemes at micron-scale wavelengths on a chip opens cross-disciplinary applications and enables the SAW electric field to drive acousto-electric currents in low-dimensional materials, including semiconducting transition metal dichalcogenides (TMDCs) [2]. Here, we study the AEC and the underlying charge-carrier dynamics in mechanically exfoliated 2D tungsten diselenide (WSe2) placed on two gold electrodes integrated into hybrid lithium-niobate-based SAW devices (150-250 MHz). Our multifunctional acousto-optoelectric setup combines current-voltage characterization, SAW-direction dependent AEC measurements and spectrally resolved scanning photocurrent (PC) spectroscopy. This allows detailed investigation of how electrical contacts affect the performance of our archetypical acoustophoto-electric device. Thus, we establish a qualitative model of the tunneling barrier and band bending induced by Schottky barriers at the Au-TMDC interface [3]. Further, tuning the optical excitation wavelength provides spectral access to energy-dependent photocurrent contributions and reveals how they are modulated by the SAW.

[1] Krenner, J. Phys. D: Appl. Phys. (2025, subm.) [2] Nat. Comm. 6 (1): 8593 (2015) [3] ACS Appl. Electr. Mat. 7 (21): 9717 (2025)

HL 36.2 Wed 17:45 POT/0081

Shift current tuned via twisting angle in moiré system — •Michele Bagaglini[1,2], Cesare Tresca[2], and Gianni Profeta[1,2] — [1]Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell'Aquila, L'Aquila, Italy — [2]CNR-SPIN c/o Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell'Aquila, L'Aquila, Italy

In recent years the interest in the two-dimensional bulk photovoltaic effect (BPVE) has been increasing in non-centrosymmetric materials. Research on 2D solar cells and optoelectronic device is focusing on these materials due to their highly efficient response. The shift current (SC) is one of the most important effect to the BPVE. The SC is second-order non-linear response that arises from the different real-space centres position of charge, a 'shift', between the valence and conduction bands. In the literature, several studies already exist on the SC in monolayer and untwisted bilayer transition-metal dichalcogenide (TMD) systems, where promising peaks have been reported from DFT calculations. In this study we focus on the evolution of the SC with the twisting angle in moiré twisted two-dimensional materials, specifically in multilayer MoS2 systems. In our case, given the large size of the systems for small twist angles, we employ a tight-binding (TB) approach with Slater-Koster (SK) parameterization to compute the SC. We show that a multiband approach improves the accuracy and allows one to reproduce the dispersions obtained from first-principles calculations.

HL 36.3 Wed 18:00 POT/0081

Theoretical investigation of the flexo-photovoltaic effect — •Juan Jose Esteve-Paredes[1], Maria N. Gastiasoro[2], and Julen Ibanez-Aspiroz[1] — [1]Materials Physics Center, University of the Basque Country, Donostia-San Sebastian, Spain — [2]Donostia International Physics Center, Donostia-San Sebastian, Spain

The bulk photovoltaic effect (BPVE) refers to the generation of a direct current in a bulk crystal under illumination. This phenomenon arises in non-centrosymmetric materials and is described by a finite electronic second-order conductivity. In recent years, experimental works have reported the realization of the BPVE in centrosymmetric media, where this effect is conventionally forbidden, by generating large strain gradients through application of local pressure with nanoscale tips [1,2]. This new effect, named the flexo-photovoltaic effect, has attracted interest regarding its microscopic origin. In this talk, we theoretically investigate this effect and demonstrate that a flexo-photovoltaic effect can indeed be predicted by considering local lattice deformations in several-layer centrosymmetric crystals, giving rise to the appearance of a finite BPVE conductivity. We employ a Slater-Koster approach to model the electronic band structure and wavefunctions within a supercell geometry and compute the associated linear and second-order optical responses. We discuss the tunability and scaling of this effect in relation to the magnitude and spatial extent of the mechanical deformation, and discuss how our theoretical predictions compare with existing experimental observations. [1] Yang et al., Science 360, 904 (2018) [2] Wang et al., Phys. Rev. Lett. 132, 086902 (2024)

HL 36.4 Wed 18:15 POT/0081

All-in-one Optoelectronic Synaptic Device with Van der Waals materials-based floating gate — •Thi Phuong Anh Bach and Sangeun Cho — Division of System Semiconductor, Dongguk University, Seoul, South Korea

Optoelectronic synaptic devices that integrate nonvolatile memory with light matter interactions offer high processing efficiency and low energy consumption for neuromorphic computing. Two-dimensional materials and their van der Waals heterostructures provide strong electronic and optical properties, while floating-gate structures emulate synaptic plasticity and enable a path toward brain-inspired, beyond-von-Neumann computation. Herein, we demonstrate a multifunctional optoelectronic synapse device based on rhenium disulfide (ReS2)/hexagonal boron nitride (hBN)/indium selenide (InSe) vdW FG structure. The device exhibits a high On/Off current ratio (>10^6), large memory window, multi-level storage behavior and excellent data retention (~10000 s) under various electrical and optical stimuli. By leveraging the thickness tunable bandgap of InSe FG and the dynamic tunneling process of photogenerated carriers across the vdWhs interface, the device capable to work under a wide range from visible to near-infrared laser with excellent synaptic plasticity. The device replicates classical conditioning (Pavlov's dog experiment) and advanced signal-discrimination learning, and also supports reconfigurable inverter logic via electrical and optical inputs, along with neuromorphic image recognition, demonstrate its multifunctionality.

HL 37: Nitrides II – Designed properties and LED

Time: Thursday 9:30–11:00 Location: POT/0006

HL 37.1 Thu 9:30 POT/0006

Designing Visible-Spectrum Nitride Alloys from First Principles — •Jan M. Waack[1,2], Michael Czerner[1,2], and Christian Heiliger[1,2] — [1]Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Germany — [2]Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, Germany

Precise band-gap engineering across the full visible spectrum is essential for emerging applications such as integrated RGB LEDs. This tunability can be achieved through alloying narrow-band-gap materials like InN or ScN with wide-band-gap semiconductors such as GaN or AlN. Among these systems, random alloys including (In,Ga)N and (Al,Sc)N require advanced theoretical treatments–such as the coherent potential approximation (CPA) and special quasi-random structures (SQS)–to capture their configurational disorder accurately.

In this work, we combine first-principles density functional theory with efficient electronic-structure methods such as LDA-1/2 and the mBJ functional to provide a comprehensive dataset for both random and ordered alloy phases. We report key structural properties including lattice parameters and bond lengths as well as elastic constants, phonon modes, thermodynamic stability, and electronic characteristics such as band gaps and Bloch spectral functions. These results offer a robust theoretical foundation for experimental detection of ordering phenomena and for the rational design of nitride alloys with tailored optical and electronic properties.

HL 37.2 Thu 9:45 POT/0006

Detailed nano-characterization of structural and optical properties of a red-emitting InGaN LED — •N. Dreyer[1], F. Bertram[1], G. Schmidt[1], J. Christen[1], Z. Chen[2], and X. Wang[2] — [1]Otto-von-Guericke-University Magdeburg, Germany — [2]Peking University, Beijing, China

A fully processed and operating red InGaN LED was grown by MOVPE on a GaN/sapphire template. The active region, which consists of three identical stacks, is surrounded by *n*- and *p*-GaN with an EBL. Each stack contains three quantum wells with different indium concentrations: two with a low indium concentration for strain relaxation, and one subsequently grown red-emitting quantum well (RQW). The structure was characterized using scanning transmission electron microscopy (STEM) and the orientation of the Burgers vector (edge- or screw type dislocation) was determined. Cross-sectional cathodoluminescence performed directly in STEM shows broad band-to-band recombination in the *n*-GaN at $T = 17$ K which is caused by band gap renormalization and conduction band filling. Line shape analysis of this emission band yields a charge carrier density of 6×10^{18} cm^{-3}. The vertical evolution of the RQW emission exhibits a shift of 123 meV within the active region. Furthermore, the lateral homogeneity

of the RQW emission will be examined. A blue-shift of the RQW emission of up to 365 meV was found around defects. The vertical and lateral trapping processes of excess carriers will be discussed in detail. The capture length of the bottom RQW was found to be 78 nm using highly spatially resolved vertical linescans across the active region.

HL 37.3 Thu 10:00 POT/0006

Determination of optical losses in AlGaN-based multimode waveguides — •Verena Kowallik[1], Martin Guttmann[2], Leonardo Wildenburg[1], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute for Physics & Astronomy, Berlin, Germany — [2]Ferdinand-Braun-Institut (FBH), Berlin, Germany

Many applications for ultraviolet photonic integrated circuits (UV PICs), such as biochemical sensing, atomic clocks, and UV Raman spectroscopy, require materials with a large bandgap energy to facilitate low optical losses. One possible candidate are AlGaN alloys which are already successfully employed for the fabrication of UV light emitting diodes (UV-LEDs) and UV lasers. However, the optical properties of AlGaN materials, especially the absorption losses have not yet been studied in detail in the UVC spectral range. In this work, the absorption losses in 200 μm wide n-$Al_{0.76}Ga_{0.24}N$ waveguides were investigated using monolithically integrated UV-LEDs emitting at 262 nm and detectors. By Monte Carlo ray-tracing simulations, we identified different contributions of the optical losses, namely, the propagation losses and scattering losses. Here, we implemented the waveguide surface roughness determined from atomic force microscopy images. Also, we investigated the portion of rays reaching the detector without beeing guided in the waveguide, e.g. scattered at the substrate's backside or the AlN/sapphire interface.

HL 37.4 Thu 10:15 POT/0006

Influence of the AlGaN multi-quantum well design on the efficiency of 233 nm far-UVC LEDs grown by MOVPE — •Rebekah Seonggyeong Kim[1], Marcel Schilling[1], Massimo Grigoletto[1,2], Jakob Höpfner[1], Tim Wernicke[1], and Michael Kneissl[1,2] — [1]Technische Universität Berlin, Institute of Physics and Astronomy, Berlin, Germany — [2]Ferdinand-Braun-Institut (FBH), Berlin, Germany

Light emitting diodes (LEDs) emitting in the far ultraviolet-C (far-UVC) spectral range are promising for applications like skin safe disinfection and gas sensing. The composition and thickness of the AlGaN-multi quantum wells and barriers are crucial for the efficiency of the LEDs. In this work we investigate the impact of the last quantum well barrier's (LB) thickness (0 nm to 10 nm) and aluminum mole fraction (76% - 86%) onto the electrooptical performance of the LEDs. The LEDs with an aluminum mole fraction of 80 % and a thickness of 5 nm exhibit the highest external quantum efficiency (EQE) of 0.32 % at 16 mA (on-wafer).

HL 37.5 Thu 10:30 POT/0006

In-rich InGaN quantum well growth for green InGaN LED — •Christoph Berger, Armin Dadgar, and André Strittmatter — Otto-von-Guericke-University, Magdeburg, Germany

Achieving high-efficiency green InGaN LEDs remains challenging due to material issues like phase instability, metallic inclusions and interface roughening. We present an optimized MOVPE growth approach that significantly improves the optical and morphological quality of green LEDs. After each QW, a growth interruption combined with a controlled temperature ramp is introduced before starting the GaN barrier growth. This sequence allows to get rid of excess indium that accumulates on the surface during QW growth, leading to smoother interfaces, a removal of indium-rich defects visible in Nomarski microscopy and consequently, a substantial suppression of a grayish appearance of the wafer. We further combine this process with hybrid MQW designs, where blue QWs are grown below a green top QW, leading to an improvement of the efficiency of the LED. The impact of different growth sequences and layer designs on the optical and structural characteristics of green LEDs will be discussed.

HL 37.6 Thu 10:45 POT/0006

Nano-characterization of polarization-doped deep UV LED structures using highly spatially resolved cathodoluminescence spectroscopy — •E. Bäker[1], F. Bertram[1], G. Schmidt[1], N. Dreyer[1], J. Christen[1], T. Kolbe[2], S. Hagedorn[2], H.K. Cho[2], J. Rass[2], S. Einfeldt[2], and M. Weyers[2] — [1]Otto-von-Guericke-University Magdeburg, Germany — [2]Ferdinand-Braun-Institut (FBH), Germany

AlGaN-based deep UV LEDs emitting below 250 nm are of great interest for many applications. Especially in the far-UVC, efficient p-doping poses major challenges, which can be effectively overcome by the concept of polarization doping. This study compares far-UVC LEDs with different AlGaN composition gradients used for polarization doping. The LEDs were grown by MOVPE on optimized AlN/sapphire templates. While the n-side of the diode uses conventional Si-doping, the p-side utilizes an AlGaN-layer with constant [Ga]-gradient. Diodes with different [Ga]-gradients but identical thicknesses are analyzed, with the Ga mole fraction increasing linearly from 0.02 to 0.45 and from 0.02 to 0.81, respectively. Using low temperature cathodoluminescence spectroscopy directly performed in a scanning transmission electron microscope, a nano-scale correlation of the optical properties with the real structure is obtained. Cross-sectional CL line scans show the different emission of the gradient layer. While the sample with the shallow gradient shows continuous emission spectral red-shift from 240 nm to 260 nm, the sample with the steep gradient shows an abrupt jump from 273 nm to 312 nm, indicating lattice relaxation.

HL 38: Materials and Devices for Quantum Technology II

Time: Thursday 9:30–12:45 Location: POT/0051

HL 38.1 Thu 9:30 POT/0051

Shadow masks for all-in-situ fabrication of InAs nanowire Josephson junctions — •Christian Schäfer, Lennart Grosch, Yurii Kutovyi, Nils von den Driesch, Thomas Schäpers, and Alexander Pawlis — PGI 9 / PGI 10 / JARA-FIT, Forschungszentrum Jülich, 52428 Jülich, Germany

Josephson junctions based on semiconductor/superconductor hybrid structures offer unique features for quantum circuits, such as gate-controllable supercurrent and quantized Andreev bound states. Clean interfaces between nanowire and superconductor are essential to leverage both effects, driving the development of in-situ contact fabrication. Shadow wall epitaxy offers both, a scalable and all-in-situ solution for nanowire growth and contact formation. Micrometer-high pre-fabricated walls shadow the molecular beams of In and As depending on their relative orientation. Since As on its own has a low sticking coefficient and In forms isolated droplets, partially shadowed regions are insulating and do not form InAs crystals. Despite the significant lattice mismatch between InAs and the GaAs substrate, we observe growth of lateral 1D-nanowires between walls spaced less than one micrometer. The same mask can additionally be used to perform selective deposition of any superconductor. We explore different mask designs to optimize electrical device isolation, nanowire growth, and junction geometry. Since no transfer or post-processing after growth is necessary, associated defects and degradation are avoided. Shadow wall epitaxy enables scalable in-situ fabrication of InAs nanowire junctions.

HL 38.2 Thu 9:45 POT/0051

Semiconductor–superconductor membranes for nanoelectronic devices — •Thies Jansen[1], Christian Reichl[2], and Thomas Sand Jespersen[1,3] — [1]Technical University of Denmark, Anker Engelunds Vej 101 2800 Kongens Lynby — [2]ETH Zürich Laboratorium für Festkörperphysik — [3]Center for Quantum Devices Niels Bohr Institute, University of Copenhagen

Semiconductor-superconductor hybrid materials have become the workhorse platform for quantum devices, owing to their clean and highly transparent semiconductor-superconductor interfaces. Indium arsenide–aluminum (InAs-Al) nanowires and quantum wells are currently the dominant material systems, each offering distinct advantages: nanowires allow transfer to arbitrary substrates, while quantum wells provide two-dimensional design flexibility. Here, we introduce a new platform that combines the strengths of both systems: a semiconductor-superconductor membrane. We present the fabrication of these membranes and their initial electrical characterization through low-temperature transport measurements. The membranes are gate-tunable, and their material properties closely resemble those of both InAs nanowires and InAs quantum wells.

HL 38.3 Thu 10:00 POT/0051

Secondary electron detector for deterministic single ion implantation — •Priyal Dadhich, Nico Klingner, and Gregor Hlawacek — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf(HZDR), Dresden, Germany

Fault tolerant quantum computers based on donor-ion solid-state qubits require highly localized placement of single donors. To achieve this, we are developing a new setup for deterministic single-ion implantation in a FIB. To detect each implanted ion, we aim to use the secondary electrons (SEs) emitted during ion impact. A windowless silicon drift detector (SDD), biased up to +10 kV, accelerates and collects these SEs. The resulting electron-hole pairs allow us to quantify the number of emitted electrons via pile-up analysis. A critical challenge for this detection approach is the intrinsic SE emission probability. As governed by Poisson statistics, the average SE yield strongly affects detection confidence. Current work examines material-dependent absolute SE yields and practical methods to enhance SE emission while maintaining efficient extraction. Given the low SE

yield per impact, optimizing the extraction geometry is crucial. A C++ simulation code using the ion-optics library IBSIMU [1] has been developed for this customised problem, to maximize SE collection and study backscattering, including possible methods to recollect backscattered electrons. References: [1] T Kalvas et. al. Rev. of Sci. Inst., 81(2), 2010.

HL 38.4 Thu 10:15 POT/0051

Spin-orbit-enabled realization of arbitrary two-qubit gates on moving spins — •David Fernández-Fernández[1], Yuta Matsumoto[2], Lieven M.K. Vandersypen[2], Gloria Platero[1], and Stefano Bosco[2] — [1]Instituto de Ciencia de Materiales de Madrid, CSIC, Spain — [2]QuTech and Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands

Shuttling spin qubits across semiconductor quantum dot arrays is emerging as a key primitive for scalable quantum information processing, enabling on-chip inter-node quantum communication and modular architectures. By analyzing the shuttling of two spin qubits towards each other using a conveyor-mode protocol, we show that controlling only two experimentally accessible parameters, the shuttling velocity and the waiting time at minimum interdot separation, is sufficient to synthesize a broad class of entangling gates. Moderate SOI provides direct access to both CPHASE(θ) and SWAP$^{\alpha}$ families, as well as native fermionic-simulation gates, all with fidelities above 99.99% neglecting decoherence. We further quantify gate accessibility through a Weyl-chamber analysis and demonstrate that strong SOI or engineered helical magnetic fields can unlock nearly complete (~ 99.98%) coverage of all locally inequivalent 2Q operations, including quantum gates such as the Berkeley gate. This work provides a realistic and scalable route toward single-step 2Q gates on mobile spin qubits, with immediate implications for distributed quantum computing, quantum simulation, and shuttling-assisted error-correcting architectures.

HL 38.5 Thu 10:30 POT/0051

Topological Superconductivity in the Presence of Contact Potentials — •Leonard Kaufhold — Institute for Theoretical Physics, Cologne, Germany

The research on Majorana bound states (MBS) has brought forth a multitude of proposed platforms and devices that are, in principle, capable of realizing such states as topological edge modes. These devices usually rely on the superconducting proximity effect induced in semiconductors with strong spin-orbit coupling or, more recently, in topological insulators. The material interface however induces another effect that can be as much as one order of magnitude larger than the electronic band gap at the surface. Due to the mismatch of work functions between the materials, a dipole layer forms at the interface, effectively creating a contact potential that modifies the electronic band structure far beyond the minimal models typically used to describe the formation of MBS. In this presentation, we will focus on different nanowire-based architectures consisting of a topological insulator in contact with an s-wave superconductor, and discuss on a theoretical level the effect of contact potentials on the formation and stability of MBS. We further outline under which parameter conditions these interface-induced effects become experimentally relevant.

HL 38.6 Thu 10:45 POT/0051

Hexagonal Germanium Nanowires as a Spin Qubit Platform — •Anirban Das[1], Baksa Kolok[1,2], Daniel Varjas[1,3], and Andras Palyi[1,2] — [1]Department of Theoretical Physics, BME, Budapest, Hungary — [2]HUN-REN-BME-BCE QTRG, BME, Budapest, Hungary — [3]IFW Dresden and Würzburg-Dresden Cluster of Excellence ct.qmat, Dresden, Germany

Hexagonal germanium (2H-Ge) offers strong spin-orbit interaction and optical activity, making it an appealing platform for semiconductor spin qubits. Recent progress in growing hexagonal Si_xGe_{1-x} nanowires enables controlled geometries suitable for quantum devices. In contrast to cubic Si or Ge, 2H-Ge supports direct band-gap transitions, opening a pathway towards a novel spin-photon interface.

We study the electronic and spin properties of 2H-Ge nanowires using a multiband k·p Hamiltonian describing low-energy states near the Γ point. By discretizing the model with open boundaries, we construct nanowires oriented perpendicular to the c-axis and compute their band structure. We analyze confinement-induced gap variations and the influence of transverse electric fields, from which we extract Rashba coefficients. Magnetic fields are included via a Peierls substitution to investigate anisotropic spin responses. The resulting effective g-tensor shows strong directional dependence, revealing regimes favorable for qubit operation in hexagonal Ge nanowires.

This research is supported by the European Union within the Horizon Europe research and innovation programme via the ONCHIPS project under grant agreement No 101080022.

15 min. break

HL 38.7 Thu 11:15 POT/0051

Low-Loss LNOI PIC Components for Quantum Interference Applications — •Mohammad Malik[1,2,3], Simon Palitza[1,2,3], and Carsten Schuck[1,2,3] — [1]Department for Quantum Technology, University of Münster — [2]Center for NanoTechnology - CeNTech, Münster — [3]Center for Soft Nanoscience - SoN, Münster

Lithium niobate on insulator (LNOI) exhibits significant potential as a platform for integrated photonics owing to its strong electro-optic response, broad transparency window, and intrinsic nonlinear properties. For on-chip quantum key distribution (QKD) and related quantum photonic applications, the precise fabrication of photonic integrated circuit (PIC) components with minimal loss and high fidelity remains a key challenge. Here, we demonstrate directional couplers (DCs) and multimode interferometers (MMIs) that achieve a 50/50 splitting ratio with insertion losses below 1.5 dB at a wavelength of 1550 nm. These results are obtained using in-house fabrication techniques, including electron-beam lithography and inductively coupled plasma reactive ion etching, enabling accurate and reproducible realization of crucial PIC components. Building on these results, we will discuss progress towards integrating superconducting nanowire single-photon detectors (SNSPDs) on the LNOI platform for realizing on-chip Hong-Ou-Mandel interference as required for integrated quantum technology applications, including measurement device independent QKD.

HL 38.8 Thu 11:30 POT/0051

Scalable and individual control of Si qubits via magnetic skyrmions — •Leander Reascos[1], Raluca Boltje[1], Kai Litzius[1], Felix Büttner[1,2], and Mónica Benito[1] — [1]Institute of Physics, University of Augsburg, 86159 Augsburg, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, 14109 Berlin, Germany

Scalable, precise control of spin qubits is essential for large-scale quantum processors with millions of qubits. Electron-spin qubits in semiconductor quantum dots are promising due to their small size, high fidelities, long coherence times, and CMOS compatibility. However, current electric-dipole spin resonance (EDSR) schemes rely on static micromagnets, which suffer from fabrication-induced inhomogeneities and limited tunability. We propose using gate-tunable nanoscale magnetic skyrmions as on-chip magnetic field sources to replace micromagnets. By controlling skyrmion geometry, the local magnetic field at a quantum dot can be tuned post-fabrication to adjust both the qubit frequency and the EDSR driving gradient. Using micromagnetic simulations and analytical modeling, we show how skyrmion geometry maps directly onto the qubit's Zeeman splitting and Rabi frequency. These results highlight skyrmion-based control as a promising route towards scalable, frequency-selective spin-qubit architectures with enhanced tunability.

HL 38.9 Thu 11:45 POT/0051

Strain modulation in Germanium: an overview for quantum applications — •Meera None[1], Ignatii Zaitsev[1], Davide Spirito[2], Patricio Farrell[3], Christian Merdon[3], Yiannis Hadjimichale[3], Daniel Fritsch[4], Marvin Hartwig Zoellner[1], and Costanza Lucia Manganelli[1] — [1]IHP-Frankfurt (Oder)-Germany — [2]BC-Materials-Leioa, Spain — [3]WIAS-Berlin — [4]Zuse-Berlin

Germanium (Ge) is a promising platform for hole-based quantum devices due to its high hole mobility, strong spin-orbit coupling, and compatibility with CMOS technology. We investigate strain engineering in an ideal structure with two silicon nitride (SiN) stressors on a Ge substrate, using FEM to study how stress level, stressor height, and design influence mechanical deformation. The resulting strain tensors, including often neglected shear components, are inserted into a fully coupled 6x6 Bir-Pikus Hamiltonian to compute heavy hole (HH) and light hole (LH) band shifts under uniaxial and biaxial stress. Our results show tunable HH-LH splitting from 36 to 165 meV for SiN stressors between 1 and 4 GPa, demonstrating that SiN stressors offer a practical, scalable route to engineer Ge band structure for quantum wells and hole spin qubits.

HL 38.10 Thu 12:00 POT/0051

Optical probing of strain fields in isotopically pure Si-28 using donor-bound excitons — •Nico Eggeling[1], Phillip Külper[1], N.V. Abrosimov[2], Jens Hübner[1], and Michael Oestreich[1] — [1]Leibniz Universität Hannover, Germany — [2]IKZ Berlin, Germany

The successful demonstration of all optical qubits in isotopically pure Si-28 utilises the donor-bound exciton transition of phosphorus dopants [1]. As a current obstacle for large-scale implementation, the challenge remains to harness inhomogeneities resulting from simple imperfections in the crystal lattice, over dopant-dependent lattice deformations, to even the hydrostatic pressure due to the sample's own weight or adjacent interfaces. We present results from spatially resolved measurements of the donor-bound exciton, revealing a distinct strain distribution in a bulk Si-28 sample at cryogenic temperatures. These are explained in the context of the Pikus-Bir formalism for silicon [2], leading to strain estimates that are well matched to the known extrinsic factors.

[1] E.Sauter, PhD Thesis (2022)
[2] Loippo et al., Phys. Rev. Mater. 016202 (2023)

HL 38.11 Thu 12:15 POT/0051

Development of heavy noble gas field ion sources using an iridium coated single crystalline tungsten emitter — •Amina Zid[1,2], Gregor Hlawacek[1], Nico Klingner[1], Arnaud Houel[2], and Anne Delobbe[2] — [1]Institute for Ion Beam Physics and Material Research, Helmholtz-Zentrum Dresden-Rossendorf — [2]ORSAY PHYSICS, 95, 3ème Avenue - ZA Saint-Charles, 13710 Fuveau, France

Gas Field Ion Sources (GFIS) provide high brightness, high current density and excellent spatial resolution[1]. Conventional GFIS use light noble gases: helium enables 0.5 nm imaging resolution, while neon allows high-resolution milling beyond Liquid Metal Ion Source (LMIS) capabilities. However, low maximum current limits material removal rates, and the light ions cause deep implantation and bubble formation, reducing efficiency for large-volume or high-aspect-ratio milling. To overcome these limits, we investigate GFIS operation in a Focused Ion Beam (FIB) using heavier noble gases.

Additionally an iridium-coated tungsten tip is investigated. Iridium forms the strongest bond with tungsten[2], enabling higher electric fields and thus higher stable beam currents. Our emitter operates from a single emission point rather than the typical trimer used in Helium Ion Microscopy. This work presents the first FIB performance evaluation of this emitter with argon and xenon, including comparison to helium and neon-based GFIS.

[1] Höflich, K. et al., Applied Physics Reviews 2023; G. Hlawacek & A. Gölzhäuser (Eds.), Helium Ion Microscopy, Springer, 2016.

[2] Oshima, C. et al., Surface Science and Nanotechnology 2018.

HL 38.12 Thu 12:30 POT/0051

Finding the kinked propagation of the I3 defect in hexagonal silicon using a machine-learned potential — •Jolijn Dellevoet — Eindhoven University of Technology, Eindhoven, The Netherlands

Hexagonal silicon-germanium (hex-SiGe) alloys have recently emerged as promising direct-bandgap semiconductors suitable for on-chip optical communication, offering a path to reduce heat production in microchips. Currently, the hex-SiGe crystal is grown in core-shell nanowire structures, but their crystal quality is hindered by the formation of I3 defects. During growth, these defects nucleate and can propagate into otherwise pristine crystal. This propagation has been observed experimentally but not reproduced in atomistic simulations, leaving the underlying mechanism unclear. This presentation reveals, at atomic resolution, a kinking mechanism that enables the I3 defect boundary to propagate within hex-Si. This mechanism and its corresponding energy landscape are obtained by using the nudged elastic band (NEB) method in combination with the machine-learned PACE potential. Although the calculations are currently limited to Si systems, future studies could focus on extending the calculations to SiGe systems. The temperature and boundary length dependence of the transition rate can ultimately be used to optimize growth conditions of the hex-SiGe core-shell nanowires.

HL 39: 2D semiconductors VII – CrSBr and related heterostructures

Time: Thursday 9:30–12:30 Location: POT/0081

HL 39.1 Thu 9:30 POT/0081

Ab initio investigation of electronic, magnetic, optical properties and proximity effect in MoS_2/CrSBr van der Waals heterostructures — •Athanasios Koliogiorgos and Karel Carva — Charles University, Prague, Czech Republic

CrSBr-MoS_2 heterostructures combine the properties of the antiferromagnetic semiconductor CrSBr and the TMD semiconductor MoS_2, yielding a promising platform for spintronic and valleytronic applications. In connection with experimental work, using density functional theory with GGA+U and hybrid HSE06 functionals, we explore the structural, electronic, magnetic and optical properties of MoS_2/CrSBr systems, where CrSBr is 1-4 layers thick and MoS_2 a monolayer. We observe induced magnetization in the MoS_2 layer via proximity effect, strongly dependent on the interlayer distance. Other proximity effects include charge transfer, bandgap renormalization and spin splitting in the band structure, while the density of states reveals a weakly hybridized system, retaining the characteristics of the separate parts. Work function and band alignment show that the material behaves as a Type-II heterostructure. The calculation of the absorption coefficient reveals distinct peaks corresponding to the CrSBr and MoS_2 layers, in agreement with the experimental photoluminescence spectrum.

HL 39.2 Thu 9:45 POT/0081

Proximity-Induced Raman Signatures in a $NbSe_2$-CrSBr Superconductor-Magnet Heterostructure — •Elena Vinnemeier[1], Jan-Hendrik Larusch[1], Kai Rossnagel[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]Institute of Experimental and Applied Physics, Kiel University, Kiel, Germany

Interfacing superconducting $NbSe_2$ with the antiferromagnetic semiconductor CrSBr provides a van der Waals platform to study proximity effects in quantum devices. The superconductivity-magnetism interplay enables Josephson junctions and superconducting quantum interference devices with field-tunable critical current and spin filtering. We study proximity effects of the spin ordered CrSBr on the specific collective modes in $NbSe_2$ in the superconducting phase at 4K and the charge-density wave phase at 15K. A magnetic field tunes CrSBr from antiferromagnetic to ferromagnetic order. The Raman response of the heterointerface, relative to bare $NbSe_2$, reveals proximity effects from the ferromagnetic CrSBr layer at the interface. Modifications of the $NbSe_2$ collective excitation spectrum demonstrate strong interaction between the proximitized magnetic order in CrSBr and correlated phases in $NbSe_2$. This project was supported by the EIC pathfinder grant 101130224 "JOSEPHINE".

HL 39.3 Thu 10:00 POT/0081

Exciton dominated anisotropic dielectric tensor in CrSBr — •Jan-Hendrik Larusch[1], Pierre-Maurice Piel[1], Aleksandra Łopion[1], Thomas Kliewer[1], Zdeněk Sofer[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, University of Münster, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Prague, Czech Republic

CrSBr is an air-stable magnetic vdW semiconductor with a direct bandgap; its anisotropic spin, lattice, and charge, drive anisotropic light-matter interaction $\varepsilon(\omega)$. We directly determine the full dielectric tensor of exfoliated CrSBr by spectroscopic imaging ellipsometry (SIE). In the paramagnetic phase, SIE verifies $\varepsilon_{xx} \times \varepsilon_{yy} \times \varepsilon_{zz}$. Room-temperature comparison of Mueller-matrix and generalized ellipsometry guides cryogenic SIE, enabling us to track changes across the Curie and Néel temperatures as the system evolves from paramagnetic over intralayer ferromagnetism to A-type antiferromagnetism. In the AFM phase, polarization-resolved magneto-reflectance with fields along c (hard), b (easy), and a (intermediate) axis yields critical fields of roughly 2.2, 1.05, and 0.3 T for transition to FM order sensed by distinct optical fingerprints. Together, these measurements quantify the anisotropic light-matter interaction and its dependence on magnetic order, linking exciton-dominated emission/absorption to the full dielectric tensor [1]. [1] J. Klein et al. ACS Nano 17, 5316-5328 (2023).

HL 39.4 Thu 10:15 POT/0081

Optical Probing of Interfacial Magnetic Properties of the CrSBr-$MnPS_3$ hetero-interface — •Thomas Kliewer[1], Aleksandra Łopion[1], Pierre-Maurice Piel[1], Jan-Hendrik Larusch[1], Zdeněk Sofer[2], and Ursula Wurstbauer[1] — [1]University of Münster, Germany — [2]University of Chemistry and Technology Prague, Czech Republic

CrSBr and $MnPS_3$ are both 2D antiferromagnetic semiconductors with different magnetic and optical properties. $MnPS_3$ has out-of-plane spin alignment while CrSBr's spins are aligned in-plane [1,2]. Interfacing these two materials is expected to result in complex interfacial spin-alignment, presumably with the stabilization of a non-collinear magnetic phase at the interface. CrSBr exhibits strong excitonic features coupled to the magnetic order [3]. This is used as a probe for the magnetic situation of the $MnPS_3$-CrSBr interface. The structures are characterized by polarization-resolved Raman spectroscopy measurements and the interfacial magnetic properties are probed by low-temperature magneto-photoluminescence and reflectance spectroscopies. We observed a peculiar influence of $MnPS_3$ on the optical response of CrSBr. A proximity-induced modification of the magnetic properties of CrSBr interfaced with $MnPS_3$ seems to induce long-range order, since the impact is observable on the CrSBr flake more than 10 μm away from the interfaced region. Our observations might be connected to the stabilization of an intermediate ordered magnetic state in CrSBr. [1] Wilson, et al. Nat. Mat. 20.12 (2021), [2] Kobets, et al. Low Temp. Phys. 35.12 (2009), [3] Heißenbüttel, et al. Phys. Rev. B 111.7 (2025)

HL 39.5 Thu 10:30 POT/0081

Coupling Between Vibrational, Electronic, and Magnetic States in CrSBr — •Daria Markina[1], Priyanka Mondal[1], Lukas Krelle[1], Sai Shradha[1], Mikhail M. Glazov[2], Regine von Klitzing[1], Kseniia Mosina[3], Zdenek Sofer[3], and Bernhard Urbaszek[1] — [1]Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 6-8, D-64289 Darmstadt, Germany — [2]St. Petersburg, Russia — [3]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Technicka 5, 166 28 Prague 6, Czech Republic

The van der Waals antiferromagnet CrSBr displays interplay between vibrational, electronic, and magnetic states, producing distinctive quasiparticle interactions. Using temperature-dependent polarization-resolved Raman spectroscopy with

optical absorption and photoluminescence excitation (PLE), we examine these effects across the magnetic phase transition. Under 1.96 eV excitation, the A_g^1, A_g^2, and A_g^3 Raman modes exhibit pronounced polarization and intensity changes near the Néel temperature, accompanied by modifications in excitonic oscillator strength and resonant PLE features. The distinct temperature evolution of Raman tensor elements indicates that individual phonons couple to specific excitonic and electronic states. The suppression of excitonic transitions above the Néel temperature links these effects to spin alignment, suggesting an indirect spin−phonon interaction mediated by exciton−phonon coupling. These findings establish CrSBr as a promising platform for studying quasiparticles in two-dimensional magnets and for potential quantum technologies.

HL 39.6 Thu 10:45 POT/0081

Evidence for a novel spin-density excitation in 2D magnetic semiconductor CrSBr — •Pierre-Maurice Piel[1], Jan-Hendrik Larusch[1], Aleksandra Łopion[1], Zdenek Sofer[2], and Ursula Wurstbauer[1] — [1]Institute of Physics, Muenster University, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Prague, Czech Republic

The van der Waals magnet CrSBr is an air-stable semiconductor with ferromagnetic layers, antiferromagnetic interlayer coupling, and a highly anisotropic bandstructure, resulting in quasi-one-dimensional excitonic states [1]. We probe the impact of magnetic order on excitons and collective modes using low temperature (4K) magneto photoluminescence and resonant Raman spectroscopy with special emphasize on the magnetic anisotropy and magnetic phase transitions. The excitonic signatures in photoluminesence show clear differences between antiferromagnetic and ferromagnetic regimes and reveal pronounced magnetic anisotropy. In resonant Raman, the first order Ag phonons remain essentially field independent, whereas additional modes appear only under excitonic resonance. We resolve a sharp mode near 248 cm-1 emerging in resonance with the A-exciton (~1.36eV) and a broad mode at 362 cm-1 occurring in A and higher-lying excitonic regimes. The mode's excitation energy and field dependence indicate selective access to different collective possibly spin-density excitations in CrSBr. [1] J. Klein et al., ACS Nano 17, 5316-5328 (2023).

15 min. break

HL 39.7 Thu 11:15 POT/0081

Tracking Magnetic Phase Evolution in CrSBr via Excitonic Emission and Absorption — •Lukas Krelle[1], Ryan Tan[1], Daria Markina[1], Priyanka Mondal[1], Kseniia Mosina[2], Kevin Hagmann[1], Regine von Klitzing[1], Zdenek Sofer[2], and Bernhard Urbaszek[1] — [1]Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 6-8, D-64289 Darmstadt, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Technicka 5, 166 28 Prague 6, Czech Republic

CrSBr is an air-stable magnetic van der Waals semiconductor, in which the interaction of excitons with the magnetic order enables the optical identification of different magnetic phases. Here, we study multi-layer samples of CrSBr inside a three-axis vector magnet and correlate magnetic order and optical transitions. We identify layer by layer switching of the magnetization through drastic changes of the optical absorption energy and strength as a function of the applied magnetic field. We find that ferromagnetic and antiferromagnetic order between layers can coexist in the same domain [1]. The photoluminescence evolution depends on the magnetic order and can differ for each emission. The intensity of energetically lower lying transitions reduces monotonously with increasing field strength whereas energetically higher lying transitions around the bright exciton increase in intensity close to the saturation field. Using this contrasting behavior we can therefore correlate transitions with each other. [1]: L. Krelle et al, ACS Nano 2025, 19, 33156

HL 39.8 Thu 11:30 POT/0081

Magnetically controllable exciton-polariton condensation in CrSBr microwires — •Christian Weidgans[1], Heng Zhang[1], Niloufar Nilforoushan[1,4], Julian Hirschmann[2], Marlene Liebich[1], Tobias Inzenhofer[1], Imke Gronwald[1], Josef Riepl[1], Kseniia Mosina[3], Zdeněk Sofer[3], Fabian Mooshammer[1], Florian Dirnberger[2], and Rupert Huber[1] — [1]University of Regensburg, Germany — [2]Technical University of Munich, Germany — [3]University of Chemistry and Technology Prague, Czech Republic — [4]Université Paris Cité, France

Coupling the macroscopic wave functions of quasiparticle condensates to other degrees of freedom, such as the electron spin, could offer valuable control knobs for future quantum applications. In particular, man-made condensates of light-matter hybrids known as exciton-polaritons have lacked a direct spin-related control mechanism. Here we demonstrate magnetically tunable exciton-polariton condensation in the antiferromagnetic semiconductor CrSBr, a van der Waals material with strongly linked optical and magnetic properties. Under photoexcitation, CrSBr microwires embedded in an optical cavity show the hallmarks of polariton condensation. The conditions for efficient optical pumping suggest a crucial role of recently discovered surface excitons. Applying an external magnetic field energetically shifts the photoemitting polariton states, enabling direct spin-based control. Our results highlight CrSBr microwires as a powerful platform for exploring magnetically tunable polariton condensates, their directional propagation and their potential for spin-based quantum devices.

HL 39.9 Thu 11:45 POT/0081

Preparation and characterization of CrSBr on opal substrtates — •Jannik Schürmann[1], Aleksandra Lopion[1], Ursula Wurstbauer[1], Alexey V. Scherbakov[2], and Giulia Magnabosco[3] — [1]University of Münster, Münster, Germany — [2]Technische Universität Dortmund, Dortmund, Germany — [3]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Ger- many

The magnetic semiconductor Chromium-Sulfur-Bromide (CrSBr) is a highly anistropic van der Waals material. To study the anisotropy of the phononic properties independent from the supporting substrate, the flakes can be detached from it either by suspending it over cavities or by transferring it to a substrate containing closely packed silica spheres (opals). This second approach was already applied to other, nonmagnetic vdW materials such as WSe2 allowing an in-depth pump-probe study of phonons in the material [1]. Accordingly, we transfer mechanically exfoliated CrSBr onto opal substrates using polycarbonate stamps (dry transfer) and thoroughly characterize the properties and qualities of the flakes on opals. Atomic force microscopy confirms that CrSBr is on top of the spheres and partially freestanding. PL and Raman measurements are performed to validate the behavior of the flake in comparison with fully supported one. The decoupled CrSBr flakes on opal substrates are suitable for pump-probe studies of phonon states in CrSBr.

[1] A. Carr et al, ACS Photonics, 11, 1147-1155 (2024) .

HL 39.10 Thu 12:00 POT/0081

Accurate electronic, optical, and magnetic properties of CrSBr via a tuned hybrid functional — •Daniel Hernangómez-Pérez[1], María Camarasa-Gómez[2], Javier Junquera[3], and Ashwin Ramasubramaniam[4] — [1]CIC nanoGUNE BRTA, Donostia, Spain — [2]Centro de Física de Materiales (CFM/MPC), Donostia, Spain — [3]Universidad de Cantabria, Santander, Spain — [4]University of Massachusetts Amherst, USA

CrSBr, a layered antiferromagnet, has attracted attention for its ambient stability, relatively high Néel temperature, and strong exciton-magnon coupling. While experiments have progressed rapidly, computational studies lag due to the high cost of many-body perturbation theory (MBPT). Here, we present a generalized Kohn-Sham density functional approach that accurately reproduces electronic bandstructures, optical spectra, exciton binding energies, and magnon spectra of bulk and few-layer CrSBr at much lower cost than MBPT. Using a minimal two-parameter set tuned to a few benchmarks, we achieve excellent agreement across a broad range of optoelectronic and magnetic properties.

M. Camarasa-Gómez, D. Hernangómez-Pérez, J. Junquera, A. Ramasubramanian (in preparation)

HL 39.11 Thu 12:15 POT/0081

Tunable exchange interaction and hysteresis observed via excitons in a van der Waals antiferromagnet bilayer — •Priyanka Mondal[1], Sonu Verma[2], Wenze Lan[1], Lukas Krelle[1], Ryan Tan[1], Regine von Klitzing[1], Kseniia Mosina[3], Zdenek Sofer[3], Akashdeep Kamra[2], and Bernhard Urbaszek[1] — [1]Institute for Condensed Matter Physics, TU Darmstadt, Hochschulstraße 6-8, D-64289 Darmstadt, Germany — [2]Department of Physics and Research Center OPTIMAS, Rheinland-Pf\"alzische Technische Universit\"at Kaiserslautern-Landau,Germany — [3]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Czech Republic

Two-dimensional magnets have emerged as key platforms for exploring layer-dependent magnetic phenomena. CrSBr is a recently identified van der Waals magnet with strong excitonic features and layered antiferromagnetic (AFM) order. While pristine bilayers show no magnetic hysteresis, we find that a ~3° twist induces clear hysteresis and can even stabilize a zero-field ferromagnetic state[1]. Field-dependent photoluminescence tracks this behavior through hysteretic exciton energy shifts that match the magnetic configuration. A two-sublattice model explains the response via twist-reduced interlayer exchange, allowing both parallel and antiparallel spin states. The bilayer behaves as an effective monodomain, switching cleanly into the AFM state without forming spin textures. These results highlight twist engineering as a route to programmable magnetic memory in 2D magnets.

[1] P. Mondal et al. arXiv preprint arXiv:2510.08018 (2025).

HL 40: Oxide Semiconductors: Transport and Spectroscopy

Time: Thursday 9:30–12:30 Location: POT/0251

HL 40.1 Thu 9:30 POT/0251

Unraveling metal-induced redox mechanisms on SrTiO3 via combined in-situ laser reflectometry and x-ray photoelectron spectroscopy — •Georg Hoffmann, Shi-Hui Liu, Serkan Sirt, Oliver Bierwagen, and Roman Engel-Herbert — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117 Berlin, Germany

SrTiO3 has long served as a key platform for emergent phenomena in perovskite oxides such as polar discontinuity driven two-dimensional electron gases (2DEGs) when interfaced with LaAlO3 [1]. Recently, increasing attention has been brought to 2-DEGs that emerge at SrTiO3 surfaces from redox-reactions induced by amorphous metal deposition on top [2]. Studying these processes, however, requires complex in-situ techniques like photoelectron spectroscopy (XPS) with long measurement cycles. Here, we introduce laser reflectometry (LR) as a complementary technique that enables monitoring of redox-reactions at oxide/metal interfaces. We show that LR in an oxide molecular beam epitaxy setup can distinguish between Al deposition on non-reactive substrates and Al oxidation, e.g. through oxygen scavenging from SrTiO3. Atomic force microscopy, Capacitance-Voltage profiling, and XPS measurements corroborate our findings. Our results demonstrate how LR can guide future investigations of redox-reactions at oxide/metal interfaces.

[1] A. Ohtomo, and H. Y. Hwang., Nature 427, 423 (2004).

[2] T. Rödel, et al., Adv. Mater. 28, 1976 (2016).

HL 40.2 Thu 9:45 POT/0251

Resonant Raman studies in rutile-Germaniumdioxide — •Kenneth Brandt[1,3], Moritz Meissner[1,3], Zbigniew Galazka[2], Tobias Schultz[2], Markus Wagner[1,3], and Hans Tornatzky[1,3] — [1]Paul-Drude-Institut, Berlin — [2]Leibniz-Institut für Kristallzüchtung, Berlin — [3]Technische Universität Berlin

Ultra-wide bandgap (UWBG) semiconductors are a new research area of interest, with promised applications in power electronics. Germaniumdioxide in the rutile phase (r-GeO_2) has been characterised to be such an UWBG Material with a Bandgap at about 4.5 eV. To be able to create homojunction devices, the material needs to be ambipolar dopable, which poses a challenge for β-Ga_2O_3, as p-type doping has yet to be achieved, while r-GeO_2 is predicted to be ambipolar dopable. Raman measurements show a non typical intensity relationship, in which explicitly the E_g mode does not follow the expected $I \propto \omega^4$ relation of the Raman-Scattering processes but decreases in intensity with higher excitation energies. We are performing resonant Raman studies, with excitation energies ranging from 1.2 eV provided by a tunable Ti:Sa Laser, as well as multiple additional single line Lasers with energies up to 5.1 eV, to investigate the atypical Raman response and electron-phonon coupling.

To quantise the measurements CaF_2 is used as a calibration standard and GaAs is included in the measurement series to compare with literature.

HL 40.3 Thu 10:00 POT/0251

Theoretical Description of a Photo-induced Hidden State in Bismuth Vanadate — •Philip Schwinghammer[1], Verena Streibel[1,2], Frederico Delgado[1], Franziska S. Hegner[1], Viktoria Kunzelmann[1,2], Konrad Merkel[1], Frank Ortmann[1], Ian Sharp[1,2], and David A. Egger[1] — [1]TUM School of Natural Sciences, Technical University of Munich, Germany — [2]Walter Schottky Institute, Technical University of Munich, 85748 Garching, Germany

Bismuth Vanadate has attracted attention in recent years as a promising photoactive material and complex model system. In order to understand new experimental results which show a light-sensitive structure at room temperature, we perform a detailed analysis of the chemical bonding and impact of the exchange-correlation functional. In addition to the use of hybrid functionals, spin-orbit coupling (SOC) stabilizes the experimentally observed monoclinic structure over its high-symmetry tetragonal counterpart. The physical mechanism behind the stabilization is explained through the increase of both covalent and ionic bonding as symmetry breaking causes shortening of select Bi-O bonds. These mechanisms are strongly affected by photo-induced excitation of charge carriers, as the states responsible for the monoclinic distortion are depleted. The alteration of the structure through light may then affect the photo-catalytic efficiencies of the material, as we also find significant differences in the optoelectronic properties of the monoclinic and tetragonal structures.

HL 40.4 Thu 10:15 POT/0251

E-field modulated phase change properties in highly epitaxial VO2 thin film monitored via Raman spectra and IR transmission — •Sonika Singh[1], Rajendra Singh[2], and Ankur Goswami[3] — [1]IIT Delhi, New Delhi, India — [2]IIT Delhi, New Delhi, India — [3]IIT Delhi, New Delhi, India

VO2 is a highly explored smart oxide semiconductor showing metal insulator transition (MIT) at near room temperature ~67 oC. It is observed that optoelectronic properties of highly epitaxial VO2 thin films offer several advantages as compared to polycrystalline film in terms of E-MIT and thermal switching. Here we investigate E-MIT on epitaxial VO2 deposited using PLD technique. Prior to electrical measurement, electrical contacts with 8 *m separation distance were made using Ti/Au metallization. The dual voltage sweep carried over the device demonstrated a high thermal switching ratio (around 30) between high resistive and low resistive state. Furthermore, the dual current sweep was performed on the devices reflected snapback transition signifying uncontrolled and rapid phase transition of VO2. Additionally, E-field dependent Raman spectroscopy revealed modulation of phase transition of VO2 monitored via Raman peaks and triggered via square signal of E-field. These findings suggest that epitaxial thin film of VO2 can be explored for further studies involving modulation of phase change properties via E-field that find direct applications in neuromorphic devices, THz transmissions, thermal switches.

HL 40.5 Thu 10:30 POT/0251

Spatially Resolved Phase Transition and Characterization in Gallium Oxide — Umutcan Bektas[1], Paul Chekhonin[2], Nico Klingner[1], Azat Abdullayev[3], Alexander Azarov[4], René Hübner[1], Zhandos Utegulov[3], Andrej Kuznetsov[4], and •Gregor Hlawacek[1] — [1]Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328, Dresden, Germany — [2]Resource Ecology, Helmholtz-Zentrum Dresden-Rossendorf, 01328, Dresden, Germany — [3]Department of Physics, Nazarbayev University, 010000, Astana, Kazakhstan — [4]Centre for Materials Science and Nanotechnology, University of Oslo, N-0316, Oslo, Norway

In this study, we investigate ion-irradiated β-Ga_2O_3 samples (varying ions and fluences) alongside α- and κ-Ga_2O_3 thin films. Using focused ion beam (FIB) irradiation, we locally modified the samples under controlled conditions by tuning beam current, size, spacing, scan type, and ion species. Structural changes in the irradiated regions were characterized via electron backscatter diffraction (EBSD) and transmission electron microscopy (TEM). Our results demonstrate that ion induced transition to the γ polymorph can be achieved also through FIB irradiation, enabling the fabrication of in-plane polymorph patterns on the nanometer scale. Furthermore, time-domain thermoreflectance (TDTR) measurements further revealed the thermal conductivity of irradiated regions, highlighting opportunities to optimize heat transport in Ga_2O_3 power electronic devices. This research is supported by the tax funds on the basis of the budget passed by the Saxonian state parliament in Germany.

HL 40.6 Thu 10:45 POT/0251

Bandgap, exciton dynamics, and anisotropic thermal transport in rutile-GeO_2 — •Markus R. Wagner[1,2], Luca S. M. Choi[2], Nils Bernhard[2], Pouria Emtenani[2], Felix Nippert[2], Moritz Meissner[1], Hans Tornatzky[1], and Zbigniew Galazka[3] — [1]Paul-Drude-Institut für Festkörperelektronik — [2]Technische Universität Berlin, Institut für Physik und Astronomie — [3]Leibniz-Institut für Kristallzüchtung

Rutile germanium dioxide (r-GeO_2) is a promising ultra-wide bandgap material, predicted to support ambipolar doping and display high thermal and electronic conductivity, making it a strong candidate for power electronics. However, essential aspects of its properties, such as exciton and phonon dynamics as well as the role of defects and impurities, remain only partially explored. Here, we present our recent spectroscopic studies on r-GeO_2. High-resolution spectroscopy of free exciton ground and excited states enables us to determine exciton binding energies and the temperature dependence of the bandgap. Polarization-resolved photoluminescence reveals pronounced differences between near-UV and visible emission bands, which we analyze regarding thermal quenching, recombination dynamics, and charge transfer through temperature- and power-dependent PL, TRPL, and PLE. Using time-domain thermoreflectance down to cryogenic temperatures, we establish the temperatur dependence of thermal conductivity and anisotropy, supported by Boltzmann transport calculations. Finally, polarization-resolved Raman spectroscopy identifies all first-order Raman-active phonons and their relative tensor elements.

15 min. break

HL 40.7 Thu 11:15 POT/0251

MESFETs based on α-$(Al_xGa_{1-x})_2O_3$ thin films — •Sebastian Köpp, Sofie Vogt, Holger von Wenckstern, and Marius Grundmann — Leipzig University, Leipzig, Germany

We present the electrical properties and key parameters of metal-semiconductor field effect transistors (MESFET) on α-$(Al_xGa_{1-x})_2O_3$. The functional thin films were grown by pulsed laser deposition. The transistors were investigated in dependence on the Al content up to x=0.1. The devices exhibit an electrical breakdown field larger than that of comparable transistors on binary α-Ga_2O_3, demonstrating the advantages of the $(Al_xGa_{1-x})_2O_3$ alloy system.

With its ultra-wide bandgap of 5.3 eV to 5.6 eV [1,2] and a high predicted breakdown field of 10 MV/cm [3], α-Ga_2O_3 is a promising material for high-power devices, as well as deep-UV photodetectors. α-Ga_2O_3, being isostructural to aluminium oxide, allows for heteroepitaxial growth on cost-efficient sapphire substrates, and also opens up the option of α-$(Al_xGa_{1-x})_2O_3$ alloys [4], with even higher dielectrical breakdown field than binary Ga_2O_3.

[1] A. Segura *et al.*, Phys. Rev. Materials 1, 024604 (2017)
[2] E. Ahmadi *et al.*, J. Appl. Phys. 126, 160901 (2019)
[3] M. Biswas and H. Nishinaka, APL Mater. 10, 060701 (2022)
[4] J. Steele *et al.*, APL Mater. 12, 041113 (2024)

HL 40.8 Thu 11:30 POT/0251

Group-III doping study of p-type oxide tin monoxide — •Nicola Gutmann, Georg Hoffmann, Aidan Campbell, and Oliver Bierwagen — Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Germany.

The use of transparent conducting oxides has so far been limited to n-type materials, hindering the development of transparent oxide-based pn-junctions and CMOS devices. In contrast, SnO shows natural p-type conduction with reported hole mobilities up to 21 cm^2/Vs [1] and well-performing p-type transistors demonstrated.

Adjustment of hole concentration by doping with Ga, Na, K and Y has been demonstrated [2]. Al is theoretically predicted to be an n-type dopant [3], which would enable SnO-based pn-homojunctions.

In this work, we comparatively explore doping of suboxide molecular beam epitaxy grown SnO by the group-III elements Al, Ga and In.

[1] M. Minohara et al., J. Phys. Chem. C, vol. 124, no. 2, pp. 1755-1760 (2020).
[2] S. Chae et al., APL Materials, vol. 13, no. 10, p. 101114 (2025).
[3] M. Graužinyte et al., Phys. Rev. Materials, vol. 2, no. 10, p. 104604 (2018).

HL 40.9 Thu 11:45 POT/0251

Realization of highly rectifying pn-heterojunctions and junction field-effect transistors on pulsed laser deposited α-Ga_2O_3 thin films — •Paul Bokemeyer, Clemens Petersen, Holger von Wenckstern, Marius Grundmann, and Sofie Vogt — University Leipzig, Felix-Bloch-Institut für Festkörperphysik, Germany

The wide band gap of about 5.3 eV[1] and a high expected breakdown field of up to 10 MV/cm[2], renders the corundum α-phase of Ga_2O_3 interesting for high power electronics. We present lateral p^+n-heterojunction diodes on α-Ga_2O_3:Sn grown by pulsed laser deposition (PLD) using a two step approach[3]. ZnCoO (ZCO) and NiO deposited by PLD at room temperature were used as p^+-type materials. Further, the influence of a remote oxygen plasma treatment prior to the deposition of the p-type layers on the device performance was investigated. High current rectification ratios of 8.2 (ZCO) and 7.8 (NiO) orders of magnitude at ± 3V were achieved. Additionally, both p-type materials were used as gate materials in the fabrication of α-Ga_2O_3:Zr junction-field-effect-transistors (JFETs), yielding on/off current ratios of more than 9 orders of magnitude and subthreshold-swings down to 119 mV/dec. Furthermore, breakdown was detected at drain voltages of up to 476 V which is estimated to a field of 1.7 MV/cm [4].

[1] A. Hassa et.al., J.Phys. D: Appl. Phys. **54**, 223001 (2021)
[2] M. Biswas et al., APL Mater. **10**, 060701 (2022)
[3] S. Vogt et al., Phys. Status Solidi A, **220** 2200721 (2023)
[4] P. Bokemeyer et al.,Phys. Status Solidi RRL, 2400388 (2025)

HL 40.10 Thu 12:00 POT/0251

Defect-Induced Resistive Switching in Titanate-based Perovskites — •Parrydeep Kaur Sachdeva[1], Wahib Aggoune[1,2], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at FHI of MPG, Berlin — [2]Institut für Physik and CSMB, Humboldt-Universität zu Berlin, Berlin

Perovskites possess strong potential for exhibiting ferroelectric resistive switching (RS), a functionality recently realized yet not understood in titanate perovskites [1]. Controlled deviation from stoichiometry has revealed high RS, indicating a defect-mediated origin. Using hybrid functional DFT calculations, we show that the Ti antisite defect (Ti-interstitial with Ca-vacancy) can induce ferroelectricity in $CaTiO_3$ which is an incipient ferroelectric, stabilized in a nonpolar state by strong octahedral tilts. The Ti-interstitial atom breaks this balance by its off-center displacement and induces a local polarization. This polarization is switchable between different off-center positions of the defect, with energy barriers in the range of 0.25 eV. Additionally, the Ti antisite defect gives rise to mid-gap states, with a charge density mainly localized around the Ti-interstitial atom. Switching the defect between equivalent off-center positions switches the polarization direction and alters the spatial distribution of the charge state. This can influence the material's overall response under external stimuli. These results are discussed with respect to the experimentally observed resistive switching in titanate-based perovskites [1], as reported by Leibniz-Institut für Kristallzüchtung (IKZ) Berlin.

[1] A. Baki, *et al.*, *Sci. Rep.*, **11**, 7497 (2021).

HL 40.11 Thu 12:15 POT/0251

ZnM_2O_4 (M = Co, Rh, Ir) spinels as potential p-type transparent conducting oxides — •Daniel Fritsch — Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24/25, 14476 Potsdam, Germany

ZnM_2O_4 (M = Co, Rh, Ir) spinels are under investigation as potential p-type transparent conducting oxides (TCOs) [1]. Here we extend our previous investigation of $ZnRh_2O_4$ into the whole series of ZnM_2O_4 (M = Co, Rh, Ir) spinels.

To this end, we perform *first-principles* calculations based on density functional theory employing a recently developed *self-consistent* hybrid exchange and correlation functional [2], and compare the results to more standard HSE06 hybrid functional calculations. In order to judge the results on the electronic and optical properties, additional calculations based on many-body perturbation theory, i.e. G_0W_0 calculations, have been performed and allow for a more detailed analysis of the applicability of ZnM_2O_4 (M = Co, Rh, Ir) spinels as potential p-type TCOs.

The obtained structural, electronic, and optical properties will be discussed alongside earlier experimental and theoretical investigations, and will open a pathway to potential applications of ZnM_2O_4 (M = Co, Rh, Ir) spinels.

[1] D. Fritsch, Electron. Mater. **2**, 504 (2021).
[2] D. Fritsch, B. Morgan, and A. Walsh, Nanoscale Res. Lett. **12**, 19 (2017).

HL 41: Quantum Dots and Point Contacts (joint session TT/HL)

Time: Thursday 11:00–12:45 Location: HSZ/0101

See TT 78 for details of this session.

HL 42: Nitrides III – Emerging thin films and electrochemistry

Time: Thursday 11:15–12:45 Location: POT/0006

Invited Talk HL 42.1 Thu 11:15 POT/0006

Transition Metal Nitride Semiconductors for Photoelectrochemical Energy Conversion — •Verena Streibel[1,2], Laura I. Wagner[1,2], Elise Sirotti[1,2], David A. Egger[2], and Ian D. Sharp[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Garching, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Garching, Germany

Transition metal nitride thin films are emerging as promising materials for (photo)electrochemical applications. However, their synthesis and defect control remain challenging. Here, we use reactive co-sputtering to synthesize and engineer nitride thin films with precise control over composition and doping in the Ti-Ta-N,[1] Zr-Ta-N,[2,3] and Hf-Ta-N materials space. Starting from orthorhombic Ta_3N_5, we show that substitutional Ti doping improves photoconversion efficiency by modulating defects and recombination dynamics. While high Ti doping forms a secondary TiN phase, Zr and Hf yield tunable solid solutions in the Zr-Ta-N-(O) and Hf-Ta-N-(O) systems, exhibiting bandgap modulation and large refractive indices. Notably, a new bixbyite-type ternary compound, $ZrTaN_3$, forms at a 1:1 Zr:Ta ratio, showing strong visible light absorption and photoanodic activity. DFT calculations reveal a tunable direct bandgap driven by cation ordering.[3] Our findings establish composition engineering as a key strategy for tailoring band structure and charge transport in emerging nitride semiconductors.

[1] Wagner, L.I. et al., Adv. Funct. Mater. 2024, 34, 2306539.
[2] Wagner, L.I. et al., Adv. Mater. Interfaces 2025, 12, 2400745.
[3] Sirotti, E. et al., Adv. Energy Mater. 2024, 202402540.

HL 42.2 Thu 11:45 POT/0006

Analysis of the interface properties of cubic nitride thin films grown on 3C-SiC/Si templates using electrochemical impedance spectroscopy — •Hannes Hergert[1,2], Mario F. Zscherp[1,2], Silas A. Jentsch[1,2], Jörg Schörmann[1,2], Sangam Chatterjee[1,2], Peter J. Klar[1,2], and Matthias T. Elm[1,2] — [1]Center for Materials Research, Heinrich-Buff-Ring 16, 35392 Giessen — [2]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Giessen

Due to its lack of internal polarization fields cubic gallium nitride (c-GaN) is a promising semiconductor material for a variety of applications, such as high-power electronics or optoelectronic devices. High quality c-GaN can successfully be grown by molecular beam epiatxy on 3C-SiC/Si templates making use of a c-AlN buffer layer, which accommodates lattice mismatch between c-GaN and the 3C-SiC template. A reliable characterization of the interface properties as well as the electrical transport properties of c-GaN is crucial for optimizing the thin film growth as well as for designing advanced functional devices. In this work we employ electrochemical impedance spectroscopy (EIS) for characterizing the transport throught c-GaN/AlN/3C-SiC/Si sample structures with different c-GaN thicknesses and for analyzing the properties of the interface, such as the trap density.

HL 42.3 Thu 12:00 POT/0006

Investigating Charge Transport Limitations in $LaTiO_2N$ Thin Films for Photoelectrochemical Water Splitting — •Oliver Brune[1,2], Gabriel Grötzner[1,2], Katarina S. Flashar[1,2], Saswati Santra[1,2], Ian D. Sharp[1,2], and Verena Streibel[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Garching, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Garching, Germany

Photoelectrochemical water splitting offers a sustainable route to hydrogen production. On the photoanode side, $LaTiO_2N$ is a promising candidate due to its visible-light absorption, favorable band alignment and n-type semiconducting properties. However, its performance is limited by inefficient charge transport, the origin of which remains unclear. In this work, we synthesize $LaTiO_2N$ thin films by spin coating and reactive sputter deposition, both followed by ammonia annealing, yielding films with controlled structure and composition as confirmed by XRD and ERDA/RBS. Synchrotron-based XAS, XPS, UV-Vis spectroscopy, and PEC measurements reveal that a larger degree of nitridation in $LaTiO_2N$ correlates with higher short-range order and crystallinity, a decreasing bandgap, and an increase in photocurrent density. To elucidate charge transport mechanisms and carrier dynamics, we use Hall effect and temperature-dependent photocurrent measurements. Our findings establish a direct link between synthesis parameters, defect chemistry, and charge-carrier dynamics in $LaTiO_2N$, providing a foundation for overcoming transport limitations in oxynitride-based photoanodes for solar hydrogen production.

HL 42.4 Thu 12:15 POT/0006

Epitaxial YbN thin films grown by nitrogen plasma-assisted molecular beam epitaxy — Yitong Chen[1,2], •Anna Meléndez Sans[1,3], Shin-ichi Kimura[2,4,5], Liu Hao Tjeng[1], and Simone Altendorf[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Department of Physics, Graduate School of Science, The University of Osaka, Toyonaka, Japan — [3]Institut de Ciència de Materials de Barcelona, Bellaterra, Spain — [4]Graduate School of Frontier Biosciences, The University of Osaka, Suita, Japan — [5]Institute for Molecular Science, Okazaki, Japan

Rare-earth mononitrides display interesting magnetic and semiconducting properties due to the strongly correlated and localized 4*f* electrons. However, extreme air sensitivity and poor stoichiometry hindered research on bulk samples when they were first discovered. Modern advancements in UHV-based thin film growth techniques have opened the possibility to synthesize and study high quality samples.

Unlike most of the rare-earths, which can break the molecular nitrogen bond, Yb does not react with nitrogen gas and therefore requires an activated nitrogen source for the synthesis of YbN.

Here we present our growth study on YbN thin films grown by nitrogen plasma-assisted molecular beam epitaxy, using different substrates (MgO and $LaAlO_3$) and growth conditions. The films were characterized *in situ* with photoelectron spectroscopy, confirming their semiconducting character and the Yb valence as 3+. Photon-energy dependence of the valence band spectra revealed a significant hybridization of the Yb 4*f* and N 2*p* states.

HL 42.5 Thu 12:30 POT/0006

Novel $TbTa(O,N)_3$ perovskite oxynitride for photoelectrochemical energy conversion — •Aleksandr Kochergov[1,2], Gabriel Grötzner[1,2], Oliver Brune[1,2], Frans Munnik[3], Saswati Santra[1,2], Verena Streibel[1,2], and Ian D. Sharp[1,2] — [1]Walter Schottky Institute, Technical University of Munich, Germany — [2]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Perovskite oxynitride semiconductors have emerged as promising candidates for photoelectrochemical (PEC) water splitting, given their smaller band gaps (~ 2 eV) compared to more extensively studied metal oxides. Previous studies show that in rare-earth lanthanide tantalum perovskite oxynitrides, PEC photocurrent density increases with the increment of the A-site cation atomic number [1]. However, no studies have investigated A-site cations heavier than gadolinium (Gd). This work presents a method for synthesizing the novel perovskite oxynitride $TbTa(O,N)_3$ as thin film via spin coating followed by a sequential two-step annealing procedure in air and ammonia. X-ray diffraction shows that proper NH_3 annealing conditions are crucial for obtaining the $TbTa(O,N)_3$ perovskite structure. The resulting films are investigated for their structural, compositional, and optoelectronic properties. The results suggest a 2.3 eV band gap and n-type conductivity. Given these favorable properties, the viability of $TbTa(O,N)_3$ as photoanode is evaluated.

[1] Zou, Qi, et al., J. Am. Chem. Soc. 2024, 146, 28182-28189

HL 43: Excursion and Network-Event at Infineon Dresden AG (joint session FM/HL)

We are organizing an Excursion and Network-Event to Infineon Dresden AG.
Only for registered and selected participants.
Please register until latest February 12th here:
https://www.icams.de/news-events/events/registration-infineon/?api=561b8d7cfcb678e9f0938830d78cf979

Time: Thursday 13:30–17:00 Location: Infineon

[-0.2mm] **HL 44: 2D Materials: Electronic structure, excitations, etc. III (joint session O/HL/TT)**

Time: Thursday 15:00–17:45 Location: HSZ/0204

See O 84 for details of this session.

HL 45: Perovskite and Photovoltaics: Spectroscopy

Time: Thursday 15:00–17:15 Location: POT/0006

HL 45.1 Thu 15:00 POT/0006

The influence of air and light exposure on alkali-metal doped $Cu(In,Ga)Se_2$ absorber materials measured with in-situ TRPL and XPS — •P. Stötzner, S. Sobisch, A. Stauffenberg, H. Kempa, R. Scheer, and S. Förster — Martin-Luther-Universität Halle-Wittenberg, Germany

Copper indium gallium diselenide ($Cu(In,Ga)Se_2$/CIGSe) is a promising thin-film solar cell absorber. Alkali-metal doping, especially in combination with heavy alkali metals, enhances solar cell efficiencies. However, air and light exposure (ALE) of the absorber reduces the solar cell efficiency. This is a result of the diffusion of sodium and oxygen toward the absorber surface, which is accompanied by a degradation of the charge-carrier lifetime of doped CIGSe absorbers [1,2].

Here, we study the ALE effect for CIGSe doped with K and cominations of Na and K as well as Na and Rb. Our studies combine X-ray photoelectron spectroscopy

(XPS) and in-situ time-resolved photoluminescence (TRPL) conducted in one ultrahigh vacuum system, addressing changes in the chemical composition and charge-carrier lifetime. The setup is completed by a high-pressure gas cell enabling for controlled exposure to specific environments.
We find that the charge-carrier lifetime of non-doped absorbers is unaffected by ALE and all alkali-metal doped absorbers degrade due to ALE. XPS shows that the most heaviest alkali metal present and oxygen are accumulated at the surface. While this effect is reversable over time, the degradation of the charge-carrier lifetime is permanent.
[1] DOI: 10.1063/1.4992116 [2] DOI: 10.1002/pip.3041

HL 45.2 Thu 15:15 POT/0006

Thermal Broadening Statistics of Photoluminescence in Tunable Lead Halide Perovskite Nanocrystals — •Luca B. Reim, Leo Luber, and Alexander S. Urban — Nanospectroscopy Group, Nano-Institute Munich, Department of Physics, Ludwig-Maximilians-Universität München, Königinstraße 10, 80539 Munich

Halide perovskite nanocrystals (NCs) exhibit excellent optoelectronic properties, including high quantum yields and composition-dependent, narrow photoluminescence (PL) that critically depend on control over NC size and uniformity. Understanding the mechanisms governing PL linewidths is therefore essential for evaluating material quality and device performance.

We synthesized size-tunable $CsPbBr_3$ nanocubes under ambient conditions using machine-learning-optimized reaction protocols.[1] The NCs were drop-cast onto substrates and investigated via temperature-dependent PL spectroscopy in a closed-cycle cryostat from 9-300 K. To quantitatively analyze the spectral evolution, we applied a novel fitting approach that enables the extraction of size dispersion, temperature-dependent exciton populations, and signatures of the local energetic environment. The latter is strongly influenced by nanocrystal quality and ligand coverage and provides a sensitive probe of inhomogeneous broadening mechanisms.

These results offer detailed insight into the fundamental limits of emission linewidths in perovskite NCs and support the targeted optimization of materials for optoelectronic applications such as LEDs.

[1] N. A. Henke, et al., Adv. Mater. 2025, e09472.

HL 45.3 Thu 15:30 POT/0006

Investigation on the efficiency limiting processes of 3C-SiC photoelectrodes using intensity modulated techniques. — •Marius Wasem[1,2], Mario F. Zscherp[1,2], Silas A. Jentsch[1,2], Jörg Schörmann[1,2], Sangam Chatterjee[1,2], and Matthias T. Elm[1,2] — [1]Center for Materials Research, Heinrich-Buff-Ring 16, 35392 Giessen — [2]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Giessen

Cubic silicon carbide (3C-SiC) is a compelling photoelectrode for photoelectrochemical water splitting due to its near-ideal band gap energy and excellent chemical stability. Here, we present the characterization of the photoelectrochemical response of epitaxially grown n- and p-type 3C-SiC using different electrochemical methods. A pH neutral phosphate buffer solution was used as electrolyte. The suitable operating conditions, such as potential range and light intensity, were determined using chopped light voltammetry. Insights of the charge carrier dynamics were gained by combining electrochemical impedance spectroscopy (EIS), intensity-modulated photocurrent spectroscopy (IMPS) and intensity-modulated photovoltage spectroscopy (IMVS). While EIS is a common and widely used method, the latter two methods are rarely discussed in the photoelectrochemical community. Here we show how a combination of all three methods enables the differentiation and quantification of key processes (recombination processes, surface effects, charge carrier lifetime) to validate the efficiency of 3C-SiC photoelectrodes.

HL 45.4 Thu 15:45 POT/0006

Nano-sensing of AC-Fields with Perovskite Quantum Dots and Electro-Switching of Luminescence — •Emanuel Eckl[1], Fabian Brütting[1], Moritz B. Heindl[1], Maryna Bodnarchuk[2], Mariia Svyrydenko[2], Maksym Kovalenko[2], and Georg Herink[1] — [1]University of Bayreuth, Bayreuth, Germany — [2]ETH Zürich, Zürich, Switzerland

Perovskite quantum dots (PQDs) currently attract significant research interest, particularly owing to their broad tunability of optoelectronic properties with applications in energy conversion, solid-state lighting and sensing technologies.

In this study, we investigate the potential of PQDs as nano-sensors for transient electric fields up to multi-Terahertz (THz) frequencies [1]. Combining electro-absorption, lifetime and photoluminescence measurements of inorganic and hybrid lead-halide PQDs, we demonstrate a massive electro-switching effect observed via luminescence. The emission modulation is directly correlated with reduced photoluminescence lifetimes and can be attributed to a switching of radiative quantum efficiency. Furthermore, we present evidence for a memory effect that exhibits significantly delayed responses in comparison to the well-understood quasi-instantaneous Quantum-Confined Stark Effect that is also observable in these PQDs. In particular, the Stark effect is utilized for the purpose of validating and comparing our measurements to those of conventional inorganic CdSe QDs, previously employed in ultrafast imaging of THz near-fields.

[1] M.B. Heindl, et al., Light Sci Appl 11, 5 (2022).

15 min. break

HL 45.5 Thu 16:15 POT/0006

Resolving Ultrafast Conductivity Dynamics in 2D-Perovskites via correlative THz-NIR Spectroscopy — •Lion Krüger[1], Fabian Brütting[1], Michael Baumann[2], Moritz B. Heindl[1], Maximilian Spies[3], Anna Köhler[3], Alexander JC Kühne[2], and Georg Herink[1] — [1]Experimental Physics VIII, University of Bayreuth, Germany — [2]Institute of Organic and Macromolecular Chemistry, Ulm University, Germany — [3]Experimental Physics II, University of Bayreuth, Germany

Quasi-2D Metal-Halide Perovskites offer flexible tuning of optoelectronic properties via composition and quantum confinement.

In this contribution we present measurements of the ultrafast carrier dynamics and mobilities of 3D- and quasi-2D-methylammonium lead iodide (MAPI) using optical-pump terahertz-probe spectroscopy (OPTP). The comparison with corresponding optical transient absorption measurements allows for the extraction of an ultrafast feature on a picosecond timescale that is correlated with the delayed hot-carrier cooling, known from 3D hybrid perovskites. Here this "hot phonon bottleneck" manifests as a 2D-specific, intensity-dependent signature in the THz-conductivity and is attributed to transient exciton formation [1].

[1] Lion Krüger, Fabian Brütting, Michael Baumann, Moritz B. Heindl, Maximilian Spies, Anna Köhler, Alexander JC Kühne, Georg Herink. "Confinement-induced Ultrafast Conductivity in 2D Perovskites resolved by correlative Terahertz-NIR Spectroscopy". 2025. In review.

HL 45.6 Thu 16:30 POT/0006

Intra- and Interlayer Excitonic Finestructure of $(PEA)_2PbI_4$ — •Patrick Grenzer[1], Fabian Lie[2], Klaus H. Eckstein[1], Linn Leppert[2], and Tobias Hertel[1] — [1]Institute of Physical and Theoretical Chemistry, Julius-Maximilians-University Würzburg, Germany — [2]MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

Layered halide perovskites exhibit strongly bound excitons shaped by reduced dimensionality, dielectric confinement, and significant spinorbit coupling. Despite extensive work, the origin of the multiple resonances in absorption and PL of $(PEA)_2PbI_4$ remains subject to debate. We investigate the excitonic fine structure in high-quality, mechanically exfoliated single crystals by combining temperature- and polarization-resolved photoluminescence with first-principles GW+BSE calculations. The polarization dependence unambiguously assigns the observed features to distinct excitonic states and resolves the contributions from exchange interactions, crystal symmetry, and interlayer coupling. We further identify and spectroscopically separate intra- and interlayer excitons and their respective transition dipole moments. The results provide a consistent microscopic picture of the exciton manifold in $(PEA)_2PbI_4$ and clarify the origins of the multi-line structure characteristic of this material class.

HL 45.7 Thu 16:45 POT/0006

Dynamic Screening Effects on Auger Recombination in Metal-Halide Perovskites from First Principles — •Utkarsh Singh — Theoretical Physics Division, IFM, Linköping University, Sweden

Auger recombination is the dominant nonradiative loss in perovskite LEDs and nanolasers at carrier densities $> 10^{17}$ cm^{-3}.[1,2] Conventional first-principles treatments[3] use static dielectric screening $W(\mathbf{q}, 0)$ and neglect its frequency dependence in polar iodide perovskites.

I present a framework that incorporates the frequency-dependent screened interaction $W_{00}(\mathbf{q}, \omega)$, computed from low-scaling GW, into direct and phonon-assisted Auger amplitudes.[4] For γ-$CsPbI_3$ and γ-$CsSnI_3$, dynamic screening enhances the dielectric response at optical energies and reduces the room-temperature Auger coefficient by 50–60% compared with the static approximation.[5] The critical crossover density is shifted by a factor of 2, with implications for efficiency roll-off and lasing thresholds in optoelectronic devices.

These results establish dynamic screening as a quantitative determinant of Auger losses in polar semiconductors and provide a transferable framework for device modeling.

[1] J. Qin *et al.*, *Trends Chem.* **3** (2021).
[2] Y. Sun *et al.*, *Appl. Phys. Rev.* **11** (2024).
[3] E. Kioupakis *et al.*, *Phys. Rev. B* **92** (2015).
[4] F. Yuan *et al.*, *Nat. Photonics* **18** (2024).
[5] U. Singh & S. I. Simak, in preparation (2025).

HL 45.8 Thu 17:00 POT/0006

Influence of static disorder on the low temperature photoexcitation dynamics in triple cation lead halide perovskites — •Alexander Schauerte[1], Anton Krüger[1], Isabel Allegro[2], Dominik Muth[1], Ian Howard[2], Uli Lemmer[2], and Marina Gerhard[1] — [1]Department of Physics and Marburg Centre for Quantum Materials and Sustainable Technologies, Hans-Meerwein-

Str. 4, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Light Technology Institute, Karlsruhe Institute of Technology, Kaiserstraße 12, 76131 Karlsruhe, Germany

We study the recombination dynamics of phase stable triple cation lead halide perovskites $Cs_{0.1}(MA_{0.17}FA_{0.83})_{0.9}Pb_{1-x}(I_{0.84}Br_{0.16})_{3-2x}$ with intentionally induced deficiencies of Pb over a broad temperature range using time-resolved photoluminescence (PL) spectroscopy. In the temperature range below 70 K, we find pronounced sub-nanosecond PL dynamics which are accompanied by an increase of the carrier diffusivity by more than one order of magnitude. The findings are attributed to the polaronic Mott transition, beyond which polaron radii overlap, leading to efficient transport and bimolecular recombination. Moreover, the observed energy dependent PL dynamics at low temperatures indicate the presence of a phonon bottleneck, which inhibits efficient cooling of the excited population. We find that a higher degree of static disorder slows down bimolecular recombination, while the phonon bottleneck effect is more pronounced, potentially because slower recombination does not effectively reduce the hot carrier population.

HL 46: Ultra-fast Phenomena II

Time: Thursday 15:00–17:15 Location: POT/0051

HL 46.1 Thu 15:00 POT/0051

Ultrafast study of out-of-plane charge carrier diffusion in perovskite thin films via pump-probe sSNOM — •Daniel Sandner[1], Branden Esses[2], Zhao Yang[3], Kai Zhu[3], Joseph Berry[2,3], Hristo Iglev[1], and Markus Raschke[2] — [1]Laser- and X-ray physics E11, TU Munich — [2]CU Boulder — [3]NREL

Despite substantial evidence for polaron formation in lead halide perovskites (LHPs), which exhibit excellent photovoltaic performance, the role of polarons in transport remains unclear. We've measured diffusion with high spatial resolution by monitoring the carrier density at the top of a thin film via the tip-localized response in pump-probe mIR-sSNOM, while exciting the sample from below. Due to the small penetration depth of the pump beam, most electrons and holes are initially located at the bottom of the perovskite layer. Consistent with previous studies, we find local variations in the diffusion coefficient. To link transport and local structure, we employ a vibrational mode as an indicator of lattice stiffness and polaron formation [JACS 2024, 146(29), 19852-19862].

HL 46.2 Thu 15:15 POT/0051

Coherent exciton-phonon coupling and many body interactions in halide perovskites probed by 2D electronic spectroscopy. — •Mohsin Sayar[1], Katrin Winte[1], Davide Caratti[2], David Cahen[2], Christoph Lienau[1], and Antonietta De Sio[1] — [1]Carl von Ossietzky Universität, Oldenburg, Germany. — [2]Weizmann Institute of Science, Rehovot, Israel

Exciton-phonon interactions are central to the unique optoelectronic properties of halide perovskites. Here we use temperature-dependent two-dimensional electronic spectroscopy (2DES) with 10 fs time resolution to study the exciton dynamics in bulk $CH_3NH_3PbBr_3$ crystals. The 2DES maps distinguish between exciton and free-carrier-induced contributions to the near-band-edge optical nonlinearity, revealing distinct signatures of exciton-exciton and exciton-carrier many-body interactions. The ultrafast dynamics further reveal coherent low-frequency phonon oscillations at $40 cm^{-1}$ and $67 cm^{-1}$, corresponding to Pb-Br-Pb bending and stretching modes that most strongly couple to the exciton. Additionally, we observe faster, 105 fs exciton amplitude oscillations across all three crystal phases, arising from coherent population oscillations between 1s and 2p excitonic states, off-resonantly driven by the low-frequency coherent phonon fields in the crystal. We rationalize these results within a phenomenological model accounting for both exciton-phonon coupling and 1s-2p exciton coupling via the phonon fields. Preliminary polarization-resolved 2DES data show that these phonon-induced exciton oscillations are retained upon spin-selective excitation.

Invited Talk HL 46.3 Thu 15:30 POT/0051

Antisymmetric vibrations in the excited state dynamics of quadrupolar dyes — Somayeh Souri[1], Katrin Winte[1], Daniel Lünemann[1], Daniel Timmer[1], Elena Mena-Osteritz[2], Sergei Tretiak[3], Christoph Lienau[1], and •Antonietta De Sio[1] — [1]Universität Oldenburg — [2]Universität Ulm — [3]Los Alamos National Laboratory

Non-equilibrium dynamics following photoexcitation in molecular materials arise from a complex interplay of electronic and vibrational motion, with antisymmetric vibrations playing a key role in ultrafast nonadiabatic dynamics, such as at conical intersections. Their direct spectroscopic identification is, however, challenging, since these modes are often Raman inactive and only weakly affect optical transitions. Here, we show experimental signatures of vibronic coupling to antisymmetric modes in the ultrafast symmetry-breaking dynamics of a quasi-quadrupolar dye[1,2] using two-dimensional electronic spectroscopy (2DES). The sub-50-fs 2DES maps reveal an asymmetric peak pattern with characteristic low-energy cross-peaks. We show that these peaks arise from stimulated emission from a double-minimum excited state potential energy surface induced by vibronic coupling to a ~1430 cm-1 antisymmetric mode[2]. Phenomenological essential state model simulations support the results. Our findings show that 2DES with sub-cycle vibrational resolution is a powerful method for identifying antisymmetric modes in the excited state dynamics prior to intramolecular vibrational relaxation and solvation. [1] Winte et al, Nature Chemistry 17, 1742 (2025); [2] Souri et al, submitted (2025)

15 min. break

HL 46.4 Thu 16:15 POT/0051

Investigating exciton dynamics and exciton–exciton interactions via optical two-dimensional photoelectron spectroscopy — •Luisa Brenneis[1], Matthias Hensen[1], Julian Lüttig[2], and Tobias Brixner[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Department of Physics, University of Ottawa, 150 Louis-Pasteur Pvt, Church St, Ontario K1N 6N5, Canada

Action-detected two-dimensional (2D) electronic spectroscopy has become a powerful technique to resolve exciton dynamics by measuring an incoherent signal proportional to the excited-state population generated by a multi-pulse sequence. However, processes that alter the excited-state population after the system's interaction with the pulse sequence, such as exciton–exciton annihilation, can obscure coupling signatures and single-exciton dynamics [1]. In optical 2D photoelectron spectroscopy (2DPES), typically a four-pulse sequence excites the system, followed by a time-delayed ionization pulse [2]. Here, we show how to disentangle exciton dynamics and interactions by varying the ionization pulse time delay. Exemplary simulations of a weakly coupled dimer demonstrate that short ionization delays reveal coupling signatures and single-exciton energy transfer, whereas longer delays reveal exciton–exciton annihilation. This concept is particularly promising for nanoscale surface studies, where 2DPES combined with photoemission electron microscopy enables spatially resolved exciton mapping.

[1] M. Bruschi et al., Phys. Chem. Lett. 14, 30, 6872 (2023).
[2] D. Uhl et al., Optica 8, 10, 1316 (2021).

HL 46.5 Thu 16:30 POT/0051

Ab initio Theory of Coherent Phonon Damping in Semimetals — •Yiming Pan and Fabio Caruso — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, 24118 Kiel, Germany

Coherent phonon plays an important role in the structural properties of the crystal lattice and ultrafast light-induced phase transition. Following its excitation, atoms oscillate coherently along the excited modes with decaying amplitudes. This dynamical process is commonly modeled with damping oscillators with phenomelogical damping rates. In this work, we derive this model by employing quantum kinetic equations [1], and attribute the damping rate and frequency renormalization of coherent phonon to the imaginary and real parts of the phonon self-energy. To valdiate our approach, we perform first-principles calculation of the damping rate of A_{1g} phonon arising from electron-phonon coupling and phonon-phonon coupling in semimetals Bi and Sb. The numerical results agree with available temperature- and fluence-dependent experimental data, thereby providing a predictive framework for determining the timescales of structural dynamics in driven solids.

[1] Y. Pan *et al.*, arXiv:2502.01529

HL 46.6 Thu 16:45 POT/0051

Probing Ultrafast Electronic and Lattice Dynamics simultaneously at the Atomic Scale with Time-Resolved Diffraction Anomalous Fine Structure (TR-DAFS) — •Moritz Meissner[1,2,6], T. C. Rossi[2], M. Rössle[2], C. Petersen[3], H. von Wenckstern[3], R. Mandal[4], M. Levantino[5], and R. M. van der Veen[2,6] — [1]Paul-Drude-Institut für Festkörperelektronik — [2]Helmholtz Zentrum Berlin — [3]Universität Leipzig — [4]Institut des materiaux de Nantes Jean Rouxel — [5]European Synchrotron Radiation Facility — [6]Technische Universität Berlin

This work presents the first successful demonstration of Time-Resolved Diffraction Anomalous Fine Structure (TR-DAFS) measurements carried out in a pump-probe (stroboscopic) scheme. We show that TR-DAFS can directly probe ultrafast structural and electronic dynamics in crystalline materials. Investigating Zinc oxide (ZnO) enables direct comparison between TR-DAFS at the Zn K-edge with time-resolved X-ray absorption spectroscopy (TR-XAS) data. TR-DAFS represents a leap forward in the study of photoexcited materials at the atomic scale by providing access to different aspects of lattice dynamics in reso-

nant and non-resonant parts of the spectrum. Preliminary ab initio calculations show that the electronic changes visible in the resonant part of the spectrum are associated with an increase of carrier temperature in the photoexcited state. This dual sensitivity to electronic and lattice degrees of freedom makes TR-DAFS a game-changer in investigating ultrafast processes in complex materials and heterostructures as represented by the results of this work.

HL 46.7 Thu 17:00 POT/0051

Theoretical Modeling of Ultrafast Phase Transitions from the Femtosecond to the Picosecond Scale — Stefano Mocatti, Giovanni Marini, Pierluigi Cudazzo, and •Matteo Calandra — Department of Physics, University of Trento, Via Sommarive 14, 38123 Povo, Italy

In this talk, I will introduce a theoretical approach to ultrafast phase transitions that captures both electron/hole and phonon dynamics following laser pumping, on time scales ranging from a few femtoseconds to several picoseconds after irradiation.

At short times, the method relies on solving the Bloch equations coupled to Ehrenfest dynamics. It includes the electric field of the pump explicitly, as well as carrier-carrier, carrier-phonon, and phonon-phonon scattering, treated entirely from first principles.

At longer times before recombination, when carrier-carrier interactions generate a photoexcited quasi-equilibrium electron-hole plasma, the approach is based on a constrained density-functional perturbation theory (cDFPT) scheme that accounts for the presence of holes in the valence band and electrons in the conduction band (two-Fermi-level approach). In this framework, the calculation of forces, phonon dispersion, and carrier-phonon coupling becomes possible, as well as molecular dynamics with machine-learning potentials in the presence of an electron-hole plasma.

I will showcase applications of the method to several materials.

This work is funded by the European Union (ERC, DELIGHT, 101052708).

HL 47: 2D Materials VIII – Quantum emitters and defects

Time: Thursday 15:00–16:00 Location: POT/0081

HL 47.1 Thu 15:00 POT/0081

Tunable phonon sidebands of defect emitters in monolayer WSe_2 heterostructures — •Felix Schaumburg[1], Cornelius Diedrich[2], Alberto Rodriguez[2], Jeniffer König[2], Corinne Steiner[3], Patricia Pesch[3], Axel Lorke[1], Michael Lorke[1], Günther Prinz[1], Martin Geller[1], and Annika Kurzmann[2] — [1]Faculty of Physics, University of Duisburg-Essen and CENIDE, Germany — [2]II. Physikalisches Institut Fachgruppe Physik, Universität zu Köln, Germany — [3]Fachgruppe Physik, RWTH Aachen, Germany

Van der Waals heterostructures hosting single-photon emitters have emerged as a versatile platform for exploring material properties, like phonon interactions. We investigate single-photon emission from a heterostructure composed of a graphite back gate, hBN dielectric layers, and a monolayer of WSe_2. A 10 nm metallic top gate enables electrical tuning of the WSe_2 layer. The entire stack is strained using lithographically defined SiO_2 nanopillars. Optically active defect centers are introduced into the WSe_2 monolayer by electron-beam irradiation. These defect centers in the strained regions exhibit clear single-photon emission, confirmed by second-order correlation function values below 0.5. Voltage-dependent measurements reveal a pronounced Stark shift of the emission lines as well as electrically tunable phonon sidebands. The intensity evolution of these sidebands can be described within the framework of a Franck-Condon model. Our results demonstrate deterministic position control, electrical control, and phonon-sideband engineering of quantum emitters in WSe_2. This paves the way towards bright, electrically tunable emission in two-dimensional materials.

HL 47.2 Thu 15:15 POT/0081

Room Temperature Visualization of Exciton Confinement in Single Photon Emitters samples — •Lucas Liberal[1], Rafael Nadas[2], Frederico B. Sousa[1], Maria Clara Godinho[3], Gabriel Jacobsen[1], Takashi Taniguchi[4], Kenji Watanabe[4], Marcio Teodoro[1], Ado Jorio[3], and Leonardo Campos[3] — [1]Departamento de Física, Universidade Federal de São Carlos, São Carlos, Brasil — [2]Institut fur Physik, Humboldt-Universitat zu Berlin, Newtonstraße 15, Berlin, Germany — [3]Universidade Federal de Minas Gerais, Belo Horizonte, MG, Brasil — [4]Research Center for Materials Nanoarchitectonics, NIMS, Tsukuba, Japan

Two-dimensional semiconductors such as monolayer WSe2 have attracted significant interest due to their remarkable quantum properties and their potential as scalable single-photon emitters. However, conventional microphotoluminescence (μ-PL) techniques are fundamentally limited by optical diffraction, preventing direct access to critical nanoscale features such as strain gradients and highly localized quantum confinement. In this study, we employ tip-enhanced photoluminescence with a spatial resolution of 10 nm to image, at room temperature, the emission landscape of monolayer WSe2 suspended over nanopillars. Our measurements reveal two distinct localization regimes consistent with leading theoretical models for single-photon activation: one arising from intervalley defect exciton hybridization and another driven purely by strain-induced confinement. These results provide practical guidelines for the deterministic nanoengineering of quantum light sources.

HL 47.3 Thu 15:30 POT/0081

Beyond static defects: temporal evolution of defect-driven reliability in WSe2 — •Madhuri Chennur[1,2], Ulrich Kentsch[1], Jens Zscharschuch[1,2], and Artur Erbe[1,2] — [1]Helmholtz-Zentrum Dresden Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany — [2]TUD Dresden University of Technology, 01062 Dresden, Germany

Two-dimensional (2D) semiconductors are emerging as promising candidates for CMOS-compatible nanoscale electronics, where defects increasingly dictate electron transport. In WSe2 transistors, chalcogen vacancies commonly degrade hole mobility, yet defect-rich surfaces or interfacial contact layers have enabled ultra-low-barrier p-type contacts. However, the electrical role of these defects is almost exclusively interpreted through static pre- and post-irradiation comparisons, leaving the time-dependent evolution of engineered defect and irradiation-induced trap dynamics essentially unexplored.

Here, we present a weeks-to-months time-resolved optical-electrical study of WSe2 FETs irradiated with a single-dose broad-beam irradiation, followed by temporal tracking of threshold voltage, subthreshold swing, and hysteresis under constant bias and ambient conditions. Raman and PL spectroscopy performed in parallel reveal lattice disorder, oxidation, and adsorbate uptake. We observe a reproducible transition with shifts in electrical parameters, demonstrating that defect is intrinsically dynamic, not static. This coupled temporal mapping provides missing insight into defect-aware reliability for realistic ambient and radiation-relevant 2D electronics.

HL 47.4 Thu 15:45 POT/0081

Physical Drivers of Metal Adsorption at 2D Interfaces for Memristive Applications — •Manoj Dey[1], Hamid Mehdipour[1,2], Peter Kratzer[2], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at the FHI of the Max Planck Society, Berlin — [2]Faculty of Physics, University of Duisburg-Essen, Duisburg

Two-dimensional (2D) materials with engineered defects are emerging as promising candidates for next-generation memristors. In these "atomristors," resistive switching (RS) arises from atomic-scale processes at the electrode-2D interface. Experiments show that adsorption and desorption of electrode metal atoms at vacancies play a key role in RS [1]. Here, we combine hybrid density functional theory with many-body dispersion corrections and the Sure Independence Screening and Sparsifying Operator (SISSO) method [2] to study metal adsorption on transition-metal dichalcogenides at gold interfaces. SISSO provides a predictive model for adsorption energies and uncovers the fundamental physical factors driving RS. Our sensitivity analysis shows how orbital hybridization and bonding interactions dominate the behavior, offering simple heuristics for understanding the atomic processes. We also build a materials-property map that highlights promising candidates and connects our predictions with experimentally demonstrated devices. Together, these results link fundamental material descriptors to RS behavior and offer clear guidance for designing future 2D atomristors.

[1] Ruijing Ge *et al.*, *Adv. Mater.*, **33**, 2007792 (2021).
[2] R. Ouyang *et al.*, *Phys. Rev. Materials*, **16**, 2, 083802 (2018).

HL 48: Heterostructures, Interfaces and Surfaces: Fabrication and Structure

Time: Thursday 15:00–17:15 Location: POT/0251

HL 48.1 Thu 15:00 POT/0251

Cross-sectional scanning tunneling microscopy (XSTM) study of nearly lattice-matched III-V semiconductor heterostructures — •Hitesh Kumar[1], Rüdiger Schott[2], Zijin Lei[2], Werner Wegscheider[2], and Stefan Fölsch[1] — [1]Paul Drude Institute for Solid State Electronics, Berlin, Germany — [2]Laboratory for Solid State Physics, ETH Zürich, Zürich, Switzerland

XSTM is a powerful technique for investigating the structural and electronic properties of III-V semiconductor heterostructures. These heterostructures are grown along the [001] direction by molecular beam epitaxy and accessible in cross-sectional view by cleaving the sample in ultrahigh vacuum to expose the (110) cleavage surface. We used this approach to study a GaSb-InAs-AlGaSb-InAs-InAsSb layered heterostructure grown on a Te-doped GaSb substrate. Voltage-dependent chemical contrast in STM imaging allows differentiation between anions and cations in the III-V semiconductors. Using this capability, we analyzed the degree of homogeneity in the ternary materials (Al-Ga mixing in the AlGaSb layer and As-Sb mixing in the InAsSb layer). With the help of scanning tunneling spectroscopy, we precisely determined the band gaps of the individual layers and locally probed the band lineup across the entire heterostructure. This allowed us to investigate the behavior of charge carriers governed by the band lineup. Specifically, we studied the spatial confinement and quantization of conduction band states in the InAs layer and their decay into the gap region of the adjacent layers.

HL 48.2 Thu 15:15 POT/0251

Theoretical Exploration of the Electronic Structure at Group-III Nitride Interfaces — •Maximilian Lauer[1,2], Christian Maas[1,2], Jan M. Waack[1,2], Michael Czerner[1,2], and Christian Heiliger[1,2] — [1]Institut für theoretische Physik, Justus-Liebig-Universität Gießen, Germany — [2]Zentrum für Materialforschung (ZfM), Justus-Liebig-Universität Gießen, Germany

Group-III nitrides are an essential group of materials at the forefront of modern optoelectronics. Recently, the metastable zincblende (In,Ga)N system emerged as a promising material for optoelectronic devices. Heterojunctions play a central role in device design, making a precise understanding of their electronic structure essential. Determining the band alignment at the interface is crucial for understanding its electronic properties.

Here, we show that the zb-GaN/zb-InN heterojunction exhibits a Type-I alignment with no states forming within the band gap at the interface. We performed KKR calculations with LDA-1/2 band gap corrections on coherently strained supercells. We report values for the band offset parameters and explore the microscopic electronic structure at the interface. Our calculations demonstrate the importance of band corrections for calculating electronic structure parameters, such as band offsets, and provide a basis for further investigations into the (Ga,In)N alloy system using the CPA.

HL 48.3 Thu 15:30 POT/0251

GaPN growth on As-Modified Si(100) for defect-reduced heteroepitaxy — •Hitha Haridas[1], Kai Daniel Hanke[1], Agnieszka Paszuk[1,2], and Thomas Hannappel[1] — [1]Technische Universität Ilmenau, Fundamentals of Energy Materials, Ilmenau,Germany — [2]BMFTR Junior Research Group PARASOL, Technische Universität Ilmenau, Germany

The Monolithic integration of III-V semiconductors with Si(100) offers a promising route toward high-efficiency,low-cost optoelectronic devices. Among these materials, GaPN is a promising candidate for III-V/Si integration because it can be grown lattice-matched to silicon, thereby minimizing strain and reducing the formation of misfit dislocations. However, structural defects generated during the earliest stages of growth can propagate into subsequent epitaxial layers, ultimately limiting device performance. In this study, we investigate the nucleation and early-stage growth behavior of GaPN on As-modified Si(100) surfaces by combining ex situ surface morphology analysis,electron channeling contrast imaging, and in situ optical spectroscopy.This integrated approach allows us to systematically evaluate how variations in the initial growth conditions influence defect formation. The insights gained provide broader guidance for improving interface quality and advancing III-V/Si heteroepitaxy through more precise control over the initial growth phases.

HL 48.4 Thu 15:45 POT/0251

Acoustoelectric effect in organic-inorganic semiconductor systems — •Paromita Bhattacharjee[1], Patrick Ganswindt[2], Alexander S. Urban[2], and Hubert Krenner[1] — [1]Institute of Physics, University of Münster, Germany — [2]Faculty of Physics, Ludwig-Maximilians-Universität München, Germany

Surface acoustic waves (SAWs) are elastic waves propagating on the surface of a piezoelectric solid and while interacting with a semiconductor, its strain and piezoelectric fields modulate the band-gap. Strain-induced field imposes an acoustoelectric (AE) drag on the charges in the direction of SAW propaga-tion, and in a photoconductive semiconductor, excitons get ionized by piezoelectric field into separate elec-trons and holes, captured and transported by SAW [1]. Utilizing these effects, we present first study of SAW-induced charge transport in hybrid organic-inorganic semiconductor system of organic polymer, poly(3-hexylthiophene) (P3HT) and halide perovskite (CsPbBr3 and CsPb(IxBr1-x)3) nanowires (HPNWs). In samples with only HPNWs the total AE current nearly vanishes due to comparable electron-hole mobilities in these materials [2]. However, in hybrid layers, weak AE effect is observed with CsPb(IxBr1-x)3 NWs and a hole dominated AE transport with CsPbBr3 NWs. The band realignment at the heterojunction explains that while for CsPb(IxBr1-x)3 -P3HT ambipolar electron-hole transport occurs via the NWs, for CsPbBr3-P3HT, electrons are limited by low electron mobility in P3HT. References: [1] J. Phys. D: Appl. Phys. 57, 423001 (2024). [2] Nano Lett., 19, 8701-8707 (2019).

15 min. break

HL 48.5 Thu 16:15 POT/0251

Ultra-high vacuum exfoliation method for the preparation of large-area single layer TMDC films — •Zhiying Dan[1], Ronak Sarmasti Emami[1], Antonija Antonija Grubisic-Cabo[1], Petra Rudolf[1], Deepnarayan Biswas[2], and Tien-Lin Lee[2] — [1]Zernike Institute for Advanced Materials, University of Groningen, 9747 AG Groningen, The Netherlands — [2]Diamond Light Source Ltd., Harwell Science and Innovation Campus, Didcot, Oxfordshire, OX11 0DE, UK

Two-dimensional transition metal dichalcogenides (2D TMDCs) are promising candidates for next-generation electronic, optical, and spintronic devices. While mechanical exfoliation yields high-quality 2D flakes, their lateral size is typically limited to tens of micrometers. Here, we report the preparation of 2D WS2 and WSe2 using a recently developed kinetic in situ single-layer synthesis (KISS) method, performed in ultra-high vacuum and tailored for surface science studies. We examine how substrate choice and chalcogen species affect film size and quality using X-ray photoelectron spectroscopy, low-energy electron diffraction, atomic force microscopy, and X-ray standing waves (XSW). Our results show that the quality of the bulk TMDC crystal is crucial for successful KISS exfoliation. Moreover, preliminary XSW data suggest that KISS does not degrade the underlying substrate, highlighting its potential as a non-destructive approach for 2D material synthesis.

HL 48.6 Thu 16:30 POT/0251

Electrical conduction and sensing properties of contacted CNTs after MOF synthesis — •Marvin J. Dzinnik[1], Adrian Hannebauer[2], Feriel Friha[1], Andreas Schaate[2], and Rolf J. Haug[1,3] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hanover, Germany — [2]Institut für Anorganische Chemie, Leibniz Universität Hannover, 30167 Hanover, Germany — [3]Laboratorium für Nano- und Quantenengineering, Leibniz Universität Hannover, 30167 Hanover, Germany

Metal-organic frameworks (MOFs) are a versatile sensor material: they are tunable, highly porous, and can be precisely grown on carbon nanotubes (CNTs).[1]

Here, we investigate how UiO-66 MOF growth affects single nanotubes. We performed DC measurements on contacted multi-walled carbon nanotubes (MWCNTs) before and after UiO-66 synthesis. We observe pronounced changes in both magnitude and character of the electrical response, indicating a strong interaction between MWCNT and MOF. AC measurements show a linear response to ethanol vapor up to 40 000 ppm, suggesting that single MWCNT-MOF hybrids are promising, tunable gas-sensing elements.

[1] Dzinnik, M. J. et al. Commun Mater 5, 38 (2024).

HL 48.7 Thu 16:45 POT/0251

Nucleation behavior for remote epitaxy of GaAs and AlAs on carbon-covered GaAs substrates — •Binamra Shrestha, Tobias Henksmeier, and Dirk Reuter — Paderborn University, Paderborn, Germany

Recently, remote epitaxy was proposed as a method that enables the growth of free-standing single-crystal layers and substrate reuse by using atomically thin 2D materials as release layers. In this work, we investigate the epitaxial growth behavior of GaAs and AlAs on ultrathin amorphous carbon layers deposited by PECVD on GaAs substrates. The amorphous carbon exhibits a graphene-like structure consisting predominantly of in-plane sp^2 bonding, thereby serving as a quasi-2D template capable of transmitting the substrate's electrostatic potential for remote epitaxial growth.

We performed controlled nucleation studies using molecular beam epitaxy (MBE). First, a GaAs buffer layer is grown on the bare GaAs to planarize the substrate surface, then the sample is covered with amorphous carbon. Subsequently, ultrathin GaAs layers ranging from 0.25 nm to 2 nm are deposited on the graphene/GaAs template at 300 °C, and the resulting nuclei are examined via atomic force microscopy (AFM). Nucleation is first observed at approximately 0.37 nm deposition thickness, with nuclei predominantly aligned along atomic

steps. This strong step-edge preference indicates that remote epitaxy is the dominant mechanism, compared to pinhole-initiated nucleation. These results highlight the suitability of PECVD-deposited amorphous carbon as an effective 2D interlayer for remote epitaxy.

HL 48.8 Thu 17:00 POT/0251

Quantum confinement in semiconductor random alloys: a case study on Si/SiGe/Si — •Daniel Dick[1,2,3,4], Florian Fuchs[1,2,3], Sibylle Gemming[2,4], and Jörg Schuster[1,2,3] — [1]Center for Micro- and Nanotechnology, TU Chemnitz, Germany — [2]Center for Materials, Architecture and Integration of Nanomembranes, TU Chemnitz, Germany — [3]Fraunhofer Institute for Electronic Nanosystems (ENAS), Chemnitz, Germany — [4]Institute of Physics, TU Chemnitz, Germany

When the size of random alloys is reduced, local fluctuations of alloy composition become more influential. Using extended Hückel theory, we study the semiconductor alloy SiGe sandwiched between Si due to its relevance in semiconductor devices. We evaluate the effects of the alloy composition, layer thickness, and local fluctuations of the Ge concentration on band alignment and the band gap. Results are compared to the finite quantum well model. This model captures the essenial physics and can act as a computationally faster surrogate model.

HL 49: Quantum Emitters in 2D Semiconductors

Time: Thursday 16:15–17:30 Location: POT/0081

Invited Talk HL 49.1 Thu 16:15 POT/0081

Phonon-mediated nonlinearity and defects in hexagonal boron nitride — •Nahid Talebi — Institute of Experimental and Applied Physics, Kiel University, Germany

Hexagonal boron nitride (hBN) hosts a rich phonon landscape whose strong oscillator strengths in the first and second Reststrahlen bands give rise to negative permittivity and support the propagation of hyperbolic phonon polaritons. In this work, we show that these phonon modes can mediate highly efficient down-conversion of optical excitation, enabling strong coupling to point defects and facilitating the coherent excitation of their electronic states. We further demonstrate that such defect states in hBN can couple efficiently to excitons in hybrid hBN*perovskite structures, establishing a robust exciton*defect interaction channel. Remarkably, we find that excitonic energy can be transported over distances up to 150 micrometers through incoherent hopping across a defect network within hBN. By combining spatially and spectrally resolved photoluminescence and cathodoluminescence spectroscopy, we identify the mechanisms governing coherent and incoherent defect excitation and reveal the interplay and strong coupling among excitons, defects, and phonons in hBN. These insights establish hBN as a versatile platform for phonon-assisted light*matter interactions and long-range energy transport in hybrid quantum nanophotonic systems.

HL 49.2 Thu 16:45 POT/0081

Spin Dynamics of Quantum Sensors Based on Hexagonal Boron Nitride — •Paul Konrad[1], Andreas Sperlich[1], Igor Aharonovich[2], and Vladimir Dyakonov[1] — [1]Experimental Physics 6, Julius-Maximilians-Universität Würzburg, 97074 Würzburg — [2]School of Mathematics and Physical Sciences, University of Technology Sydney, Ultimo, NSW 2007, Australia

Colour centres in solid-state materials show great potential in quantum information technology and sensing applications. The spin triplet system of the lately discovered negatively charged boron vacancy (V_B^-) in hexagonal boron nitride (hBN) can be exploited in terms of its application as temperature, magnetic field, and pressure sensor.[1] Increasing the sensitivity of these nano-scale sensors is a crucial step towards application and requires not only controlled generation[2] but deep knowledge about the dynamics of the system. This includes predicted but experimentally hardly accessible intermediate states.

In this study, we achieve a direct measurement of a 24.0(3) ns relaxation time from the dark intermediate state to the ground state at room temperature, which approximately doubles at low temperatures. These findings are corroborated by detailed simulations of populations. Accounting for this relaxation considerably enhances spin manipulation efficiency, allowing substantial optimization of the quantum sensor's sensitivity based on boron vacancies.[3]

[1] Gottscholl et al., *Nat. Commun.*, **12**, 4480 (2021).
[2] Patra et al., *Adv. Funct. Mater.* e17851 (2025).
[3] Konrad et al., *arXiv* preprint arXiv:2503.22815 (2025).

HL 49.3 Thu 17:00 POT/0081

Exciton-enhanced light emission in pristine and doped MoS_2 from ab initio calculations — •Adriana Bocchini[1], Djennane Khaoula[2], Henry Hübschmann[1], Nikita Siverin[3], Andreas Farenbruch[3], Maja Groll[1], Klaus Jöns[1], Gerhard Berth[1], Dmitri Yakovlev[3], Wolf Gero Schmidt[1], and Uwe Gerstmann[1] — [1]Universität Paderborn, Germany — [2]Yahia Fares University of Medea, Algeria — [3]Technische Universität Dortmund, Germany

Two-dimensional transition metal dichalcogenides (2D-TMDs) are emerging as a suitable alternative in a variety of electronic and optoelectronic devices [1,2]. The properties of this family, in fact, can be systematically customized upon structural modification, e.g., via exfoliation or dopants. Notably, most of these properties are strongly determined by excitons, the formation of which is strongly facilitated by defects [3]. In this study, we use DFT routines to systematically investigate the influence of excitons on the optical properties of MoS_2 films. Thereby, we do not only analyze the dependency of the optical response on the layer thickness, but also their evolution upon the application of external electric fields or by twisting the layers relative to each other. In addition, we model MoS_2-based Janus structures by selectively substituting some of the S atoms with heavier chalcogens and analyze the suitability of these configurations as possible light-emitting solid-state quantum dots.

[1] R. Thayil,, *et al.*, Small **21**, 2412467 (2025)
[2] S. Joseph, *et al.*, Mater. Chem. Phys. **297**, 127332 (2023)
[3] J. Qu *et al.*, ACS Nano **18**, 34322 (2024)

HL 49.4 Thu 17:15 POT/0081

Thermodynamic properties of quantum defects in boron nitride using machine-learned force fields — •Ariel Moises Cabrera Aguilar and Carla Verdi — The University of Queensland, Brisbane, Australia

Hexagonal boron nitride (hBN) has emerged as an excellent host material for bright single-photon emitters. Experimental and computational studies associate these single-photon emitters (SPEs) in hBN predominantly with carbon-related defects. However, the lack of first-principles calculations at finite temperatures and with sufficiently large supercells hinders the establishment of a consensus on the most likely defect candidates for quantum-technology applications. Machine-learned force fields (MLFFs) provide highly accurate finite-temperature simulations because they can be trained to reproduce first-principles energies and forces across diverse configurations. We trained a MLFF capable of describing various carbon cluster defects (C_B, C_N, C_BC_N, C_BV_N, C_BC_i, and C_NC_i) at temperatures up to approximately 2000 K. To evaluate the accuracy of the force field in reproducing atomic positions, interatomic energies, and forces across these structures, we compute formation energies, phonon dispersions, and photoluminescence spectra, and compare these quantities with available experimental data. The force field successfully reproduces the line shape of several defects in multilayered systems of different supercell sizes. The MLFF is used to investigate multiple defects in large supercells over long molecular dynamics simulation times, allowing us to capture metastable structures that emerge at finite temperature.

HL 50: Members' Assembly

Organized by Rudolf Bratschitsch, Alexander Holleitner and Axel Lorke

Time: Thursday 17:45–19:15 Location: POT/0051

All members of the Semiconductor Physics Division are invited to participate.

HL 51: 2D Materials: Stacking and heterostructures (joint session O/HL/TT)

Time: Friday 9:30–12:30 Location: HSZ/0401

See O 95 for details of this session.

HL 52: THz and MIR Physics in Semiconductors

Time: Friday 9:30–10:45 Location: POT/0006

HL 52.1 Fri 9:30 POT/0006

Probing Terahertz Emission and Structural Dynamics in Quasi-two-dimensional $NbOI_2$ — •Daniel Geyer[1], Rieke von Seggern[1], Soufiane El-Kabil[1], Zouchen Fu[3], and Sascha Schäfer[1,2] — [1]Department of Physics, University of Regensburg, Germany — [2]Regensburg Center for Ultrafast Nanoscopy (RUN), Germany — [3]Nankai University, Tianjin, China

Optically induced processes in matter, captured via time-resolved imaging methodologies, uncover a variety of transient phenomena evolving on ultrafast time scales. Layered ferroelectric niobium oxide dihalides $NbOX_2$ (X=I, Cl, Br) have garnered significant interest in this context, as they combine pronounced optical nonlinearities [1,2] with a ferroelectric order parameter that can be controlled via optical stimuli [3]. In this work, we investigate the $NbOI_2$ compound as a material platform in which both regimes of ultrafast light-matter interaction can be accessed within different experimental approaches.

At first, we explore thin $NbOI_2$ flakes as promising stackable terahertz (THz) emitters. We demonstrate broadband THz generation via nonlinear optical rectification, characterized using a time-domain THz emission spectroscopy setup.

Secondly, we discuss the photoinduced evolution of the material's ferroelectric polarization, employing time-resolved electron diffraction in an ultrafast transmission electron microscope (UTEM).

[1] Guo et. al., Nature **613**, 53-59 (2023)
[2] Chen et. al., Adv. Mater. **36**, 2400858 (2024)
[3] Wang et. al., Nat. Comm. **16**, 8132 (2025)

HL 52.2 Fri 9:45 POT/0006

AlGaN/GaN-based grating-gate plasmonic crystals for nonlinear THz applications — Pavlo Sai[1], Vadym V. Korotyeyev[2], Serhii Kukhtaruk[2], Dmytro B. But[1], Maksym Dub[1], Alexej Pashkin[3], Stephan Winnerl[3], Wojciech Knap[1], and •Martin Mittendorff[4] — [1]Institute of High Pressure Physics PAS ul. Sokołowska 29/37, Warsaw 01-142, Poland — [2]V. Ye. Lashkaryov Institute of Semiconductor Physics (ISP) NASU prospect Nauky 41, Kyiv 03028, Ukraine — [3]Helmholtz-Zentrum Dresden-Rossendorf 01328 Dresden, Germany — [4]Universität Duisburg-Essen Fakultät für Physik 47057 Duisburg, Germany

We present time-resolved THz measurements on grating-gate plasmonic crystals, based on the two-dimensional interface electron gas in epitaxial GaN/AlGaN heterostructures. The free-electron laser FELBE at Helmholtz-Zentrum Dresden-Rossendorf served as tunable source for intense, narrowband THz pulses at about 1.8 THz, the plasmon frequency was tuned via the grating-gate. The strongest pump-probe signals are observed at resonance, where a rather low pump fluence of about 200 nJ/cm^2 leads to a pump-induced change in transmission of more than 40% [1]. The signal decays within about 50 ps. The experimental results are complemented by a finite-difference time-domain electrodynamic simulation, allowing to identify the main driving mechanisms for the observed strong nonlinearity, e.g. near-field effects and hot charge carriers.

[1] P. Sai et al., Adv. Optical Mater. 2025, 13, 2500716; https://doi.org/10.1002/adom.202500716

HL 52.3 Fri 10:00 POT/0006

Plasmonic nonlinearity in AlGaN/GaN-based rectangular patches — •Nandita Bajpai[1], Pavlo Sai[2,4], Maksym Dub[2,4], Alexej Pashkin[3], Stephan Winnerl[3], Wojciech Knap[2,4], and Martin Mittendorff[1] — [1]Department of Physics, University of Duisbur-Essen,Duisburg,Germany — [2]Institute of HighPressurePhysics,Warsaw,Poland — [3]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [4]Center for Terahertz Sciences and Applications CENTERA -CEZAMAT Warsaw University of Technology, Warsaw, Poland

Recent observation of enhanced nonlinear THz absorption by resonant excitation of 2D plasmons in the AlGaN/GaN based plasmonic crystal has revealed a strong pump-induced transparency of probe upto 45%[1].Here, we investigate the nonlinear coupling between the perpendicular plasmonic modes in AlGaN/GaN-based rectangular patches. To this end, we performed a two colour pump probe experiment at the free-electron laser facility at the Helmholtz-Zentrum Dresden-Rossendorf. The spectrally narrow pump pulse was used to drive the plasmonic resonance at 1.95 THz whereas a broadband THz pulse from a synchronized table-top time domain spectroscopy setup was exploited to probe the plasmonic mode at 1.38 THz. We observed a relative pump - induced change in transmission of probe upto 12%, which is attributed to the excitation of hot carriers that decays within 25ps.

[1] P.Sai et al., Adv. Optical Matter.2025,13,2500716; https://doi.org/10.1002/adom.202500716

HL 52.4 Fri 10:15 POT/0006

Elucidating carrier dynamics in bismuth thin film with time-resolved terahertz spectroscopy — •Guriviredy Yettapu, Fabian Thiemann, Michael Horn-von Hoegen, and Martin Mittendorff — University of Duisburg-Essen, Duisburg, Germany

Bismuth (Bi) is a Peierls distorted semimetal in its bulk state that transforms into a semiconductor for thicknesses below ~30 nm [1]. Time-resolved terahertz spectroscopy is an ideal tool to investigate the charge carrier dynamics by following the pump-induced change in electric field with pump-probe delay. Herein, we employed optical-pump terahertz-probe spectroscopy to elucidate the carrier dynamics in single crystalline Bi film with a thickness ~36 nm, including spectrally resolved measurements to determine the frequency dependent complex conductivity. At a pump fluence of 30 uJ/cm2, we observe a pump-induced change of the electric field of about 20 %, followed by an exponential decay with a relaxation time of ~7 ps. Our results reveal that carrier relaxation times are hardly affected by the pump fluence, the complex conductivity can be well described by the Drude model. Our future studies include thickness- and temperature-dependent measurements to gain insights about the carrier-lattice interactions in the semiconductor and semimetal phase. [1] C. A. Hoffman et al., Phys. Rev. B. 48, 11431-11434 (1993).

HL 52.5 Fri 10:30 POT/0006

Identifying the semiconductor doping range addressable by terahertz time-domain spectroscopy — •Joshua Hennig[1,2], Jens Klier[1], Stefan Duran[1], Mirco Kutas[1,2], Georg von Freymann[1,2], and Daniel Molter[1] — [1]Department for Materials Characterization and Testing, Fraunhofer Institute for Industrial Mathematics ITWM, 67663 Kaiserslautern, Germany — [2]Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany

Semiconductors are essential materials for the technological advancements of the 21st century. With the growing demand for semiconductor devices going along with this, the need for fast and non-destructive characterization techniques is growing quickly, too. Terahertz time-domain spectroscopy (THz-TDS) has proven to be capable of measuring the desired properties of various semiconductors over the last decades. Yet, it is still not widely established for this purpose. One reason is that for each combination of material, doping concentration and thickness the possibility to characterize the sample has to be evaluated individually. Therefore, we are developing a simulation-based tool that can help identify the accessible doping ranges. Based on simulations of the interaction between a terahertz pulse and an arbitrary layer stack of doped semiconductor materials, a well-founded estimate of the characterizability with reflection THz-TDS is retrieved. These simulations allow for a better understanding of the suitability of a THz-TDS characterization for specific semiconductor samples and hence to establish THz-TDS further in the semiconductor industry.

HL 53: Organic Semiconductors: Carrier Dynamics

Time: Friday 9:30–11:15 Location: POT/0051

Invited Talk HL 53.1 Fri 9:30 POT/0051

Organic semiconductors: Opening new perspectives in sustainable electronics — •Karl Leo — IAPP, TU Dresden

Organic semiconductors enable a variety of novel applications for flexible, lightweight, and environmentally friendly electronics. One unique advantage of these carbon-based materials is their compatibility with body tissue, thus opening perspetives for completely new medical applications on and even in the human body. Furthermore, the materials set available in this technology allows biodegradability and thus sustainable electronics without the serious environmental issue of conventional electronics. In the first part of my talk, I will show examples how organic electronic devices can be used in postsurgical monitoring, avoiding life-threatening complications. In the second part of the talk, I will address lignocellulose leaf skeleton structures (Leaftronics) as basis for a variety of novel applications, such as semitransparent electrodes.

HL 53.2 Fri 10:00 POT/0051

Unveiling the role of disorder on carrier concentration transients in electrochemical transistors — •Tobias Krebs and Martijn Kemerink — IMSEAM, Heidelberg University, Germany

Already the drain current transients in organic electrochemical transistors hint for not yet fully understood underlaying device physics, as they show a generally slower turn on compared to turn off, with the difference between these on- and off- switching times varying over orders of magnitude between materials and driving voltages. Tracking the charge carrier concentration during switching then completes this asymmetric picture: A sharp doping front entering the device during turn on, followed by gradual bulk de-doping during turn off. We measure these concentration transients optically, using the red-shifted absorption in the doped state of the redox active polymers we investigated. Comparison of this data with drift-diffusion simulations revealed a strong dependence of this asymmetry on the broadness of the density of states, which in our simulations both modulates the carrier density dependence of hole mobilities and influences the maximum charge carrier concentration for a set gate voltage. Our simulation framework also allowed us to study the surprisingly small effect of ionic mobilities in the semiconductor on switching times, above a device specific mobility threshold. The results can be used to guide the rational design of improved devices.

HL 53.3 Fri 10:15 POT/0051

Simulation of Coulomb Glass Behavior in Organic Semiconductor Devices at high carrier densities — •Magdalena Dörfler[1], Heinz Bässler[2], Anna Köhler[1,2], and Harald Oberhofer[3] — [1]Soft Matter Optoelectronics and Bayerisches Polymerinstitut (BPI), Experimental physics II, University of Bayreuth, Universitätsstr. 30, Bayreuth, Germany — [2]Bayreuth Institute of Macromolecular Research (BIMF), University of Bayreuth, Universitätsstr. 30, Bayreuth, Germany — [3]Chair for Theoretical Physics VII and Bavarian Center for Battery Technologies, University of Bayreuth, Universitätsstr. 30, Bayreuth, Germany

Recent advances in organic transistors (OFETs, EGOFETs, OECTs) enable device operation at high charge carrier densities where Coulomb interactions between carriers become significant.

Using Kinetic Monte Carlo simulations, we investigate carrier-carrier Coulomb interactions in OFET-like structures. Comparing simulations with and without these interactions reveals reduced carrier mobility and increased activation energy when interactions are included, with effects increasing for higher carrier densities.

Our results indicate a transition to correlated transport with a Coulomb gap in a dynamic density of states. The system exhibits Coulomb glass behavior, where the activation energy reflects structural reorganization of the carrier ensemble.

Notably, the Coulomb gap appears at ambient temperature and does not require variable-range hopping, unlike to the situation in electron liquids and inorganic semiconductors.

HL 53.4 Fri 10:30 POT/0051

Dual Ferroelectric and Semiconducting behaviour in supramolecular organics — •Tara Vollus[1], Sophia Klubertz[1], Shyamkumar Vadakket Haridas[2], Oleksandr Shysho[2], Max von Delius[2], and Martijn Kemerink[1] — [1]IMSEAM, Heidelberg University, Germany — [2]Institute of Organic Chemistry, Ulm University, Germany

The combination of interacting conductive and ferroelectric properties, resulting in a multifunctional material, has the potential to simplify the structure of memory devices. It has been demonstrated that the organic ferroelectric material C6H6F5O-C3-amide (M3) exhibits both these properties, showing ferroelectricity and an unexpected DC conductivity.[1][2] It has been shown that the latter is related to the presence of interfacial dipoles that allow efficient charge injection from (oxidation and/or reduction by) metal contacts and is enhanced by a supramolecular arrangement formed at higher temperatures and under an applied electric field. Here, we demonstrate the effects of alignment and, especially, the presence of both n- and p-type doping-like processes, suggesting that M3 is a wide-bandgap organic semiconductor that reversibly can be reduced and oxidized. Kelvin probe force microscopy measurements revealed filament-like potential structures that may act as pathways for bipolar charge transport, and suggest the formation of dynamic pn-junctions.[3]

[1] Mager et al., arXiv:2507.11309 [cond-mat.mtrl-sci] [2] Mager et al., arXiv:2506.02673 [cond-mat.mtrl-sci] [3] Matyba et al., DOI:10.1038/nmat2478

HL 53.5 Fri 10:45 POT/0051

Backbone Alignment and Morphology Formation in PBTTT Thin Films: Insights from In-Situ GIWAXS — •Robin M. Teichgreber[1], Christopher R. McNeill[2], and Eva M. Herzig[1] — [1]Dynamics and Structure Formation - Herzig Group, University of Bayreuth, Universitätsstr. 30, Bayreuth — [2]Material Science and Engineering, Monash University, 20 Research Way, Clayton

The performance of organic electronic devices strongly depends on the morphology of the organic semiconductor thin film [1]. Enhancing the understanding on fundamental structure-function relationships is therefore crucial to improve the performance of such devices in the future. Highly aligned films can furthermore be used to study fundamental charge separation processes. Controlling the alignment of polymer backbones is a challenge in the first place, demanding further research on the processes of structure formation resulting in aligned films. Using PBTTT as a model system, the influence of different coating parameters on the kinetics of film formation during the deposition thin films via blade-coating is investigated by employing time-resolved in-situ GIWAXS measurements. Furthermore, the formation of high degrees of alignment during the post-deposition annealing process was studied with temperature-resolved GIWAXS. [1] Herrmann, N.J., von Coelln, N., Teichgreber, R.M., Höfener, S., Huck, C., Ghalami, F. et al. (2023) J. Mater. Chem. C, 11, 10185-10197.

HL 53.6 Fri 11:00 POT/0051

Multiscale Modelling of the Density of States in PEDOT:Tosylate Films — •Melissa Kim Meinel and Igor Zozoulenko — Laboratory of Organic Electronics, Linköping University, Norrköping, Sweden

A key descriptor of the electronic structure is the density of states (DOS), which directly affects properties such as charge mobility, intrinsic capacitance, and optical absorption. Structural disorder and the local electrostatic environment strongly influence the DOS but are rarely captured in full detail in computational studies that often rely on small model systems or simplified methods. We present a multiscale modelling approach for computing the DOS of realistic PEDOT:Tosylate films. Molecular dynamics simulations generate film structures that capture the complex packing and disorder of PEDOT chains and counterions. These configurations are analysed within a quantum mechanical/molecular mechanical (QM/MM) framework, where molecular mechanics accounts for large-scale heterogeneity while quantum calculations resolve local electronic states under explicit electrostatic embedding of the environment. Steric effects are treated at the MM level, while the QM region can be limited to a single chain. Accurate results require optimally tuned range-separated hybrid functionals, geometry optimisation of the QM chain, and iterative adaptation of charge distributions to capture realistic environmental effects. This framework enables quantitatively realistic, morphology-sensitive predictions of the electronic structure and has been applied to systems at different oxidation levels.

HL 54: 2D Materials IX – Photonic properties and devices

Time: Friday 9:30–12:45 Location: POT/0081

HL 54.1 Fri 9:30 POT/0081

Signature of interference between second and fourth order nonlinearities in atomically thin crystals — •Paul Herrmann[1], Jonas Margraf[1], Sebastian Klimmer[1], Sebastian Piehler[2], Maximilian Graml[2], Muhammad Sufyan Ramzan[3], Caterina Cocchi[3], Jan Wilhelm[2], and Giancarlo Soavi[1,4] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Germany — [2]Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, Germany — [3]Institute of Condensed Matter Theory and Optics, Friedrich Schiller University Jena, Germany — [4]Abbe Center of Photonics, Friedrich Schiller University Jena, Germany

Transition metal dichalcogenides (TMDs) are a well studied class of two-dimensional materials, whose opto-electronic properties are dominated by excitons and exhibit strong light-matter interaction. The relaxed phase matching in TMD monolayers facilitates the emission of many orders of nonlinearities with approximately equal efficiency. Thus, one can in principle observe interference effects between nonlinearities of different orders N (N=2,3,4,...). Here, we observe a previously unseen modulation of the generated second harmonic upon rotation of the input fundamental polarization. By combining wavelength and power dependent measurements with macroscopic, symmetry-based calculations and microscopic density functional theory simulations, we can assign this modulation to an interference between second and fourth order terms of the nonlinear polarization.

HL 54.2 Fri 9:45 POT/0081

Measurement of optically induced broken time-reversal symmetry in atomically thin crystals — •Florentine Friedrich[1], Paul Herrmann[1], Shridhar Shanbhag[2], Sebastian Klimmer[1], Jan Wilhelm[2], and Giancarlo Soavi[1] — [1]Institute of Solid State Physics, University of Jena, Germany — [2]Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, Germany

Time-reversal symmetry (TRS) and space-inversion symmetry (SIS) are fundamental properties underlying phenomena like magnetism and non-trivial spin

textures in crystals. Transition Metal Dichalcogenides (TMDs) offer a tunable platform to study the interplay of these symmetries, which can be engineered by tuning the number of layers and via all-optical bandgap modulation. We propose a powerful, all-optical approach using third harmonic (TH) Faraday rotation to probe broken TRS, regardless of the SIS [1]. By exciting mono- and bilayer TMDs with elliptically polarized light, we achieve spin-selective bandgap modulation, consequently breaking TRS. This symmetry reduction modifies the nonlinear susceptibility tensor, causing a measurable rotation of the emitted TH polarization. Our experimental results are supported by analytical theory for both mono- and bilayer TMDs and provide a unique tool to investigate spin, valley, and layer coupling in atomically thin semiconductors, thereby contributing to the understanding of the relation between crystal symmetries and the nonlinear optical response of a material.

[1] Friedrich et al., Nat. Photon., 10.1038/s41566-025-01801-2 (2025).

HL 54.3 Fri 10:00 POT/0081

Analytical Theory Of Third Harmonic Generation In Two-Dimensional Materials — •Shridhar Sanjay Shanbhag[1], Florentine Friedrich[2], Paul Herrmann[2], Sebastian Klimmer[2], Giancarlo Soavi[2], and Jan Wilhelm[1] — [1]Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, 93053 Regensburg, Germany — [2]Institute of Solid State Physics, Friedrich Schiller University Jena, 07743 Jena, Germany

Valleytronics explores the valley degree of freedom in materials like transition metal dichalcogenides (TMDs), using electrons in ±K valleys as binary states for information encoding. In valleytronics applications, efficient valley readout is crucial. We show that third harmonic generation (THG) provides an ultrafast solution to valley readout for both centrosymmetric and non-centrosymmetric materials [1].

We solved the semiconductor Bloch equations perturbatively to derive an analytical expression for the polarization state of the emitted third harmonic signal. Our analysis shows how material parameters influence the polarization and attributes polarization rotation to spin and valley dependent optical Stark and Bloch-Siegert shifts in TMDs. Our theoretical predictions closely align with experiments, providing the microscopic mechanism and thus helping advance valleytronic readout mechanisms.

[1] Friedrich, F., Herrmann, P., Shanbhag, S.S. et al. Nat. Photon. (2025). https://doi.org/10.1038/s41566-025-01801-2

HL 54.4 Fri 10:15 POT/0081

Nonlinear optical characterization of oxidized thin layered MoS2 — •Henry Hübschmann[1], Gerhard Berth[1], Klaus Jöns[1], Katharina Burgholzer[2], and Alberta Bonanni[2] — [1]Paderborn University, Paderborn, Germany — [2]Johannes Kepler University Linz, Linz, Austria

In the field of two-dimensional structures the class of transition metal dichalcogenides (TMDs) has sparked great interest in the last decades. Semiconductor materials like molybdenum disulfide (MoS2) have found many applications in photonic and optoelectronic devices [1,2]. An important characteristic is the tunability of the band structure and therefore consequently the possibility for modification of electronic and optical properties [3]. Within this work we conduct comprehensive second order nonlinear optical analysis on thermally oxidized mechanically exfoliated MoS2. In this context a layer number dependent investigation of the nonlinear response up to seven-layer configurations of AB-stacked 2H-MoS2 is performed. Here we found fingerprints of induced structural modifications identified which manifest themselves in the strength of the nonlinear response and a resulting symmetry break of centrosymmetric media.

HL 54.5 Fri 10:30 POT/0081

quantum electrodynamics of excitons in bilayer graphene — •abraham nava mireles — the institut of photonic sciences, castelldefels, spain.

Cavity quantum electrodynamics has been a cornerstone in understanding light-matter interactions. In the so-called strong-coupling regime, these interactions cannot be described as a simple combination of their light and matter components. Instead, light and matter form new hybrid states. This project aims to push beyond into the ultrastrong coupling (USC) regime, where the interaction strength becomes comparable to the system's transition frequencies. In this regime, quantum vacuum fluctuations and elementary excitations become significant. This enables not only the control of quantum effects but also the modification of a material's ground state, even in the absence of external light. To that end, we explore the coupling between confined hyperbolic phonon polaritons (HPhPs) in hexagonal boron nitride (hBN) and excitons in bilayer graphene (BLG). The hyperbolic nature enables deep subwavelength confinement, enhancing the photonic density of states. In BLG, extended dipole transitions exhibit a nonlocal optical response, in which propagating HPhPs allow momentum-dependent transitions and access to a continuum of electronic final states. This leads to enhanced emission rates and to each exciton effectively coupling to multiple polaritonic modes, ultimately reaching a regime where the coupling strength compares to the transition frequency. This platform opens new possibilities for quantum technologies and non-perturbative light-matter engineering.

HL 54.6 Fri 10:45 POT/0081

All-TMDC nanobeam cavities with embedded $MoSe_2$ monolayers for enhanced light-matter interaction — •Aris Koulas-Simos[1], Pietro Metuh[2], Athanasios Paralikis[2], Kartik Gaur[1], Maximilian Klonz[1], Imad Limame[1], Chirag Palekar[1], Battulga Munkhbat[2], and Stephan Reitzenstein[1] — [1]Institut für Physik und Astronomie, Technische Universität Berlin, Berlin, Germany — [2]Department of Electrical and Photonics Engineering, Technical University of Denmark, Kongens Lyngby, Denmark

All-TMDC photonic structures enable enhanced light-matter interaction by combining high index contrast with atomically thin excitonic materials in a homogeneous platform [1]. Recent theoretical work [2] shows that all-TMDC nanostructures can support very large Purcell factors, highlighting their potential for nanoscale lasing. We realize WS_2 nanobeam cavities with a $MoSe_2$ monolayer embedded inside the dielectric cavity for improved field-exciton coupling compared to the conventional evanescent coupling schemes. Simulations predict a cavity mode at 766 nm with $Q \approx 4 \cdot 10^3$, a mode volume of approximately 2.6 $(\lambda/n)^3$, and a confinement factor $\Gamma \approx 0.8\%$. Cross-polarized reflectivity at room temperature reveals resonances between 725 and 760 nm with Q-factor values of 100-300, and low-temperature photoluminescence confirms coupling of the $MoSe_2$ monolayer to the cavity mode. These results establish a monolithic TMDC platform for future all-TMDC nanolasers and quantum emitters.

[1] B. Munkhbat et al., Laser Photon. Rev. 17, 2200057 (2023) [2] F. Binkowski, A. Koulas-Simos et al., arXiv:2508.05333 (2025), accepted

15 min. break or similar.

HL 54.7 Fri 11:15 POT/0081

Temperature-Dependent Moiré Polariton Formation in Bilayer MoSe2 Integrated in DBR based Microcavities — •Chirag Palekar[1], Aris Koulas-Simos[1], Imad Limame[1], Stephan Reitzenstein[1], and Bárbara Rosa[1,2] — [1]Institut für Physik und Astronomie, Technische Universität Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany — [2]University of Campinas, R. Sérgio Buarque de Holanda, 777, 13085-636, Brazil

Twisted bilayer (tBL) MoSe2, which hosts moiré polaritons, when integrated into microcavities, provides a versatile platform for exploring light-matter interactions in moiré-engineered quantum materials. In the absence of the cavity, we observed the PL spectrum of the tBL exhibits multiple resonances corresponding to distinct moiré excitons. When embedded within a DBR cavity, such moiré excitons enter the strong coupling regime with the confined cavity photon mode, leading to the formation of moiré exciton-polaritons. Temperature-induced resonance tuning enables systematic control over the exciton-photon detuning, allowing modulation of the coupling strength. Remarkably, these moiré polaritons remain observable even at temperatures exceeding 150 K, underscoring the robustness of the hybridized light-matter states. Modeling the system using a coupled oscillator approach reveals a Rabi splitting as large as 11 meV. Our results demonstrate that temperature serves as an efficient external control parameter for engineering and tuning moiré exciton polaritons in twisted, atomically thin semiconductors, opening pathways toward reconfigurable polaritonic devices based on van der Waals heterostructures.

HL 54.8 Fri 11:30 POT/0081

Cavity polaritons in a hybrid van-der-Waals superconductor-semiconductor structure — •Seyma Esra Atalay, Hangyong Shan, Martin Esmann, and Christian Schneider — Carl von Ossietzky Universität Oldenburg, Germany

Monolayers of transition metal dichalcogenides (TMDs) offer new possibilities to study superconductivity. In this project, we investigate hybrid heterostructures of $NbSe_2/MoSe_2$ van der Waals layers, in the framework of cavity experiments. $NbSe_2$ and $MoSe_2$ are TMDs; superconductivity occurs in $NbSe_2$ [1], and the monolayer $MoSe_2$ is a direct band gap semiconductor that hosts excitons with high oscillator strength. By embedding the $NbSe_2/MoSe_2$ heterostructure in an open cavity [2], we achieve strong coupling between the $MoSe_2$ excitons and the cavity photons, forming exciton-polaritons, as evidenced by the pronounced Rabi gap seen in subsequent longitudinal and transversal cavity modes in where we tuned the open cavity length. This implementation of a hybrid superconductor-semiconductor monolayer polariton cavity forms the foundation of experiments to gain insight into how exciton-polariton coupling can influence the superconductive phase of $NbSe_2$ and allow us to further investigate optically tunable superconducting hybrid systems.

References [1]Xi, X., Wang, Z., Zhao, W. et al. Ising pairing in superconducting $NbSe_2$ atomic layers. Nature Phys 12, 139-143 (2016)., Journal 100, 101101 (2009) [2]J.C., Drawer et al., Nano Letters 2023 23 (18), 8683-8689

HL 54.9 Fri 11:45 POT/0081

Room temperature hybrid exciton-polaritons in a Perovskite-TMD heterostructrue — •Marti Struve[1], Hamid Pashaei Adl[1], Oliwia Janikwska[2], Sven Stephan[3], Jamie Fitzgerald[4], Paulina Plochocka[2,5], Christian Schneider[1], and Martin Esmann[1] — [1]Carl von Ossietzky Universität, Oldenburg, Germany — [2]Wrocław University of Science and Technology, Wrocław, Poland — [3]University of Applied Sciences Emden, Emden, Germany —

[4]Philipps-University Marburg, Marburg, Germany — [5]Laboratoire National des Champs Magnetiques Intenses, Toulouse, France

Chemically synthesized quasi-2D halide perovskites (HaP) exhibit strong excitonic resonances with large oscillator strength, high binding energy and tunable emission, making them an interesting platform for polariton physics at room temperature. Transition metal dichalcogenide (TMD), while showing lower oscillator strength, offer access to K-valley selective rules, opening the access to polarized excitonic states. In this work, we demonstrate the formation of hybrid exciton-polaritons in a quasi-2D HaP-TMD heterostructure embedded in a planar open cavity at room temperature. Using the tunability of our open cavity we first confirm strong coupling of our materials separately. When combined the system exhibits three polaritonic branches, showing a hybridization of the polariton modes that is reproduced using a three-oscillator Hamiltonian, revealing a state where both excitonic fractions become comparable. Our results lay the foundation to imprint the accessibility of the K-valley selection rules to HaP-polaritons devices leading to additional degrees of freedom.

HL 54.10 Fri 12:00 POT/0081

Tunable Room-Temperature Polaritons Achieving the Very Strong Coupling Regime in Quasi-2D Layered Perovskites — •Hamid Pashaei Adl[1], C. Bennenhei[1], M. Struve[1], P. Peksa[2], M. Dyksik[2], M. Baranowski[2], K. W. Song[3], M. Gittinger[1], C. Lienau[1], J. K. König[4], J. M. Fitzgerald[4], N. P. Jasti[5], F. Eilenberger[6], P. Plochocka[2], E. Malic[4], O. Kyriienko[7], M. Esmann[1], and C. Schneider[1] — [1]Carl von Ossietzky Universität Oldenburg, Germany. — [2]Wroclaw University of Science and Technology, Wroclaw, Poland. — [3]Xiamen University Malaysia, Sepang, Malaysia. — [4]Philipps-Universität, Marburg, Germany. — [5]JNCASR, Bangalore, India. — [6]Max Planck School of Photonics, Jena, Germany. — [7]University of Sheffield, UK.

Layered halide perovskites are organic and inorganic 2D or quasi-2D layers, which self-assemble in solution realizations of quantum well stacks with giant exciton oscillator strengths, tunable emission spectra and very large exciton binding energies. In this contribution, we discuss widely tunable room-temperature cavity exciton polaritons at the cross-over from the strong coupling to the very strong coupling regime, in mechanically exfoliated quasi-2D Ruddlesden-Popper iodide perovskite integrated into an open microcavity. We gradually increased the cavity length and observed a pronounced anti-crossing behavior associated with successive longitudinal cavity modes. The Rabi splitting exhibited a systematic reduction with increasing cavity length; however, the scaling behavior deviated from the conventional square root dependence typically observed in the strong coupling regime.

HL 54.11 Fri 12:15 POT/0081

Optical Gain in Lasers Based on Two-Dimensional TMD Semiconductors — Tommy Schulz[1], •Daniel Erben[1], Alexander Steinhoff[2], Weng Chow[3], and Frank Jahnke[1] — [1]Institute for Theoretical Physics and Bremen Center for Computational Materials Science, University of Bremen, P.O. Box 330 440, 28334 Bremen, Germany — [2]Institute for Physics, Faculty V, Carl von Ossietzky University Oldenburg, 26129 Oldenburg, Germany — [3]Sandia National Laboratories, Albuquerque, New Mexico 87185, USA

We present a direct comparison of the optical gain in InGaAs quantum wells (QWs) and transition-metal dichalcogenide (TMD) monolayers on SiO_2 and encapsulated in hBN. A central objective of this work is to theoretically quantify the gain and to identify its microscopic origin. As a result, we find a substantially larger magnitude of the gain in TMDs - especially in WS_2 - and comparable transparency carrier densities in both systems. The enhanced interband Coulomb interaction in TMDs provides this superior gain performance, although the valley-rich conduction band makes sustaining population inversion more challenging than in InGaAs/GaAs QWs. Encapsulating WS_2 in hBN - a common approach to improve optical quality - proves advantageous, as it reduces carrier drain into side valleys, which lowers the transparency carrier density compared with WS_2/SiO_2. Lastly, we investigate the Henry factor (α), which governs key laser properties such as linewidth behaviour. InGaAs QWs exhibit large α values near transparency, hBN-encapsulated WS_2 shows weakly negative values - an indication towards more favourable lasing performance.

HL 54.12 Fri 12:30 POT/0081

Room-temperature polariton condensate in a quasi-2D hybrid perovskite — M. Struve[1], C. Bennenhei[1], H. Pashaei Adl[1], K.W. Song[2], H. Shan[1], N. Matukhno[1], J.-C. Drawer[1], S. Stephan[1], F. Eilenberger[3], N.P. Jasti[4], D. Cahen[4], O. Kyriienko[5], C. Schneider[1], and •M. Esmann[1] — [1]Carl von Ossietzky Universität Oldenburg — [2]Xiamen University, Sepang, Malaysia — [3]Frauenhofer IOF, Jena — [4]Weizmann Institute of Science, Rehovot, Israel — [5]University of Sheffield, UK

Quasi-2D halide perovskites are chemically synthesized quantum well stacks with large exciton oscillator strength and binding energy. Although promising for polaritonics, bosonic condensation and polariton lasing have so far remained elusive in quasi-2D perovskites at ambient conditions. Here, we demonstrate room-temperature cavity exciton-polariton condensation in mechanically exfoliated crystals of $(BA)_2(MA)_2Pb_3I_{10}$ in an in-situ tunable optical microcavity [1]. We observe a polariton condensation threshold of 0.41 μJcm^{-2} per pulse and detect a strong non-linear response. Interferometric measurements confirm the spontaneous emergence of spatial coherence across the polariton condensate. Our results lay the foundation for a new class of room-temperature polariton lasers based on quasi-2D halide perovskites with great potential for heterointegration with other van-der-Waals materials, photonic crystals and waveguides.

[1] M. Struve et al. arXiv:2408.13677 (Nat. Comms. accepted 2025)

HL 55: Quantum Dots and Wires: (Single) Photonics

Time: Friday 9:30–12:30 Location: POT/0251

HL 55.1 Fri 9:30 POT/0251

Fabrication of a III/V SiO2/SiN hybrid cavity incorporating a single Stark tunable (In,Ga)As quantum dot for high rate single photon generation — •Imad Limame, Kartik Gaur, Sarthak Tripathi, Setthanat Wijitpatima, Aris Koulas-Simos, Chirag Chandrakant Palekar, and Stephan Reitzenstein — Institute for Physics and astronomy, Technical University of Berlin, Berlin, Germany

The advancement of quantum photonic technologies, particularly secure communication based on semiconductor quantum dots (QDs), relies on the on-demand generation of high-quality quantum light. Emission of single photons with high brightness, purity, and indistinguishability is essential for scalable quantum networks. However, the photon emission rate of QDs is fundamentally limited by their nanosecond-scale radiative lifetime. To overcome this, QDs are integrated into photonic nanostructures that enhance light-matter interaction via the Purcell effect, accelerating emission dynamics. Yet, such approaches often require complex bonding and alignment, hindering scalability.

We demonstrate a scalable hybrid cavity platform integrating a Stark-tunable QD within a p-i-n diode into a resonator composed of an epitaxially grown III-V bottom mirror and a PECVD-deposited dielectric top DBR. Deterministic QD positioning using marker-based EBL ensures precise spatial and spectral alignment, improving photon extraction and reducing the radiative lifetime. This approach enables scalable, high-brightness, coherent quantum light sources, providing a solid foundation for next-generation integrated quantum photonics.

HL 55.2 Fri 9:45 POT/0251

Deterministic single-photon source with on-chip GHz acoustic clock — •Alexander Kuznetsov[1], Meysam Saeedi[1], Zixuan Wang[2], Kevin Silverman[2], and Klaus Biermann[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e. V., Hausvogteiplatz 5-7, 10117 Berlin, Germany — [2]National Institute of Standards and Technology, Boulder, Colorado 80305, USA

Solid state single-photon sources are a key component in quantum communication. Their efficiency depends strongly on the single-photon (SP) emission rates. Typically, the latter can be enhanced via Purcell effect by embedding quantum dots (QDs) in optical microcavities (MC), which requires the energy matching between MC optical mode and QD energies. Here, we demonstrate triggering of QD SP emission using dynamic Purcell effect induced by acoustic strain at a frequency of several GHz. To this end, InAs QDs are integrated in a hybrid photon-phonon AlGaAs microcavity, where the density of optical states is tailored by the lateral confinement of photons in um-sized traps defined lithographical patterning of the microcavity spacer. We demonstrate modulation of QD energy up to 14 GHz using quasi-monochromatic strain of a piezoelectrically excited bulk acoustic wave. The modulation periodically shifts the QD transition in resonance with a spectrally narrow confined optical mode, leading to an enhancement of emission, i.e., the dynamic Purcell effect. In combination with high-Q MCs this approach is promising for SP rates above 10 GHz under continuous wave optical excitation. [arXiv:2510.22826]

HL 55.3 Fri 10:00 POT/0251

Beyond-Dipole Radiative Lifetimes of Excitons and Biexcitons in GaAs/AlGaAs Quantum Dots — •Petr Klenovský — Masaryk University, Brno, Czech Republic — Czech Metrology Institute, Brno, Czech Republic

Semiconductor quantum dots are promising sources of on-demand single and entangled photons, but a quantitative microscopic description of their radiative lifetimes remains challenging. We theoretically investigate Coulomb-correlated multi-particle states (X^0, $X^{\pm}$, XX) in weakly confining GaAs/AlGaAs quantum dots using an 8-band $\mathbf{k}\cdot\mathbf{p}$ model combined with continuum elasticity and configuration interaction (CI). Polarization-resolved oscillator strengths and radiative rates are computed both in the dipole approximation and in a quasi-electrostatic beyond-dipole formulation based on a Poisson reformulation of the dyadic Green tensor. For the dots studied, the beyond-dipole treatment yields exciton and biexciton lifetimes in quantitative agreement with experiment. We further analyze electric-field tuning of the multi-particle spectrum and the resulting indistinguishability, characterized by $P = \tau^X/(\tau^X + \tau^{XX})$, and discuss the sensitivity to CI-basis size and to electron-electron and hole-hole exchange.

HL 55.4 Fri 10:15 POT/0251

High-quality single photons from cavity-enhanced biexciton-to-exciton transition — •Nils Heinisch[1], Francesco Salusti[1], Timon L. Baltisberger[2], Mark R. Hogg[2], Malwina A. Marczak[2], Rüdiger Schott[3], Sascha R. Valentin[3], Andreas D. Wieck[3], Arne Ludwig[3], Klaus D. Jöns[1], Richard J. Warburton[2], and Stefan Schumacher[1] — [1]Department of Physics, CeOPP, and PhoQS, Paderborn University, Germany — [2]Department of Physics, University of Basel, Switzerland — [3]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Germany

Generating high-quality photons using the biexciton-exciton cascade benefits from the separability of the photons from the two-photon excitation laser pulse. However, the intrinsic lifetime ratio between biexciton (XX) and exciton (X) states leads to a fundamental limit for the achievable indistinguishability of the single photons [1]. Therefore, the XX must decay much faster than the X. We achieve this with an optical resonator that resonantly enhances the XX-X transition. By optimizing the cavity parameters and avoiding phonon-mediated cavity feeding, we show that high-quality cavity photons originating from XX can be generated. Furthermore, we show that spectral filtering restores single-photon quality in regimes of XX binding energies, where X emission into the cavity is not initially excluded. Our theoretical investigations are joined by key results from the experimental demonstration, which make this approach a major advance in the realization of practical quantum light sources. [1] E. Schöll et al., PRL 125, 233605 (2020). D. Bauch et al., Adv. Quantum Technol. 7, 2300142 (2024).

HL 55.5 Fri 10:30 POT/0251

Photon-mediated electron capture into a single quantum emitter — •Daniel Oppers[1], Hendrik Mannel[1], Luca Henrichs[1], Fabio Rimek[1], Arne Ludwig[2], Axel Lorke[1], and Martin Geller[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg, Germany — [2]Chair of Applied Solid State Physics, Ruhr-University Bochum, Germany

Single-photon emitters are one of the key components of quantum information technology. Especially single self-assembled quantum dots in a p-i-n diode structure for charge control are still a promising candidate. We use an InAs/GaAs quantum dot in a bias regime, where the dot is uncharged and drive the exciton transition optically resonant with a cw diode laser. A second off-resonant cw laser with a lower energy than any optical transition is used to induce an internal photoeffect [1], exiting electrons from the electron reservoir in the diode, that are captured into the quantum dot. Consequently, we observe a quenching of the exciton transition, which can no longer be driven resonantly. This electron capture by photo-excitation of electrons from the reservoir (see also [2]) is measured here in real-time, observing every quantum jump from an uncharged to a charged quantum dot in a random telegraph signal. Evaluating the telegraph signal using waiting time distributions we observe a linear increase in the electron capture rate scaling up with increasing excitation power of the off-resonant laser. Our findings reveal that photo-induced quenching is a possible source of exciton dephasing.

[1] P. Lochner et. al., Phys. Rev. B **103**, 075426 (2021)
[2] A. Kurzmann Appl. Phys. Lett. **108**, 263108 (2016)

HL 55.6 Fri 10:45 POT/0251

Influence of the internal photoelectric effect on the indistinguishability of single quantum dot photons — •Luca Henrichs[1], Fabio Rimek[1], Hendrik Mannel[1], Daniel Oppers[1], Arne Ludwig[2], Martin Geller[1], and Axel Lorke[1] — [1]Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg — [2]Chair of Applied Solid State Physics, Ruhr-University Bochum, Germany

A single self-assembled quantum dot (QD) is one of the promising candidates as a bright (high photon rate) and stable (Fourier-limited) linewidth single photon source [1]. For applications in photonic devices or in quantum communication networks the dephasing process is an important property, where besides spin- and charge noise, the Auger-Meitner [2] and the photoeffect [3] could play an important role.

Here, we investigate the impact of the internal photoelectric effect on the indistinguishability of single QD photons. We used pulsed Hong-Ou-Mandel measurements at different excitation intensities of the exciton transition to determine the photon indistinguishability in various driving regimes, ranging from coherent scattering (the Heitler regime) to the incoherent regime above the saturation intensity. Above saturation, we observe the influence of the photoeffect, which reduces the indistinguishability. Our findings represent an important step toward understanding the decoherence of single photons in this important quantum system.

[1] N. Tomm et al., Nat. N. **16**, 399*403 (2021). [2] H. Mannel et al., AIP, **15**, 134 (2023). [3] P. Lochner et al, PR, **7**, 103, (2021).

15 min. break

HL 55.7 Fri 11:15 POT/0251

An ultra-compact deterministic source of maximally entangled photon pairs — Moritz Langer[1], Pavel Ruchka[2], Ahmad Rahimi[1], Sara Jakovljevic[2], Yared G. Zena[1], Sai Abhishikth Dhurjati[1], Alexey Danilov[1], Mandira Pal[1], Riccardo Bassoli[3], Frank H. P. Fitzek[3], Oliver G. Schmidt[4], Harald Giessen[2], and •Caspar Hopfmann[1,2] — [1]Institute for Emerging Electronic Technologies, IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [2]4th Physics Institute and Research Center SCoPE, University of Stuttgart, 70569 Stuttgart, Germany — [3]Deutsche Telekom Chair of Communication Networks, Technische Universität Dresden, Dresden, Germany — [4]Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Chemnitz, Germany

We demonstrate an ultra-compact source of on-demand, maximally entangled photon pairs using single GaAs quantum dots in monolithic microlenses, efficiently fiber-coupled in a cryogenic environment. A 3D-printed micro-objective facilitates near-diffraction-limited performance at 3.8 K. The system achieves high single-photon emission rates (392(20) kHz) and purities (0.992(5)) via two-photon resonant excitation. Leveraging the exciton-biexciton cascade, it produces near-maximally entangled photon pairs (peak entanglement negativities of 2n=0.96(2)). This quantum light source combines state-of-the-art performance and stability with a dramatically reduced footprint, well-suited for seamless industrial integration.

HL 55.8 Fri 11:30 POT/0251

Spectral shadows of a single GaAs quantum dot — •Jens Hübner[1], Kai Hühn[1], Lena Klar[1], Fei Ding[1], Arne Ludwig[2], Andreas D. Wieck[2], and Michael Oestreich[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany

Semiconductor quantum dots are today's leading candidates for generating single and entangled photons. However, even the most advanced devices face performance limitations due to charge state fluctuations within the quantum dot and its surrounding environment. We have carried out detailed time-resolved resonance fluorescence measurements on an individual charge-tunable GaAs quantum dot, providing new insight into the spectral signatures generated by the complex landscape of unintentional impurities. For the neutral exciton and the negatively charged trion transitions, we uncover multiple Stark-shifted resonances, linked to rare spectral jumps smaller than the homogeneous linewidth. In other experiments, these jumps are typically obscured by measurement noise. In contrast, the positively charged and doubly negatively charged trions exhibit distinctly different behaviors. We quantify the underlying impurity charge dynamics over timescales ranging from sub-milliseconds to several seconds, and demonstrate that the hole population of the positively charged trion is limited in our state-of-the-art pin-structure by fast hole loss combined with slow hole recapture.

[Hühn et al., arXiv:507.20290 (2025)]

HL 55.9 Fri 11:45 POT/0251

Adhesive bonding of In(Ga)As - QD membrane on Silicon for evanescent light coupling — •J. Unfried[1], R. Vijayan[1], U. Pfister[1], D. Wendland[2], S. Oberle[1], M. Weiss[1], M. Jetter[1], S. Portalupi[1], and P. Michler[1] — [1]IHFG, University of Stuttgart, Allmandring 3, 70569 Stuttgart, Germany — [2]AG Pernice, Universität Münster, Heisenbergstraße 11, 48149 Münster, Germany

Hybrid integration of III-V materials with silicon photonics involves combining efficient III-V light emitters with low-loss, CMOS-compatible Si platforms. This allows high-performance PICs to be realised. Adhesive bonding is a scalable and flexible method for achieving this integration. It provides and enables lithography-defined alignment. However, this approach also presents significant challenges. Efficient coupling between the III-V active membrane and Si waveguides (WG) requires an extremely thin, optically transparent bonding layer to enable strong evanescent coupling. Such thin layers restrict the thermal budget available for post-bonding processes, and may result in delamination during subsequent fabrication steps. Reliable integration therefore necessitates an optimised bonding process and carefully controlled fabrication conditions. This work focuses on integrating an InGaAs membrane with C-band InAs QDs

onto a Si photonic platform using an optimised adhesive bonding scheme. A simulation-guided design approach is employed to identify suitable waveguide and taper geometries, and a reproducible bonding process is used to fabricate uniform, thin bonding layers and tapered InGaAs waveguides that efficiently couple QD emission into Si waveguides.

HL 55.10 Fri 12:00 POT/0251

Revisiting Quantum Well Thickness Fluctuation Quantum Dots as a Source of Single Photons — •Tom Fandrich[1], Frederik Benthin[1], Yiteng Zhang[1], Benjamin Bohn[1], Maximilian Heller[1], Johan Hilbig[1], Tom Rakow[1], Arijit Chakraborty[1], Doaa Abdelbarey[1], Eddy P. Rugeramigabo[1], Michael Zopf[1,2], and Fei Ding[1,2] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover — [2]Laboratorium für Nano- und Quantenengineering, Leibniz Universität Hannover, Schneiderberg 39, 30167 Hannover

Semiconductor-based quantum dots (QDs) are promising candidates for quantum network applications due to their ability to generate single, entangled, and indistinguishable photons on demand. Modern epitaxial III-V quantum emitters based on local droplet etching with nanohole infilling or Stranski-Krastanov growth exhibit excellent properties from the near-infrared to the telecom bands. An alternative from the early days of QD research involved QDs formed by thickness fluctuations in quantum well (QW) heterostructures. These QW thickness fluctuation (QWTF) QDs can naturally display strong light-matter interaction due to giant oscillator strengths, yet have not been the focus of recent research as quantum emitters for single-photon applications. In this work, we investigate the optical properties of naturally formed QWTF QDs in GaAs QWs emitting near 780 nm. Our results demonstrate that their distinctive properties justify revisiting QWTF QDs with today's standard for single-photon sources competing against state-of-the-art epitaxial approaches.

HL 55.11 Fri 12:15 POT/0251

Single-Photon Emission with High Spectral Purity from Site-Controlled InGaN Quantum Dots — •Nima Hajizadeh[1,2], Nils Bernhardt[2], Richard Zimmermann[2], Felix Nippert[2], Luca Sung-Min Choi[2], Benjamin Damilano[3], Jean-michel Chauveau[4], and Markus Wagner[1,2] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V. — [2]Technische Universität Berlin, Institute of Solid State Physics — [3]Université Côte d'Azur, CNRS, CRHEA — [4]Université Paris Saclay, Université Versailles Saint Quentin, CNRS, GEMaC

The development of high-quality Single-Photon Emitters (SPEs) based on Indium Gallium Nitride (InGaN) Quantum Dots (QDs) is essential for advancing quantum technologies. We present a comprehensive investigation of SPEs based on novel top-down fabricated, site- and size-controlled InGaN QDs. In this work, the optical and quantum optical properties of these isolated QDs are comprehensively investigated using high-resolution, time-correlated micro-photoluminescence (μ-PL) spectroscopy, including temperature-, power- and polarization-dependent measurements, as well as hyperspectral PL mapping of their excitonic emission. The purity of the single-photon emission is evaluated by measuring the second-order intensity autocorrelation function $g^{(2)}(\tau)$ in a Hanbury-Brown and Twiss (HBT) setup. We show that the emitter exhibits an exceptionally sharp emission bandwidth below 0.02 nm and pronounced anti-bunching with $g^{(2)}(0) < 0.36$. These results confirm the potential of our site-controlled growth methodology to deliver high-purity SPEs with narrow spectral lines.

HL 56: Quantum Emitters in 3D Semiconductors

Time: Friday 11:15–12:30 Location: POT/0006

HL 56.1 Fri 11:15 POT/0006

Electrically driven single-photon sources for scalable quantum photonics operating at the telecommunication wavelengths — •Alessandro Puddu[1,2], Junchun Yang[2], Shengqiang Zhou[1], Artur Erbe[1,2], Ahmad Echresh[1], Kambiz Jamshidi[2], and Yonder Berencén[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstrasse 400, Dresden, 01328, Germany — [2]Technische Universität Dresden, Dresden, 01069, Germany

Silicon-based quantum technologies provide a scalable platform for photonics due to their CMOS compatibility and ease of integration. Single-photon sources operating at telecom wavelengths are key components for low-loss quantum communication networks and the emerging quantum internet. Integrating these emitters with reconfigurable photonic elements such as multiplexers, modulators, filters, etc. and on-chip single-photon detectors is essential for realizing scalable quantum hardware. Optical excitation methods, however, rely on complex and alignment-sensitive laser systems, limiting their integration potential. Electrically driven color centers offer a compact and fully integrable alternative. This paper is focused on achieving electrically driven single-photon emission from individual color centers embedded in a silicon PIN diode. Emission in the telecom O- and L-bands is particularly advantageous, as it aligns with low-loss and low-dispersion regions in standard optical fibers. To improve emission efficiency and on-demand single photon generation, a single-color center will be coupled to a CMOS-compatible optical cavity, enabling Purcell-enhanced emission and efficient integration into silicon photonic circuits.

HL 56.2 Fri 11:30 POT/0006

Liquid Metal Alloy Ion Sources for Quantum Emitters — •Nico Klingner[1], Lukas Prager[1], Gregor Hlawacek[1], Stefan Findeisen[1], Wolfgang Pilz[2], and Paul Mazarov[2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden - Rossendorf (HZDR), Bautzner Landstr. 400, 01328 Dresden, Germany — [2]Raith GmbH, Konrad-Adenauer-Allee 8, 44263 Dortmund, Germany

Liquid metal alloy ion sources (LMAIS) have evolved into powerful emitters for generating focused ion beams (FIBs) of a wide range of elemental species. In recent years, they have become a key enabling tools for quantum technologies, supporting applications such as deterministic single-ion implantation, the controlled creation of defect centers acting as single-photon sources, or for local isotopic purification of silicon for quantum-grade materials.

In this contribution, we present an overview of the LMAIS fabrication process, inluding eutectic alloy phase diagrams in selecting suitable compositions, the microfabrication and sharpening of emitter needles, and the challenges of alloy wetting and reservoir filling. As the alloy chemistry and emitter surface are highly susceptible to contamination, all steps are recently carried out under ultra-high-vacuum conditions to prevent oxidation and ensure reproducible operating characteristics.

Finaly we will show a summary and an outlook on single photon emitter production that benefit from the unique versatility of LMAIS-based ion beams.

HL 56.3 Fri 11:45 POT/0006

Defect-based quantum emitters in aluminum nitride — •Annkathrin Köhler, Jan Böhmer, and Carsten Ronning — Friedrich Schiller Universität, Jena, Deutschland

Aluminum nitride (AlN) has recently gained attention as a promising platform for integrated quantum photonic applications, where single-photon emitters (SPEs) play a key role in quantum communication and on-chip information processing. Its wide bandgap, CMOS compatibility, and established role in optoelectronic technologies make AlN an attractive host for stable, room-temperature SPEs. However, the microscopic origin and controllability of its defect-based emission remain insufficiently understood, challenging the implementation in scalable quantum photonic devices. Here, we investigated the defect-related luminescence in commercially available PVD-grown AlN thin films using micro-photoluminescence spectroscopy and second-order correlation measurements. By characterizing both intrinsic defects and extrinsic impurities introduced through controlled ion irradiation, we aim to identify routes toward reproducible and deterministic creation of optically active defect centers. Ion irradiation provides a tunable method for introducing specific defect types and spatially localized emitters, potentially enabling on-demand SPE fabrication. This study supports the development of AlN as a viable wide-bandgap host for quantum light sources and outlines directions for integrating AlN-based SPEs into future photonic architectures.

HL 56.4 Fri 12:00 POT/0006

Atomic force lithography positioned circular Bragg cavities for high performance quantum dot based quantum light sources. — •Abhishikth Dhurjati[1], Moritz Langer[1], Yared Zena[1], Ahmad Rahimi[1], Liesa Raith[1], Martin Bauer[1], Riccardo Bassoli[2], Frank Fitzek[3], and Caspar Hopfmann[2] — [1]Institute for Emerging Electronic Technologies, IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [2]Quantum Communication Networks research group, Deutsche Telekom Chair of Communication Networks, Dresden University of Technology, Germany — [3]Deutsche Telekom Chair of Communication Networks, Dresden University of Technology, Germany

Semiconductor quantum dots (QDs) are excellent quantum emitters, but their random spatial distribution hinders deterministic cavity integration. We present a room-temperature atomic force microscopy (AFM) assisted nano-oxidation technique enabling deterministic QD positioning with a radial displacement of 51(28) nm. Free-standing circular Bragg gratings fabricated around positioned GaAs QDs exhibit a 245-fold photoluminescence enhancement and fine-structure splitting comparable to bulk QDs. Polarization-resolved measurements and simulations show robust cavity-coupled emission for in-plane displacements up to 50 nm and devices with Stokes imbalance below 5 percent, confirming precise alignment and a scalable route toward high-performance quantum light sources.

HL 56.5 Fri 12:15 POT/0006

Bright quantum dot light sources using monolithic microlenses on gold back-reflectors — •Moritz Langer[1,2,3], Sai A Dhurjati[1], Yared Zena[1], Ahmad Rahimi[1], Mandira Pal[1], Liesa Raith[1], Sandra Nestler[1], Riccardo Bassoli[2,3], Frank H P Fitzek[3], Oliver G Schmidt[4], and Caspar Hopfmann[1,2,3] — [1]Institute for Emerging Electronic Technologies - IFW Dresden, Dresden, Germany — [2]Quantum Communication Networks Research Group, Dresden University of Technology, Germany — [3]Deutsche Telekom Chair of Communication Networks, Dresden University of Technology, Germany — [4]Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Germany

We present a scalable approach for fabricating bright GaAs quantum-dot photon sources by integrating QDs into broadband monolithic AlGaAs microlens arrays on gold-coated GaAs substrates. Thermally reflowed photoresist templates are transferred into AlGaAs thin films using an optimized 3D reactive-ion etching process, enabling large-area arrays with highly uniform lens geometries. Photoluminescence statistics reveal brightness enhancements of up to *200, occurring in roughly 1 out of 200 lenses, in good agreement with our developed fabrication-yield model. Finite-difference time-domain simulations predict extraction efficiencies of up to 62% for free-space collection and 37% for fiber-coupling. These results highlight the strong potential of this platform for compact, scalable entangled-photon sources in future quantum networks.

HL 57: Nitrides IV – Optical properties

Time: Friday 11:30–12:45 Location: POT/0051

HL 57.1 Fri 11:30 POT/0051

Optical Properties of Sn-doped n-type GaN — •Hannah Bendin[1], Elias Kluth[1], Kazuki Ohnishi[2], Kansuke Hamasaki[2], Shugo Nitta[2], Naoki Fujimoto[2], Hirotaka Watanabe[2], Yoshio Honda[2], Hiroshi Amano[2], Rüdiger Goldhahn[1], and Martin Feneberg[1] — [1]Otto-von-Guericke-Universität Magdeburg, Germany — [2]Nagoya University, Japan

GaN is at the heart of many contemporary electronic and optoelectronic applications. To increase the efficiency of high-power devices, the preparation of degenerately doped n-type GaN of high quality is required. Generally, Si and Ge are introduced as dopants, each giving rise to their own challenges. For example, high Si-doping is counteracted by carrier compensation and an increase in tensile stress. Recently, Sn has also gained interest as a dopant in GaN. Initial theoretical and experimental studies show promising results, introducing Sn as a candidate for strain control in n-type GaN via co-doping with Si or Ge, as the radius mismatch between Ga and Sn causes compressive strain, unlike Si or Ge. Here, we investigate Sn-doped samples with different carrier concentrations grown by halide vapor phase epitaxy by employing a variety of optical techniques. To determine the influence of the carrier concentration in GaN:Sn on the optical properties, we apply spectroscopic ellipsometry, Raman spectroscopy, and photoluminescence. Two sets of samples have been investigated: (I) GaN:Sn on a GaN/sapphire template and (II) GaN:Sn on a freestanding GaN substrate.

HL 57.2 Fri 11:45 POT/0051

Optical properties of ScAlN: investigation by spectroscopic ellipsometry — •Christina Harms[1], Jona Grümbel[1], Duc V. Dinh[2], Zhuohui Chen[3], Oliver Brandt[2], Martin Feneberg[1], and Rüdiger Goldhahn[1] — [1]Otto-von-Guericke-Universität, Institut für Physik, Magdeburg, Germany — [2]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V., Berlin, Germany — [3]Huawei Technologies Canada Co., Ltd., Kanata, Canada

$Sc_xAl_{1-x}N$ alloys are of increasing interest due to their unique ferroelectric and optoelectronic properties. In this work, we investigate the dielectric function of this material using spectroscopic ellipsometry. A series of $Sc_xAl_{1-x}N$ samples with $0 \leq x \leq 0.35$, grown on AlN/Si by plasma-assisted molecular beam epitaxy, were measured in the infrared (IR) and ultraviolet (UV) spectral range. In the IR range, the E_1(TO) phonon mode is characterized in terms of its resonance frequency ω and broadening γ, which are analyzed as a function of Sc content. Additionally, the dielectric limit ε_∞ is derived. With increasing Sc content, ω decreases, while both γ and ε_∞ increase. In the UV range, we determine the optical bandgap E_g as well as the corresponding ε_∞ and describe the observed trends across the composition range. Here, E_g decreases systematically with increasing Sc content and ε_∞ increases accordingly. The results are compared with recent results from literature, showing consistent trends in the optical properties throughout the investigated composition range.

HL 57.3 Fri 12:00 POT/0051

Near-lattice-matched AlScN/GaN heterostructures studied by spectroscopic ellipsometry and photoluminescence — •Alwin Wüthrich[1], Rajendra Kumar[2], Oana Malis[2], Rüdiger Goldhahn[1], and Martin Feneberg[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Germany — [2]Department of Physics and Astronomy, Purdue University, USA

Understanding the fundamental properties of the novel ferroelectric material AlScN, such as ferroelectricity, tunable lattice constants, a wide and tunable band gap, and high piezoelectric coefficients, is crucial for its correct implementation in modern applications. Examples include processing units based on non-volatile memory and the design of infrared devices that utilize transitions between strongly confined electronic states, i.e., intersubband transitions. Here, near-lattice-matched AlScN layers (with 4–25% Sc) were grown by molecular beam epitaxy (MBE) on MBE-grown GaN layers. The samples were investigated by spectroscopic ellipsometry from the near-infrared to the far-ultraviolet range, probing infrared-active phonons and interband transitions. Additionally, the samples were studied by temperature-dependent photoluminescence, revealing luminescence from a two-dimensional electron gas.

HL 57.4 Fri 12:15 POT/0051

Near-Infrared Photocurrent Spectroscopy of InN Two-Terminal Devices — •Alexandra V. Nemmaier[1,2], Maximilian A. Gruber[1,2], Abhilash Ulhe[1,2], Gregor Koblmüller[1,2], and Alexander W. Holleitner[1,2] — [1]Walter Schottky Institute, TU Munich, Germany — [2]Exzellenzcluster e-conversion, Munich, Germany

The semiconductor InN, with its narrow bandgap, high electron mobility, and specific carrier cooling mechanisms, is a promising platform for optoelectronics and hot carrier solar cells. We investigate epitaxial InN layers grown on GaN by near-infrared photocurrent spectroscopy. We measure the spatially resolved photocurrent to characterize the photoresponse in gated two-terminal devices. This approach offers a new perspective on hot carrier generation, charge carrier transport, and relaxation mechanisms close to the bandgap of the material.

HL 57.5 Fri 12:30 POT/0051

Structural and vibrational properties of strain-free $Al_{1-x}Sc_xN$ nanowires — Adriano Notarangelo[1], Ileana Florea[2], Philippe Vennéguès[2], Aidan Campbell[1], Hans Tornatzky[1], Jonas Lähnemann[1], Thomas Auzelle[1], Lutz Geelhaar[1], Oliver Brandt[1], and •Philipp John[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz-Institut im Forschungsverbund Berlin e.V. 10117 Berlin, Germany — [2]Université Côte d'Azur, CRHEA, CNRS, 06905 Sophia-Antipolis Cedex, France

The incorporation of Sc into the wurtzite crystal lattice of AlN enhances its piezoelectricity and induces ferroelectricity, making $Al_{1-x}Sc_xN$ an attractive material for novel types of group-III nitride based devices. Yet, the lattice distortions giving rise to these functionalities are superimposed to distortions arising from residual strain introduced during the heteroepitaxy on lattice-mismatched substrates.

In this work, self-assembled wurtzite $Al_{1-x}Sc_xN$ nanowires are grown by molecular beam epitaxy, varying the Sc content x from 0 to 0.38. The nanowire geometry allows elastic relaxation to occur, resulting in strain-free, bulk-like $Al_{1-x}Sc_xN$. A non-linear evolution of lattice parameters and a continuous redshift of the E_2^{high} and A_1(TO) phonon modes as a function of Sc content are found, confirming its incorporation into the wurtzite lattice and revealing modifications of anion-cation bond strength and coordination environment.

Our results highlight the advantages of bulk-like $Al_{1-x}Sc_xN$ for probing its fundamental properties, laying the ground work for further device applications.

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Overview of Invited Talks and Sessions

(Lecture halls HSZ/0002, HSZ/0004, POT/0112, POT/0151, POT/351, and POT/361; Poster P2 and P4)

Invited Talks

MA 1.1	Sun	16:00–16:30	TRE/PHYS	**Recent advances and challenges in magnetic structure determination** — •Dmytro Inosov
MA 4.1	Mon	9:30–10:00	POT/0151	**From ML to Kinetics: Modeling the Switching in Ferroelectric Wurtzites** — •Andrew Rappe, Drew Behrendt, Atanu Samanta, Von Braun Nascimento
MA 4.2	Mon	10:00–10:30	POT/0151	**Topological order parameter switching** — •Sergey Artyukhin
MA 4.3	Mon	10:30–11:00	POT/0151	**Optical Control of Ferroaxial Order via Circular Phonon Excitation** — •Zhiyang Zeng, Michael Först, Michael Fechner, Dharmalingam Prabhakaran, Paolo Radaelli, Andrea Cavalleri
MA 10.1	Mon	15:00–15:20	POT/0112	**Multi-field analysis of magnetic materials: Phase-field based simulations of magnetic domains and phase transition** — •Mobina Alaeddini, Jörg Schröder, Maximilian Vorwerk
MA 10.2	Mon	15:20–15:40	POT/0112	**Realistic Modelling of Finite Temperature Electron Transport Properties in Ferromagnets** — •Fabian Engelke, Christian Heiliger
MA 10.3	Mon	15:55–16:20	POT/0112	**Exploring magneto- and multicaloric materials for room and cryogenic temperature applications** — •Benedikt Beckmann
MA 10.4	Mon	16:20–16:45	POT/0112	**Nonlinear magnon dynamics: From the discovery of Floquet magnons to CMOS-compatible magnon computing** — •Christopher Heins
MA 10.5	Mon	16:45–17:10	POT/0112	**The geometric memory of quantum wave functions** — •Niclas Heinsdorf
MA 10.6	Mon	17:10–17:35	POT/0112	**Altermagnets and Odd-parity-wave Magnets** — •Anna Birk Hellenes
MA 14.1	Tue	9:35–10:20	HSZ/0002	**Femtophonomagnetism** — •Sangeeta Sharma, John Dewhurst
MA 14.2	Tue	10:20–10:50	HSZ/0002	**THz-driven dynamical ferroicity in paraelectric and diamagnetic perovskites** — •Martina Basini
MA 14.3	Tue	10:50–11:20	HSZ/0002	**Angular momentum transfer and chiral phonons from first principles** — •Markus Weissenhofer, Philipp Rieger, MS Mrudul, Luca Mikadze, Sergiy Mankovsky, Svitlana Polesya, Hubert Ebert, Ulrich Nowak, Peter M. Oppeneer
MA 14.4	Tue	11:35–12:05	HSZ/0002	**Inertial Spin Dynamics: A Signature of Non-Markovian Interactions in Ferromagnets** — •Vivek Unikandanunni, Felix Hartmann, Matias Bargheer, Eric Fullerton, Stefano Bonetti, Janet Anders
MA 14.5	Tue	12:05–12:35	HSZ/0002	**Atomistic simulations of ultrafast spin-lattice dynamics** — •Richard Evans, Mara Strungaru
MA 18.1	Tue	9:30–10:00	POT/0151	**Magnetic Cooling: From applications at room temperature to hydrogen liquefaction** — •T. Gottschall, E. Bykov, M. Strassheim, T. Platte, C. Fujta, D. Benke, M. Fries, W. Liu, A. Döring, K. Skokov, O. Gutfleisch, J. Wosnitza
MA 25.1	Wed	9:30–10:00	HSZ/0002	**Coherent phononic control of chirality** — •Michael Först
MA 25.2	Wed	10:00–10:30	HSZ/0002	**Towards a modern theory of chiralization (and can chiral phonons help us get there?)** — •Nicola Spaldin
MA 25.5	Wed	11:15–11:45	HSZ/0002	**Observation and control of chiral phonons in non-centrosymmetric materials** — •Hiroki Ueda
MA 27.1	Wed	9:30–10:00	HSZ/0004	**Towards sub-10fs magnetization switching** — Reza Rouzegar, Oliver Franke, Gal Lemut, Oliver Gueckstock, Junwei Tong, Dieter Engel, Xianmin Zhang, Georg Woltersdorf, Piet W. Brouwer, Tobias Kampfrath, •Quentin Remy
MA 29.1	Wed	9:30–10:00	POT/0112	**Exploring the interplay between spin and chirality** — •Angela Wittmann

MA 35.1	Wed	15:00–15:30	POT/0112	**Magneto-optic Kerr effects of higher order in magnetization in thin films of different crystal orientations** — •Timo Kuschel
MA 40.1	Thu	9:30–10:00	HSZ/0002	**Magnetic order induced chiral phonons in a ferromagnetic Weyl semimetal** — •Luyi Yang
MA 40.6	Thu	11:15–11:45	HSZ/0002	**Thermal Hall Effects of Magnons and Phonons** — •Alexander Mook
MA 43.1	Thu	9:30–10:00	POT/0112	**Defect-Induced Phase Transitions in the 2D Magnetic Semiconductor CrSBr** — •Shengqiang Zhou
MA 44.1	Thu	9:30–10:00	POT/0151	**2D and 3D racetracks: Interplay of geometric and magnetic chiralities** — •Stuart Parkin
MA 44.2	Thu	10:00–10:30	POT/0151	**Combined MFM/KPFM at the Ultimate Sensitivity Limit for Probing Curvature-Engineered Micromagnetic States** — •Emily Darwin, Reshma Peremadathil Pradeep, Luca Berchialla, Daniel Rotthardt, Ales Hrabec, Hans Hug
MA 44.3	Thu	10:30–11:00	POT/0151	**Curvilinear magnetism in superconducting spintronics** — •Sol Jacobsen
MA 44.4	Thu	11:15–11:45	POT/0151	**Advanced Control of Magnetic Nanostructures via Metasurface Engineering and Voltage-Driven Functionalities** — •Anna Palau
MA 44.5	Thu	11:45–12:15	POT/0151	**Magnetic tomography of noncollinear spin textures in curvilinear geometries** — •Sandra Ruiz-Gomez

Invited Talks of the joint Symposium SKM Dissertation Prize 2026 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	HSZ/0002	**Stochastic-Calculus Approach to Non-equilibrium Statistical Physics** — •Cai Dieball
SYSD 1.2	Mon	10:00–10:30	HSZ/0002	**Nonuniform magnetic spin textures for sensing, storage and computing applications** — •Sabri Koraltan
SYSD 1.3	Mon	10:30–11:00	HSZ/0002	**Anomalous Quantum Oscillations beyond Onsager's Fermi Surface Paradigm** — •Valentin Leeb
SYSD 1.4	Mon	11:00–11:30	HSZ/0002	**Coherent Control Schemes for Semiconductor Quantum Systems** — •Eva Schöll
SYSD 1.5	Mon	11:30–12:00	HSZ/0002	**On stochastic thermodynamics under incomplete information: Thermodynamic inference from Markovian events** — •Jann van der Meer

Invited Talks of the joint Symposium Fluids with Broken Time-Reversal Symmetry: Odd/Hall Viscosity between Active Matter and Electron Flows (SYBS)

See SYBS for the full program of the symposium.

SYBS 1.1	Tue	9:30–10:00	HSZ/AUDI	**Odd viscosity in three-dimensional fluids: flows, wakes, and eddies** — •Tali Khain
SYBS 1.2	Tue	10:00–10:30	HSZ/AUDI	**Odd viscosity in two-dimensional hydrodynamic electron transport** — •Igor Gornyi, Dmitry Polyakov
SYBS 1.3	Tue	10:30–11:00	HSZ/AUDI	**Odd slip on chiral active surfaces** — •Andrej Vilfan, Yuto Hosaka
SYBS 1.4	Tue	11:15–11:30	HSZ/AUDI	**Parity-odd transport in electron fluids** — •Johanna Erdmenger
SYBS 1.5	Tue	11:30–11:45	HSZ/AUDI	**Curved Odd Elasticity** — Lazaros Tsaloukidis, Yuan Zhou, Jack Binysh, Nikta Fakhri, Corentin Coulais, •Piotr Surówka

Invited Talks of the joint Symposium Beyond Transistors: Material-Based Edge Computing Paradigms (SYBT)

See SYBT for the full program of the symposium.

SYBT 1.1	Wed	9:30–10:00	HSZ/AUDI	**Finding Neuromorphic Advantage with Magnetism** — •Johan Mentink
SYBT 1.2	Wed	10:00–10:30	HSZ/AUDI	**Accelerating Neural Networks Computation with Ferroelectric Oxides** — •Laura Bégon-Lours, Nikhil Garg, Alexandre Baigol, Anwesha Panda, Nathan Savoia, Alexander Flasby
SYBT 1.3	Wed	10:30–11:00	HSZ/AUDI	**a photonic approach to probabilistic computing** — •Wolfram Pernice
SYBT 1.4	Wed	11:15–11:45	HSZ/AUDI	**Tackling Reliability and Scalability in Neuromorphic Computing via Noise-aware Learning** — •Eleni Vasilaki
SYBT 1.5	Wed	11:45–12:15	HSZ/AUDI	**Bayesian nanodevices for trustworthy artificial intelligence** — •Damien Querlioz

Invited Talks of the joint Symposium Interacting Degrees of Freedom in Ultrathin Quantum Films (SYQF)

See SYQF for the full program of the symposium.

SYQF 1.1	Fri	9:30–10:00	HSZ/AUDI	**Exciton dressing by extreme nonlinear magnons in a layered semiconductor** — •Geoffrey M. Diederich
SYQF 1.2	Fri	10:00–10:30	HSZ/AUDI	**A tale of demons and decay in two-dimensional (alter)magnets** — •Alexander Mook
SYQF 1.3	Fri	10:30–11:00	HSZ/AUDI	**Magnetism, light and matter - Role of excitons in two-dimensional magnets** — •Florian Dirnberger
SYQF 1.4	Fri	11:15–11:45	HSZ/AUDI	**Advantages and challanges of resonance Raman scattering with infrared excitation energy** — •Leonetta Baldassarre
SYQF 1.5	Fri	11:45–12:15	HSZ/AUDI	**Shining light on 2D antiferromagnets** — •Dmytro Afanasiev

Sessions

MA 1.1–1.2	Sun	16:00–18:15	TRE/PHYS	**Hands-On Tutorial: Magnetic Structure Determination Using Fullprof and SARAh Representation Analysis (joint session MA/TUT)**
MA 2.1–2.12	Mon	9:30–12:45	HSZ/0004	**Altermagnets I**
MA 3.1–3.12	Mon	9:30–12:45	POT/0112	**Complex Magnetic Oxides**
MA 4.1–4.6	Mon	9:30–12:00	POT/0151	**Focus Session: Novel mechanisms of ferroic switching (joint session MA/FM)**
MA 5.1–5.9	Mon	9:30–12:00	POT/0351	**Surface Magnetism and Topological Insulators (joint session MA/TT)**
MA 6.1–6.12	Mon	9:30–12:45	POT/0361	**Magnetic Imaging Techniques I**
MA 7.1–7.86	Mon	9:30–12:30	P2	**Poster Magnetism I**
MA 8.1–8.13	Mon	15:00–18:30	HSZ/0002	**Altermagnets II**
MA 9.1–9.13	Mon	15:00–18:30	HSZ/0004	**Magnonics I**
MA 10.1–10.6	Mon	15:00–18:05	POT/0112	**INNOMAG e.V. Prizes 2026 (Diplom-/Master and Ph.D. Thesis)**
MA 11.1–11.11	Mon	15:00–18:00	POT/0151	**Electron Theory of Magnetism and Correlations (joint session MA/TT)**
MA 12.1–12.6	Mon	15:00–16:30	POT/0351	**Terahertz Spintronics**
MA 13.1–13.9	Mon	15:00–17:15	POT/0361	**Magnetic Heuslers and Semiconductors**
MA 14.1–14.5	Tue	9:30–12:40	HSZ/0002	**PhD Focus Session: What about the lattice? Lessons from (ultrafast) magnetism**
MA 15.1–15.7	Tue	9:30–12:45	HSZ/0003	**Focus Session: Quantum Sensing with Solid State Spin defects I (joint session TT/MA)**
MA 16.1–16.12	Tue	9:30–12:45	HSZ/0004	**Skyrmions I**
MA 17.1–17.11	Tue	9:30–12:30	POT/0112	**Multiferroics and Magnetoelectric Coupling (joint session MA/FM)**
MA 18.1–18.7	Tue	9:30–11:30	POT/0151	**Caloric Effects in Ferromagnetic Materials (joint session MA/TT)**
MA 19.1–19.11	Tue	9:30–12:30	POT/0361	**Frustrated Magnets I (joint session MA/TT)**
MA 20.1–20.6	Tue	14:00–15:30	HSZ/0002	**Altermagnets III**
MA 21.1–21.6	Tue	14:00–15:30	HSZ/0004	**Skyrmions II**
MA 22.1–22.5	Tue	14:00–15:30	BEY/0138	**Focus Session: Materials Discovery II – High throughput searches for functional magnetic materials (joint session FM/MA)**
MA 23.1–23.6	Tue	14:00–15:30	POT/0151	**Cooperative Phenomena: Spin Structures and Magnetic Phase Transitions (joint session MA/TT)**
MA 24.1–24.6	Tue	14:00–15:30	POT/0361	**Weyl Semimetals (joint session MA/TT)**
MA 25.1–25.9	Wed	9:30–12:45	HSZ/0002	**Focus Session: Chiral phonons and crystals coupled to magnetic order I**
MA 26.1–26.7	Wed	9:30–12:45	HSZ/0003	**Focus Session: Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects I (joint session TT/DS/MA)**
MA 27.1–27.11	Wed	9:30–12:45	HSZ/0004	**Ultrafast Magnetization Effects I**
MA 28.1–28.4	Wed	9:30–10:30	HSZ/0101	**Focus Session: Quantum Sensing with Solid State Spin defects II (joint session TT/HL/MA)**
MA 29.1–29.11	Wed	9:30–12:45	POT/0112	**Spin Transport and Orbitronics, Spin-Hall Effects I (joint session MA/TT)**
MA 30.1–30.12	Wed	9:30–12:45	POT/0151	**Functional Antiferromagnetism**
MA 31.1–31.12	Wed	9:30–12:45	POT/0361	**Frustrated Magnets II (joint session MA/TT)**
MA 32	Wed	14:00–17:30	HZDR	**Excursion: Current and Future High-Field THz User Facilities at HZDR**
MA 33.1–33.13	Wed	15:00–18:30	HSZ/0002	**Altermagnets IV**
MA 34.1–34.13	Wed	15:00–18:30	HSZ/0004	**Computational Magnetism I**
MA 35.1–35.10	Wed	15:00–18:00	POT/0112	**Spintronics (other effects) (joint session MA/TT)**
MA 36.1–36.13	Wed	15:00–18:30	POT/0151	**Molecular Magnetism and Magnetic Particles / Clusters I**
MA 37.1–37.9	Wed	15:00–17:15	POT/0351	**Non-Skyrmionic Magnetic Textures**

MA 38.1–38.14	Wed	15:00–18:45	POT/0361	**Ultrafast Magnetization Effects II**
MA 39.1–39.25	Wed	18:00–21:00	P2	**Poster Magnetism II**
MA 40.1–40.10	Thu	9:30–12:45	HSZ/0002	**Focus Session: Chiral phonons and crystals coupled to magnetic order II**
MA 41.1–41.11	Thu	9:30–12:30	HSZ/0003	**Focus Session: Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects II (joint session TT/DS/MA)**
MA 42.1–42.11	Thu	9:30–12:30	HSZ/0004	**Molecular Magnetism and Magnetic Particles / Clusters II**
MA 43.1–43.6	Thu	9:30–11:15	POT/0112	**Spin-Dependent Phenomena in 2D**
MA 44.1–44.8	Thu	9:30–13:00	POT/0151	**Focus Session: Curvilinear magnetism: Magnetics with nanoscale curved geometries (joint session MA/TT)**
MA 45.1–45.6	Thu	9:30–11:00	POT/0351	**Magnetic Relaxation and Gilbert Damping**
MA 46.1–46.5	Thu	9:30–10:45	POT/0361	**Magnetic Imaging Techniques II**
MA 47.1–47.11	Thu	15:00–18:00	HSZ/0002	**Altermagnets V**
MA 48.1–48.11	Thu	15:00–18:00	HSZ/0004	**Magnonics II**
MA 49.1–49.9	Thu	15:00–17:15	POT/0112	**Magnetic Imaging, Information Technology, and Sensors**
MA 50.1–50.9	Thu	15:00–17:15	POT/0151	**Bulk Materials: Soft and Hard Permanent Magnets**
MA 51.1–51.8	Thu	15:00–17:00	POT/0361	**Spin Transport and Orbitronics, Spin-Hall Effects II (joint session MA/TT)**
MA 52.1–52.40	Thu	15:00–17:00	P4	**Poster Magnetism III**
MA 53	Thu	18:00–19:00	HSZ/0002	**Members' Assembly**
MA 54.1–54.11	Fri	9:30–12:30	HSZ/0002	**Altermagnets VI**
MA 55.1–55.12	Fri	9:30–12:45	HSZ/0004	**Skyrmions III**
MA 56.1–56.6	Fri	9:30–11:30	BEY/0E40	**Focus Session: (Anti)ferroic states – Magnetic and magnetoelectric III (joint session FM/MA)**
MA 57.1–57.6	Fri	9:30–11:00	POT/0112	**Thin Films: Magnetic Coupling Phenomena / Exchange Bias and Magnetic Anisotropy**
MA 58.1–58.12	Fri	9:30–12:45	POT/0151	**Computational Magnetism II**
MA 59.1–59.11	Fri	9:30–12:30	POT/0361	**Magnonics III**

Members' Assembly of the Magnetism Division

Thursday 18:00–19:00 HSZ/0002

- Bericht
- Wahl
- Verschiedenes

Sessions

– Invited Talks, Topical Talks, Tutorials, Contributed Talks, and Posters –

MA 1: Hands-On Tutorial: Magnetic Structure Determination Using Fullprof and SARAh Representation Analysis (joint session MA/TUT)

The functionalities of many materials of contemporary interest are related to complex types of magnetic ordering. Accurate magnetic structure determination is thus crucial for understanding and optimizing such materials.

After an introduction into the subject, participants of the tutorial will gain hands-on experience on the methods for magnetic structure determination.

Time: Sunday 16:00–18:15 Location: TRE/PHYS

Invited Talk MA 1.1 Sun 16:00 TRE/PHYS

Recent advances and challenges in magnetic structure determination — •Dmytro Inosov — Institut für Festkörper- und Materialphysik, TU Dresden, Germany

In this introductory tutorial talk, I will provide an overview of magnetic structure determination in the context of recent advances in magnetic materials. I will focus on the limitations and challenges of magnetic structure refinement, and explain why it is important to use the full range of complementary experimental methods alongside conventional diffraction in order to develop a consistent understanding of magnetic structures. This is particularly important when dealing with complex types of magnetic order, such as noncollinear and multi-Q spin textures, altermagnets, and systems with multiple magnetic sublattices or very weak and/or fluctuating magnetic moments.

Tutorial MA 1.2 Sun 16:30 TRE/PHYS

Hands-On Tutorial: Magnetic Structure Determination Using Fullprof and SARAh Representation Analysis — •Matthias Frontzek — Oak Ridge National Laboratory, Neutron Scattering Division, One Bethel Valley Road, 37831 Oak Ridge, TN, USA

The determination of magnetic structures is a crucial aspect of materials science, particularly for understanding the magnetic properties of novel materials. Given the limited availability of neutrons with the closure of smaller sources, competitive access to beam time, and the high hurdles associated with software usage, there is an increasing need for training in the analysis of magnetic structures. This tutorial aims to provide participants with practical skills in magnetic structure determination using SARAh and Fullprof, two powerful tools frequently utilized in this field.

Participants will:

-Gain hands-on experience with the tools and techniques necessary for magnetic structure determination.

-Refine nuclear and magnetic structures using real data sets.

-Understand key concepts in diffraction techniques and steps involved in the magnetic structure determination process.

Important: for Hands-on participation, please bring a laptop with a working installation of Fullprof (https://www.ill.eu/sites/fullprof/).

For links to Fullprof, SARAh stand-alone and tutorial data visit: https://neutrons.ornl.gov/wand/users

MA 2: Altermagnets I

Time: Monday 9:30–12:45 Location: HSZ/0004

MA 2.1 Mon 9:30 HSZ/0004

Electric Control of Spin and Valley Polarization in the XMoTeO6 Family of Two-dimensional Altermagnets — •Avijeet Ray[1], Fatemeh Haddadi[2], Antimo Marrazzo[3], and Marco Gibertini[1,4] — [1]University of Modena and Reggio Emilia, Italy — [2]EPFL, Switzerland — [3]SISSA, Italy — [4]Istituto Nanoscienze-CNR, Italy

Altermagnets are a special class of antiferromagnets with zero net magnetization but spin-split bands, even in the absence of spin-orbit-coupling. In semiconducting altermagnets, this spin-splitting can give rise to spin-valley locking, where valleys located at specific k-points have a well-defined spin. Still, symmetries connecting the spin sublattices impose an overall degeneracy between valleys of opposite spins. An external electric field can break these symmetries, enabling controllable spin (and valley) polarization. This is particularly promising in two-dimensional (2D) materials where it is easy to apply a vertical electric field in a double-gate field-effect setup, provided that 2D altermagnets with suitable crystal symmetries are found. Here, by using first-principles simulations, not only we put forward an interesting family of 2D altermagnets that display the correct symmetries, but we also show that the electric field effect is sizable in these materials and reaches the requirements needed for applications in spin-valleytronics.

MA 2.2 Mon 9:45 HSZ/0004

Zeeman Quantum Geometry as a Probe of Unconventional Magnetism — •Snehasish Nandy[1], Neelanjan Chakraborti[2], and Sudeep Kumar Ghosh[2] — [1]National Institute of Technology Silchar, Silchar, India — [2]Indian Institute of Technology Kanpur, Kanpur, India

Unconventional magnets with momentum-dependent spin-splitting but zero net magnetization form a recently identified class of collinear magnets that are challenging to probe via conventional means. We show that these systems can be distinguished through intrinsic gyrotropic magnetic (IGM) currents, enabled by the Zeeman quantum geometry, which captures the coupled response of electronic states to momentum translation and spin rotation. Examining two prototypical two-dimensional unconventional magnets with Rashba spin-orbit coupling, a time-reversal-broken d-wave altermagnet and a time-reversal-symmetric p-wave magnet, we uncover a direct link between crystalline symmetry, spin-split band structures, and transport signatures. The d-wave altermagnet exhibits both transverse conduction and longitudinal displacement IGM currents, whereas p-wave magnet supports only transverse conduction IGM current. Remarkably, the mixed d-wave altermagnet supports all four types of IGM currents, including a longitudinal conduction current enabled by symmetric (Zeeman) Berry curvature that is forbidden in conventional quantum geometry. These responses, measurable via Hall transport and optical probes, persist even when conventional quantum geometry-driven linear responses vanish, offering unique access to hidden spin-split band structures.

MA 2.3 Mon 10:00 HSZ/0004

Spin demons in d-wave altermagnets — •Pieter Gunnink[1], Jairo Sinova[1], and Alexander Mook[2] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Staudingerweg 7, Mainz 55128, Germany — [2]University of Münster, Institute of Solid State Theory, 48149 Münster, Germany

Demons are a type of plasmons, which consist of out-of-phase oscillations of electrons in different bands. Here, we show that d-wave altermagnets, a recently discovered class of collinear magnetism, naturally realize a spin demon, which consists of out-of-phase movement of the two spin species [1]. The spin demon lives outside of the particle-hole continuum of one of the spin species, and is therefore significantly underdamped, reaching quality factors of > 10. We show that the spin demon carries a magnetic moment, which inherits the d-wave symmetry. Finally, we consider both three and two dimensional d-wave altermagnets, and show that spin demons exists in both.

[1] Gunnink, Sinova, Mook, Phys. Rev. Lett. 135, 126701 (2025)

MA 2.4 Mon 10:15 HSZ/0004

Altermagnetism in magnetic nanoisland arrays — •Rhea Hoyer[1], Lukas Körber[2], Tobias Wagner[3], and Alexander Mook[1] — [1]Institut für Festkörpertheorie, Universität Münster, Münster, Germany — [2]Institute of Molecules and Materials, Radboud University, Nijmegen, The Netherlands — [3]Department of Physics, Johannes Gutenberg University Mainz, Mainz, Germany

We present a macrospin model for magnetic island arrays engineered with altermagnetic symmetries. The islands interact purely via dipole-dipole coupling, which makes the strict spin-orbit-free limit of altermagnetism inaccessible. Although the magnon dispersion is split by spin-orbit coupling, the magnon bands

remain spin-polarized, exhibiting a characteristic d-wave-like pattern of the spin expectation value across the Brillouin zone. This residual altermagnetic character gives rise to direction-dependent spin dynamics and suggests the possibility of anisotropic spin-transport phenomena in mesoscopic artificial magnets.

MA 2.5 Mon 10:30 HSZ/0004

Magnons in Antialtermagnets — •Robin R. Neumann[1,2,3], Rodrigo Jaeschke-Ubiergo[2], Ricardo Zarzuela[2], Jairo Sinova[2,4], and Alexander Mook[1,2] — [1]University of Münster, Münster, Germany — [2]Johannes Gutenberg University Mainz, Mainz, Germany — [3]Martin Luther University Halle-Wittenberg, Halle, Germany — [4]Texas A&M University, College Station, USA

Altermagnets and antialtermagnets are unconventional magnetic phases with compensated magnetization and nonrelativistic spin splitting in their electronic band structures. In altermagnets, this spin splitting has even parity, whereas in antialtermagnets it has odd parity. In this talk we go beyond electrons and demonstrate that magnons, the collective spin excitations of magnetically long-range ordered systems, inherently feature an odd-parity spin polarization in antialtermagnets without spin-orbit or dipolar coupling. We present minimal model spin Hamiltonians free of spin-orbit coupling that stabilize antialtermagnetic ground states, discuss their symmetries, and characterize the spin-polarized magnon band structures.

MA 2.6 Mon 10:45 HSZ/0004

Magnetization processes and spin-lattice coupling in the hexagonal easy-plane altermagnet α-MnTe — •Sahana Rössler[1], Victoria Ginga[1], Ece Uykur[2], Yurii Skourski[3], Jeremy Sourd[3], Sergei Zherlitsyn[3], Marcus Schmidt[4], Yurii Prots[4], Helge Rosner[4], Ulrich Burkhardt[4], Ulrich K. Rössler[5], and Alexander A. Tsirlin[1] — [1]Felix Bloch Institute for Solid State Physics, Leipzig University, Leipzig, Germany — [2]HZDR, IBP and Materials Research, Dresden, Germany — [3]HLD, HZDR, Dresden, Germany — [4]MPI CPfS, Dresden, Germany — [5]Institute for Theoretical Solid-State Physics, Leibniz IFW Dresden, Germany

We investigated the magnetization dynamics associated with domain behavior in α-MnTe using magnetization, magnetostriction, sound velocity, and attenuation measurements. Angle- and field-dependent magnetization data reveal complex magnetic responses with a distinct anomaly around 1 T, reflecting domain-related processes. Magnetostriction and elastic constant measurements indicate strong lattice effects at the field-induced reorientation transition. These features were analysed using a phenomenological micromagnetic model incorporating higher-order anisotropic exchange interactions that couple the weak ferromagnetic component to the antiferromagnetic order parameter. The model successfully reproduces the generic behaviour of the magnetic states and demonstrates that the observed uniaxial and unidirectional anisotropies arise from metastable domain configurations and irreversible magnetization processes [1].

[1] S. Rößler et al., arXiv:2511.01388

15 min break

MA 2.7 Mon 11:15 HSZ/0004

Emergent Altermagnetism in Antiferromagnetic Surfaces — •Colin Lange[1], Rodrigo Jaeschke Ubiergo[1], Alexander Mook[2], and Jairo Sinova[1] — [1]Institut für Physik, Johannes Gutenberg Universität Mainz, Germany — [2]Institut für Festkörpertheorie, Universität Münster, Germany

Three-dimensional altermagnets with collinear compensated order and nonrelativistic spin splitting have recently been realized, but experimental access to their 2D counterparts remains limited. We show that surfaces of the most abundant class of collinear magnets – conventional 3D antiferromagnets – provide a general route to 2D altermagnetism through surface-induced symmetry breaking. We implement this in a semi-infinite stack geometry, effectively modeling a thin film to establish a direct connection to experimental systems. This way, the symmetry analysis made here has direct implications for readily available experiments and materials. Using our novel definition of "surface spin groups", which lies between the 3D and 2D cases due to the semi-infinite geometry, we provide a full symmetry classification of all possible cases of altermagnetic surface termination. We scan available databases of magnetic materials, and conclude that almost half of the collinear antiferromagnets can host an altermagnetic surfaces. We present calculations of spin-split surface states in realistic candidates, that can serve for future experimental verification of surface induced altermagnetism. Our work positions the broadly accessible landscape of antiferromagnets as a promising foundation for 2D altermagnetism, whose experimental realization remains limited.

MA 2.8 Mon 11:30 HSZ/0004

Angle-dependent magnetoresistance induced by interface-generated spin current in RuO_2/permalloy heterostructures — Akashdeep Akashdeep[1], Ewiese Mohammad Ababneh[2], Christin Schmitt[1], Edgar Galíndez-Ruales[1], Felix Fuhrmann[1], Timo Kuschel[1], Mathias Kläui[1], Vivek Amin[2], and •Gerhard Jakob[1] — [1]Johannes Gutenberg University, Mainz, Germany — [2]Indiana University, Indianapolis, USA

Ruthenium dioxide (RuO_2) is a promising altermagnetic candidate. In our PLD grown films clear signs of altermagnetism were found by photoemission [1] and optically induced spin polarization with d-wave symmetry [2]. However, recent reports suggest that RuO_2 may be nonmagnetic in its ground state. (100)-oriented RuO_2 films are expected to generate spin currents with transverse spin polarization parallel to the Neel vector. We investigated magnetotransport in epitaxial RuO_2/permalloy (Py) heterostructures to examine spin Hall magnetoresistance and interfacial effects. Our measurements revealed a pronounced negative angular-dependent magnetoresistance that we attribute to interface-generated spin current (IGSC) at the RuO_2/Py interface supported by drift-diffusion calculations. The interface effects predominate over possible altermagnetic contributions [3]. This finding is in accord with recent muon spin resonance on our films [4].

[1] O. Fedchenko et al., Sci. Adv. 10, eadj4883 (2024);
[2] M. Weber et al., arXiv2408.05187 (2024);
[3] A. Akashdeep et al., Phys. Rev. Appl. 24, 054018 (2025);
[4] A. Akashdeep et al., arXiv2510.08064 (2025);

MA 2.9 Mon 11:45 HSZ/0004

X-ray magnetic circular dichroism of altermagnet α-Fe2O3 based on multiplet ligand-field theory using Wannier orbitals — Ruiwen Xie, Hamza Zerdoumi, and •Hongbin Zhang — TU Darmstadt, Darmstadt, Germany

Hematite α-Fe2O3 is a g-wave altermagnet, possessing an easy-axis and easy-plane weak ferromagnetic phase below and above Morin temperature, respectively. The presence of these phases renders it a good candidate to study the characteristic spin splitting in altermagnets under the impacts of relativistic effect and finite temperature. We have calculated the band structure of α-Fe2O3 based on density functional theory (DFT) considering the Coulomb correction and spin-orbit coupling effects. Additionally, the DFT + dynamical mean-field theory calculations have been performed at finite temperatures. It is found that the spin splitting in α-Fe2O3 preserves with either SOC or temperature effect included. Furthermore, we present a numerical simulation of the x-ray magnetic circular dichroism (XMCD) of the L2,3 edge of Fe using a combination of DFT with multiplet ligand-field theory. In terms of the different Néel vectors present in α-Fe2O3, we calculate the x-ray absorption spectroscopy of the L2,3 edge of Fe in the form of conductivity tensor and analyze the XMCD response from a perspective of symmetry. A characteristic XMCD line shape is expected when the Néel vector is along [010] direction and the light propagation vector is perpendicular to the Néel vector, which can be further distinguished from the XMCD response originated from weak ferromagnetism with the light propagation vector parallel to the Néel vector.

MA 2.10 Mon 12:00 HSZ/0004

Magnetic circular dichroism in resonant Auger electron diffraction from altermagnets — •Peter Krüger — Chiba University, Chiba, Japan

Recently we demonstrated that in altermagnets, there exists a large magnetic circular dichroism (MCD) in resonant photoelectron diffraction (RPED) [1]. The MCD-RPED signal is time-reversal odd and characteristic of the altermagnetic state. It is proportional to the local XMCD signal from a single magnetic sublattice and thus provides a direct probe of the sublattice magnetization. Here we show that MCD-RPED occurs in all altermagnets independently of the orientation of the Néel vector. This is a major difference to the weak XMCD observed in some altermagnets [2]. We also extend the theory to resonant Auger electron diffraction, whose MCD gives similar information as that of RPED, while being conceptually simpler. We discuss the symmetry properties of the MCD signal and explain its physical origin with a simple model. [1] P. Krüger, Phys. Rev. Lett. 135, 196703 (2025). [2] A. Hariki et al, Phys. Rev. Lett. 132, 176701 (2024).

MA 2.11 Mon 12:15 HSZ/0004

Heisenberg models of altermagnets — •Volodymyr Kravchuk[1,2], Kostiantyn Yershov[1,2], and Jeroen van den Brink[1] — [1]Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany — [2]Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, 03143 Kyiv, Ukraine

Being collinear-compensated magnets, altermagnets differ from conventional antiferromagnets by a more complex symmetry transformation that connects two sublattices. Due to the specific local nonmagnetic surroundings of the magnetic atoms, the symmetry transformation also involves rotation or mirror reflection, in addition to translation and time reversal. Here we propose Heisenberg models for a number of materials, including d-wave (rutiles), bulk g-wave (CrSb, MnTe), and planar g-wave (FeS2) alternagnets. The models capture the altermagnetic properties due to the additional superexchange interactions whose bonds orientations respect the symmetry of the local nonmagnetic surrounding of the magnetic atoms. Using our models, we reproduce the altermagnetic splitting in the magnon spectra, and predict a number of new effects induced by altermagnetism, namely fluctuation-induced piezomagnetism and thermal spin conductivity for d-wave altermagnets, and emergent magnetization of domain walls for both d- and g-wave altermagnets. For planar g-wave altermagnets, we demonstrate that mechanical stress can induce the effective g-wave – d-wave

transition for low-energy magnons. As a result, the stress-induced thermal spin conductivity appears.

MA 2.12 Mon 12:30 HSZ/0004

Multiferroic altermagnet $BiFeO_3$ investigated by DFT+DMFT and XMCD — •Hamza Zerdoumi, Ruiwen Xie, Fu Li, and Hongbin Zhang — Institute of Materials Science, TU Darmstadt, 64287 Darmstadt, Germany

As an emergent magnetic ordering, altermagnets with finite non-relativistic spin splitting exhibit a wide spectrum of fascinating properties. In this work, combining density functional theory (DFT) and dynamical mean-field theory (DMFT), we investigate how such splitting evolves as a function of temperature in $BiFeO_3$. Moreover, by solving the DFT-derived atomic Hamiltonian, we evaluated x-ray magnetic circular dichoism (XMCD) with detailed symmetry analysis, which can be considered as a characteristic feature for altermagnetic ordering. Furthermore, as $BiFeO_3$ is a well-established multiferroic compound, we evaluate the nonlinear transport properties such as shift current originated from the quantum geometry, and further explore how such altermagnetic properties can be tailored by external electric fields.

MA 3: Complex Magnetic Oxides

Time: Monday 9:30–12:45 Location: POT/0112

MA 3.1 Mon 9:30 POT/0112

Twisted planar freestanding La0.7Sr0.3MnO3 junctions — •Alejandro Martín Merodio, Victor Rouco, Fernando Gallego, David Sanchez-Manzano, Carlos León, and Jacobo Santamaria — GFMC, Dpto. de Física de Materiales, Facultad de Ciencias Físicas, Universidad Complutense de Madrid, 28040 Madrid, Spain

The recent realization of membranes of transition metal oxides has enabled their mechanical assembly in twisted bilayers opening avenues to wards oxide twistronics. The ferroic orders hosted by transition metal oxides, many of which are stable at room temperature, offer exciting opportunities for the search of chiral ferroic properties in twisted ox ide membranes. In this work we present the growth, fabrication and characterization of twisted stacks made of La0.7Sr0.3MnO3 (LSMO), a half-metallic ferromagnetic perovskite with highly tunable properties. We have studied the temperature dependent magnetotransport across the interface of two twisted LSMO membranes for different twisting angles. These samples exhibit a large low temperature magnetoresistance MR up to 32% which switches abruptly at small (10 mT) magnetic fields. These MR values are well above the 0,01% AMR typically observed in single LSMO flakes. This approach allows exploring material combinations which are not possible in epitaxial heterostructures and opens promising avenues towards oxide based CMOS compatible spintronic devices.

MA 3.2 Mon 9:45 POT/0112

Controlling Magnetic Anisotropy in Barium Hexaferrite by Cation Doping — •Jakob Baumsteiger[1,2] and Cesare Franchini[1,2] — [1]Faculty of Physics and Center for Computational Materials Science, University of Vienna, Vienna, Austria — [2]Department of Physics and Astronomy "Augusto Righi", Alma Mater Studiorum - Università di Bologna, Bologna, Italy

Circulators are essential components in many radio-frequency systems, including 5G base stations. Their operating frequency is primarily determined by the magnetic properties of the ferrite core - specifically the anisotropy field and the saturation magnetization. Experimental studies suggest that both quantities can be actively modified in barium hexaferrite - one of the ferrites commonly used in circulators - through cation doping. However, the relationship between doping and the resulting magnetic properties is highly complex and not yet fully understood. We investigate the electronic structure of pristine and cobalt-doped barium hexaferrite using density functional theory. Our calculations show that the additional electron introduced by cobalt plays a key role in modifying the material's magnetocrystalline anisotropy. By occupying a localized orbital at the cobalt site, it locally activates spin-orbit interactions, leading to substantial changes in the magnetocrystalline anisotropy energy even at low doping concentrations. The insights gained from our results support the design of miniaturized circulators capable of operating over broad frequency bands.

MA 3.3 Mon 10:00 POT/0112

Emergent magnetic ordering in high-entropy oxides — •Laura T. Corredor[1,2], Augustè Stanionytė[3], Richard Matyšek[3], Anja U. B. Wolter[4], Carlos F. Eugenio[2,5], Andrea Kirsch[2,5], Giuditta Perversi[6], and Anna Isaeva[1,2,3] — [1]TU Dortmund University, Germany — [2]Research Center Future Energy Materials and Systems, Germany — [3]University of Amsterdam, The Netherlands — [4]Leibniz IFW Dresden, Germany — [5]Ruhr University Bochum, Germany — [6]Maastricht University, The Netherlands

Magnetism in high-entropy oxides (HEOs) has emerged as a compelling topic due to the unique behavior arising from extreme cationic disorder. HEOs offer a rich platform for fundamental studies and are promising for applications like energy-efficient magnetic devices and catalysts. Recently, long-range magnetic order was reported in some HEOs, e.g. the AFM rocksalt $(Co_{0.2}Ni_{0.2}Cu_{0.2}Mg_{0.2}Zn_{0.2})O$[1] and cubic perovskite $La(Cr_{0.2}Mn_{0.2}Fe_{0.2}Co_{0.2}Ni_{0.2})O$[2], demonstrating that HEOs can host long-range magnetic order despite substantial chemical disorder. We present the exploration of magnetism across three HEO families: (1) cubic perovskites $BaIn_{1-x}M_xO_{3-\delta}$[3], (2) spinel M_3O_4 and (3) rocksalt MO. The M site is shared by up to five (post-)transition metals. Some members of the M_3O_4 family exhibit remarkably high T_N up to 618 K, highlighting its potential for stabilizing robust magnetic interactions. In contrast, $BaIn_{1-x}M_xO_{3-\delta}$ display glassy behavior. We examine how chemical complexity shapes magnetic properties across these families. [1] Chem. Mat. 2019 31 (10), 3705-3711. [2] Adv. Sci. 2022, 9, 2200391. [3] Solid State Ionics (2024) 427, 116901.

MA 3.4 Mon 10:15 POT/0112

Exploring the electronic structure of (111)-oriented $La_{0.7}Sr_{0.3}MnO_3$ through soft X-ray ARPES and DFT — •Øyvind Finnseth, Sverre M. Selbach, Hendrik Bentmann, and Ingrid Hallsteinsen — NTNU, Trondheim, Norway

While $La_{0.7}Sr_{0.3}MnO_3$ (LSMO) has been widely studied due to its room-temperature ferromagnetism and half-metallicity, the majority of work has been focused on thin films in the (001)-orientation. The less conventional (111)-orientation has received far less attention despite its distinct intriguing properties, including sixfold in-plane magnetic anisotropy and enhanced interfacial coupling in heterostructures. As such, a full description of the electronic structure of LSMO in this orientation is lacking. Here, we consider epitaxial thin films of LSMO grown by pulsed laser deposition on (111)-oriented $SrTiO_3$ substrates. We first develop an in-vacuum methodology for surface preparation of the films by annealing in an oxygen atmosphere. The electronic band structure of the films is probed by soft X-ray angle-resolved photoemission spectroscopy (ARPES) using a synchrotron lightsource. The tunability of the photon energy allows for precise control of the probed out-of-plane momentum, yielding a full description of the LSMO electronic band structure. Density functional theory (DFT) calculations are performed to obtain the theoretical band structure of bulk LSMO modeled through the use of the special quasirandom structures approach. By comparing the calculated band structure to the experimental results, we find that the DFT calculations are able to accurately predict the LSMO electronic band structure.

MA 3.5 Mon 10:30 POT/0112

Unveiling the Origins of Strong Magnetostriction in Cobalt Ferrite using neutron scattering. — •Guratinder Kaur — School of Physics and Astronomy, The University of Edinburgh, UK

Cobalt ferrite (CoFe2O4, CFO) stands out among advanced functional materials due to its exceptional magnetostrictive behaviour. This property allows its shape to be influenced by its magnetic state, making it desirable for various technological applications such as electronic devices, ferrofluids, magnetic drug delivery, microwave devices, and high-density information storage1-3. The present study provides a comprehensive investigation using neutron diffraction to explore the interplay between CFO's nuclear and magnetic structures4 across varying temperatures. This study complements our recent inelastic neutron scattering (INS) experiments on single crystal and powder samples. The combined data, along with our INS findings and developed excitonic theory, will provide a deeper understanding of the underlying mechanism responsible for CFO's strong magnetostrictive effect5. This knowledge will be valuable for designing novel materials with precisely controlled magnetostrictive properties for applications in areas like sensors and actuators6. References: 1)*Slonczewski J C, Phys. Rev. 110 1341 (1958). 2)*Zheng H et al., Science 303 661 (2004). 3)*Bhame S D et al., J. Appl. Phys. 100 113911 (2006). 4)*Teillet et al., J. Mag. Magn. Mater. 123, 93 (1993). 5)*Lane et al., Adv. Funct. Mater. 2025, e16830. 6)*Chen Y, et al., IEEE Trans. Magn. 35 3652 (1999).

MA 3.6 Mon 10:45 POT/0112

Polarized Neutron Scattering Studies on SDW Order in $Sr_{1.5}Ca_{0.5}RuO_4$ and $Sr_2Ru_{0.95}Co_{0.05}O_4$ — •Felix Wirth[1], Yvan Sidis[2], Paul Steffens[3], Kevin Jenni[1], Agustinus Agung Nugroho[4], Karin Schmalzl[5], Mechthild Enderle[3], and Markus Braden[1] — [1]II. Physic. Inst., Univ. Cologne, Germany — [2]LLB, CEA Saclay, France — [3]ILL, Grenoble, France — [4]Inst. Teknologi, Bandung, Indonesia — [5]JCNS Outst. ILL, Grenoble, France

Superconductivity in Sr_2RuO_4 emerges close to magnetic instabilities from Fermi-surface nesting at incommensurate $Q^{\alpha\beta}$ ≈(0.3,0.3,L) and Q^{γ} ≈(0.15,0.15,L)[1]. In $Sr_{1.5}Ca_{0.5}RuO_4$ the anisotropic fluctuations at $Q^{\alpha\beta}$

condense into a c-axis polarized spin-density-wave[2]. Polarized inelastic neutron scattering reveals an unusual hierarchy of excitations with enhanced longitudinal modes. In contrast, transverse modes are suppressed, although their energy dependence remains similar to that of the parent compound. Above the SDW transition, longitudinal and transverse contributions show a split response, incompatible with tetragonal symmetry and suggestive of electronic nematicity. Ti^{4+} and Mn^{3+} substitution stabilise the same static order at $Q^{\alpha\beta}$[3]. By contrast, 5% Co doping does not yield the expected ferromagnetic cluster glass but a new magnetic order at Q≈(0.2,0.2,0) with intensity following the Ru^{4+} form factor that cannot be attributed to the known nesting vectors in this system. [1] Jenni, K. et al., Phys. Rev. B 103, 104511 (2021), [2] Kunkemöller, S. et al., Phys. Rev. B 89, 045119 (2014), [3] Braden, M. et al., Phys. Rev. Lett. 88, 197002 (2002)

15 min break

MA 3.7 Mon 11:15 POT/0112

Magnetic structure and magnetic excitations of the triple layer $Sr_4Ru_3O_{10}$ — •Lara Kiefer[1], Zahrasadat Ghazinezhad[1], Felix Wirth[1], Jens Mettler[1], Ursula Bengaard Hansen[2], Paul Steffens[2], Oksana Zaharko[3], Vladimir Pomjakushin[3], Karin Schmalzl[4], Devashibhai Adroja[5], Augustinus Agung Nugroho[6], and Markus Braden[1] — [1]Inst. Phys. 2, Cologne, Germany — [2]ILL, Grenoble, France — [3]PSI, Villingen, Switzerland — [4]JCNS Out. ILL, Grenoble, France — [5]ISIS, Didcot, UK — [6]FMIPA ITB, Badung, Indonesia

The triple-layer transition-metal oxide $Sr_4Ru_3O_{10}$ is a member of the Ruddlesden-Popper series with a layered orthorhombic structure. It is a ferromagnetic metal (T_C=105 K) with an additional metamagnetic transition below 60 K. The nature of the intermediate phase is still under debate. Using multiple neutron diffraction techniques, we were able to determine its magnetic structure. Our inelastic neutron experiments revealed a parabolic, isotropic dispersion with a stiffness constant comparable to that of $SrRuO_3$ [1,2]. However, the spin-wave scattering at low constant energy transfer deviates from the expected isotropic ring, and the stiffness increases upon heating, mirroring $SrRuO_3$ [1,2]. Polarized neutron measurements reveal longitudinal spin excitations inside the ferromagnetic phase. These amplitude-type fluctuations are unexpected in a standard Heisenberg ferromagnet, suggesting the emergence of a new class of magnetic excitations beyond conventional transverse magnons. [1] K. Jenni et al., Phys. Rev. B 107, 174429 (2023). [2] K. Jenni et al., Phys. Rev. Lett. 123, 017202 (2019).

MA 3.8 Mon 11:30 POT/0112

Multi-length scale investigation of the Perovskite-Brownmillerite topotactic phase transition in $La_{0.7}Sr_{0.3}MnO_{3-\delta}$ thin films — •C. Yin[1,2], X. Bai[3], Z. Xu[4], V. Lauter[5], S. Zhou[6], F. Gunkel[7], L. Cao[2,8], G. Puebla Hellmann[4], R.E. Dunin-Borkowski[3], and O. Petracic[2,1] — [1]Faculty of Mathematics and Natural Sciences, Heinrich Heine University Düsseldorf — [2]Jülich Centre for Neutron Science (JCNS-2), JARA-FIT, Forschungszentrum Jülich GmbH — [3]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons (ER-C), JARA-FIT, Forschungszentrum Jülich GmbH — [4]QZabre LLC, Zürich, 8050, Switzerland — [5]Neutron Scattering Division, Neutron Sciences Directorate, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA — [6]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf (HZDR) — [7]Peter Grünberg Institut (PGI-7), JARA-FIT, Forschungszentrum Jülich GmbH — [8]School of Advanced Materials, Peking University, Shenzhen Graduate School, Shenzhen, 518055, China

In $La_{0.7}Sr_{0.3}MnO_{3-\delta}$, the introduction of oxygen vacancies induces a topotactic phase transition from the perovskite phase to an oxygen-vacancy ordered Brownmillerite phase. The influence of oxygen vacancies on near-surface magnetic domains is probed via Nitrogen-Vacancy (NV) magnetometry. Polarized Neutron Reflectometry (PNR) provide depth-resolved magnetization profiles and oxygen stoichiometry. Scanning Transmission Electron Microscopy (STEM) elucidates the atomic structure and depth-dependent oxidation states.

MA 3.9 Mon 11:45 POT/0112

Probing Spin-Waves and Spin-Phonon Coupling in a Double Perovskite Oxide: A Raman Study — •Akriti Singh and Surajit Saha — Indian Institute of Science Education and Research Bhopal, Bhopal, India

Double perovskites have emerged as a promising class of materials to explore the novel magnetic phenomena. This includes high-TC magnetic orderings, spin-reorientation, magnetostriction, and multiferroicity due to the presence of complex spin arrangements, competing exchange pathways or magneto-elastic couplings. Here, we report the evolution of magnetic excitations in Ca2NiWO6 using inelastic light scattering and explore the complex interplay between the lattice and spin degrees of freedom. To get insights into the underlying magnetic dynamics, we performed temperature-dependent magnetization, x-ray diffraction, and Raman spectroscopic measurements. Our results indicate an antiferromagnetic ground state below 50 K along with signatures of magnetostriction and spin-phonon coupling. Additionally, we employ magneto-Raman spectroscopy to probe the low-energy spin-waves (magnons), providing evidence of the nature and origin of magnetism in the system. Taken together, our findings on Ca2NiWO6 highlight its potential as a fertile ground to study the complex magnetic phenomena arising due to its exchange interactions, suggesting that it may be a possible candidate for applications in spintronics, magnonics, and other advanced spin-based technologies.

MA 3.10 Mon 12:00 POT/0112

resonant inelastic x-ray scattering spectra of the dynamic jahn-teller Cu^{2+} center in $CuAl_2O_4$ — •Takumi Gengo[1], Kenta Touge[2], Ara Go[3], and Naoya Iwahara[1] — [1]Graduate School of Engineering, Chiba University, Chiba, Japan — [2]Department of Materials Science, Faculty of Engineering, Chiba University, Chiba, Japan — [3]Department of Physics, Chonnam National University, Gwangju, South Korea

Cu spinel compounds such as $CuAl_2O_4$ and $CuGa_2O_4$ attract attention as spin-orbit entangled magnets. The density mean-field theory calculations show that the spin-orbit coupling on the Cu site suppresses the Jahn-Teller deformation in the ground state, which is consistent with the x-ray diffraction data. On the contrary, recent resonant inelastic x-ray scattering (RIXS) measurement of $CuAl_2O_4$ suggests the possibility that the Jahn-Teller deformation develops. Such a contradictory situation could occur due to the development of the dynamic Jahn-Teller effect .

This study aims to theoretically elucidate the nature of quantum states on Cu sites induced by the competition between spin-orbit and electron-phonon (vibronic) couplings. We successfully reproduced the Cu L_2- and L_3-edge RIXS spectra based on our model with the quantum mechanical treatment of the lattice degrees of freedom (i.e., dynamic Jahn-Teller effect), which is consistent with the structural data. This study supports the former theoretical prediction that $CuAl_2O_4$ is a 3d spin-orbit coupled magnet.

MA 3.11 Mon 12:15 POT/0112

EMCD analysis of ferrimagnetic moments changes in Ti-doped barium hexaferrite — •Hitoshi Makino[1], Rolf Erni[2], Devendra Singh Negi[3], Ján Rusz[4], Bernd Rellinghaus[1], and Darius Pohl[1] — [1]DCN, TU Dresden, Dresden, Germany — [2]Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland — [3]Indian Institute of Technology Jodhpur, Jodhpur, India — [4]Uppsala University, Uppsala, Sweden

Barium hexaferrite ($BaFe_{12}O_{19}$) is a robust permanent magnet material with good thermal and environmental stability. Small substitutions of Fe by Ti are known to enhance the coercivity at elevated temperatures. Our goal is to reveal changes of the ferrimagnetic arrangement of the moments by the Ti doping using electron energy-loss magnetic chiral dichroism (EMCD), an element- and site-specific probe of magnetic moments via electron energy-loss spectroscopy (EELS). We modified a highly accurate classical EMCD methodology with an improved signal-to-noise ratio, enabling the quantitative deconvolution of the Fe-$L_{2,3}$ edges into oxidation- and site-resolved magnetic contributions. The results suggest that the magnetic structure changes primarily at the tetrahedral site. Using the recently established atomic-resolution electron vortex beam EMCD, we verified these results from an alternative perspective. These measurements reveal a threefold supersymmetry in the magnetic-moments, consistent with the symmetry of the site occupied by Ti substitution identified in the STEM-EELS elemental map. These observations deepen our understanding of magnetic structure changes induced by Ti doping in barium hexaferrite.

MA 3.12 Mon 12:30 POT/0112

Long-range spin density wave order in bilayer nickelates revealed by neutron diffraction — •Igor Plokhikh — TU Dortmund University, Department of Physics, 44227 Dortmund, Germany — Research Center Future Energy Materials and Systems, 44227 Dortmund, Germany

The observation of pressure-induced superconductivity in Ruddlesden Popper nickelates has triggered renewed interest in their magnetic ground states as potential precursors to unconventional superconductivity [1]. Using high-intensity neutron powder diffraction (NPD) complemented by muon-spin rotation/relaxation (μSR), we directly resolve long-range spin-density-wave (SDW) order in bilayer $La_3Ni_2O_7$ and $La_2PrNi_2O_7$ below 150 K [2].

Magnetic Bragg reflections appear at propagation vectors $q_1 = (0, \frac{1}{2}, 0)$ for both compounds and an additional vector $q_2 = (\frac{1}{2}, \frac{1}{2}, 0)$ exclusively in undoped $La_3Ni_2O_7$. Representation analysis reveals amplitude-modulated SDW structures composed of alternating low- (≈ 0.05 μ_B) and high-moment (≈ 0.7 μ_B) Ni sites forming antiferromagnetically stacked bilayers along the c-axis. The coexistence of two distinct stacking polymorphs corresponding to q_1 and q_2 reflects quasi-two-dimensional magnetic order intrinsic to this system.

These findings provide the first direct neutron evidence for SDW order in bilayer nickelates and offer crucial insights into their ground state.

[1] Wang et al., Chinese Phys. Lett. 41, 077402 (2024).
[2] Plokhikh et al., arXiv:2503.05287(2025).

MA 4: Focus Session: Novel mechanisms of ferroic switching (joint session MA/FM)

This focus session highlights recent advances in ferroic switching across ferroelectric, multiferroic, ferroaxial and magnetic systems. Topics include topologically protected order-parameter dynamics, ultrafast non-thermal switching, and complex domain-wall phenomena revealed by atomistic modeling, ultrafast optics and advanced imaging. Contributions span machine-learning-based simulations of domain kinetics, optical control of ferroaxial and structural orders, multiferroic multi-cell memory concepts, and theoretically predicted unidirectional domain-wall motion with time-crystal behavior. Together, these works uncover new switching pathways and robust functional mechanisms, offering promising routes toward energy-efficient memory and quantum devices.

Organizer: Andrei Pimenov, andrei.pimenov@tuwien.ac.ac

Time: Monday 9:30–12:00 Location: POT/0151

Invited Talk MA 4.1 Mon 9:30 POT/0151

From ML to Kinetics: Modeling the Switching in Ferroelectric Wurtzites — •Andrew Rappe, Drew Behrendt, Atanu Samanta, and Von Braun Nascimento — Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323 USA

We present a series of works, from the development of a new force field (MLFF) for multi-scale simulations of bulk AlN, through application of MLFF to understand the atomistic switching mechanism, to the development of a new kinetic model to uncover how switching changes as a function of experimental conditions.

We train our MLFF to 1000s of DFT calculations, so the underlying calculations are as accurate as DFT with the flexibility in simulation size of classical MD. Powered by the MLFF, we can predict the energies, forces, and phonon dispersions of AlN at dramatically lower cost, thus enabling the study of emergent and long-range effects, such as the frequency-dependent dielectric functions and multiple FE domains.

Applying the AlN MLFF, we uncover the atomistic mechanism of domain wall (DW) migration and domain growth in wurtzites. We find that the critical nucleus is a single broken Al-N bond along the polar axis; this creates a cascade of bond breaking in a single column of atoms due to the stability of the 180° DW in wurtzites. We reveal the switching mechanism of 1D atomic columns propagating from a slow-moving 2D fractal-like DW in the basal plane.

Finally, we develop an analytical extension to the KAI model that accounts for fractal FE domains. To do this, we take the traditional model of circles that can nucleate and grow and add a budding term.

Invited Talk MA 4.2 Mon 10:00 POT/0151

Topological order parameter switching — •Sergey Artyukhin — Quantum Materials Theory, Genova, Italy

Ferroic orders are widely used to encode information in data storage devices and may provide a beneficial way to circumvent Boltzmann tyranny affecting conventional MOSFET memory [1]. However, information writing involves order parameter switching, facilitated by domain nucleation and motion of domain walls across a disordered material, which leads to energy dissipation. Recently, an alternative order parameter switching paradigm has been introduced, where the ordered state tracking the free energy minimum continuously rotates the order parameter direction as the free energy surface is deformed by an external driving [2]. The process is analogous to Thouless pumping and is topologically protected. A related mechanism allows pumping of topological spin textures in space [3].

[1] S. Manipatruni, D. E. Nikonov, I. A. Young, Nature Physics 14, 338 (2018)
[2] L. Ponet et al., Nature 607, 81-85 (2022)
[3] L. Maranzana et al., arXiv:2502.13083

Invited Talk MA 4.3 Mon 10:30 POT/0151

Optical Control of Ferroaxial Order via Circular Phonon Excitation — •Zhiyang Zeng[1,2], Michael Först[1], Michael Fechner[1], Dharmalingam Prabhakaran[2], Paolo Radaelli[2], and Andrea Cavalleri[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Department of Physics, Clarendon Laboratory, University of Oxford, Oxford, United Kingdom

Ferroaxial order is a distinct ferroic order in crystal systems characterized by a rotational texture of electric dipoles. Its unique symmetry prohibits direct coupling to static fields or stress, making conventional control approaches ineffective.

Based on symmetry analysis, we identify a coupling between the ferroaxial order and circularly driven optical phonons, which can be resonantly excited with circularly polarized mid-infrared light. Exploiting this coupling, we experimentally achieve reversible, deterministic switching of the ferroaxial order in the prototype material RbFe(MoO4)2 using single-shot excitation.

This work establishes a new mechanism for manipulating ferroaxial order via light-driven phonons, enabling dynamic control of ferroic properties in complex materials.

15 min break

MA 4.4 Mon 11:15 POT/0151

Coherent Control of Competing Structural Orders in SrTiO3 — •M. Fechner[1], H. Wang[2], M. Foerst[1], G. Orenstein[2], A. Disa[3], M. Trigo[2], and A. Cavalleri[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Stanford Pulse Institute, SLAC National Accelerator Laboratory, Menlo Park, CA, USA — [3]School of Applied & Engineering Physics, Cornell University, Ithaca, NY USA

The interplay between antiferrodistortive (AFD) rotation and polar instability prevents the formation of ferroelectric order in SrTiO3 yet keeps the paraelectric-to-ferroelectric transition on the verge of emerging. Light excitation has been shown to induce metastable ferroelectricity[1], but the response of the AFD order to such optical driving remains unclear. Here we use time-resolved X-ray scattering to track AFD-order dynamics, launched by mid-infrared excitation of the Ti-O stretching vibration, from 10 K to 135 K above the cubic transition. In the tetragonal phase below 110 K, the AFD order transiently increases before the AFD angle is reduced, whereas in the cubic phase rotational fluctuations initially grow before being strongly suppressed[2]. A unified lattice model, incorporating nonlinear coupling of the excited infrared phonon to the AFD mode and to strain, captures both regimes. With a single set of coupling parameters, we reproduce behaviors for both phases, indicating a common underlying mechanism that also constrains explanations for the light-induced ferroelectric state.

[1] T.F., et al. Nova Science 364, 1075 (2019), [2] M. Fechner, et al. NatMat, 23, 363 (2024)

MA 4.5 Mon 11:30 POT/0151

Multi-cell unit storage based on a multiferroic — •Maksim Ryzhkov[1], Alexey Shuvaev[1], Maxim Mostovoy[2], Andrei Pimenov[1], Anna Pimenov[1], and Sergey Artyukhin[3] — [1]Institute of Solid State Physics, Vienna University of Technology, Vienna, Austria — [2]Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands — [3]Quantum Materials Theory, Istituto Italiano di Tecnologia, Genova, Italy

Recent advances in multiferroic materials offer promising prospects for next-generation memory and data-processing devices. Previous studies [1,2] have shown that rare-earth manganates RMn_2O_5, particularly with R = Gd, are strong candidates for storage applications due to their topologically protected four-state magnetoelectric switching and the efficient electric-field control of this switching.

In this work, we demonstrate that this system enables the realization of a multi-cell storage unit capable of encoding and decoding at least five bits. We show that only two key ingredients are required:

(i) the four-state magnetoelectric switching observed during magnetic-field sweeps, and

(ii) a ferroelectric domain structure in the bulk together with local inhomogeneities (e.g., internal mechanical stresses) that produce a distribution of the spin-flop critical field H_c across different domains.

Thus, the magnetoelectric domains in $GdMn_2O_5$ are not an unwanted bug but an essential feature enabling multi-cell functionality.

[1] L. Ponet, et al., Nature 607, 81-85 (2022)
[2] H. Wang, et al., PRL 134, 016708 (2025)

MA 4.6 Mon 11:45 POT/0151

E-field induced unidirectional motion of domain wall in a ferromagnet and time crystals — •Margherita Parodi[1,2], Sergey Artyukhin[1], and Maxim Mostovoy[3] — [1]Quantum Materials Theory, Italian Institute of Technology, Genova, Italy — [2]Physics Department, University of Genova, Italy — [3]Theory of Condensed Matter, Zernike Institute for Advanced Materials, Groningen, The Netherlands

Noncollinear spin textures may break inversion symmetry and induce ferroelectric polarization, giving rise to multiferroicity. Here we study the most basic non-collinear spin texture: a domain wall in a collinear (anti)ferromagnet. The spin chirality of the domain wall is analogous to that in spiral multiferroics and like-

wise leads to ferroelectric polarization. Here we find that oscillating magnetic and electric fields can drive a unidirectional motion of the magnetic texture, similar to how electrons are transported by the Thouless pump. Furthermore, for certain periods of a driving field, the domain wall demonstrates complex behaviour akin to a time crystal, with the period equal to an integer multiple of the driving periods. The phenomenon arises due to a mismatch between the natural timescale of the domain wall motion and the driving field period.

MA 5: Surface Magnetism and Topological Insulators (joint session MA/TT)

Time: Monday 9:30–12:00 Location: POT/0351

MA 5.1 Mon 9:30 POT/0351

Impact of keV He-ion bombardment on the magnetic proximity effect in Pt/Fe bilayers — •Mika Ossenschmidt[1], Arne Vereijken[1], Yahya Shubbak[1], Varun Vanakalapu[1], Maik Gaerner[2], Arno Ehresmann[1], and Timo Kuschel[2] — [1]University of Kassel, Germany — [2]Bielefeld University, Germany

The static magnetic proximity effect (MPE) describes the occurrence of spin polarization at the interface of nominally paramagnetic materials caused by its adjacency to a ferromagnetic material. KeV-He light ion bombardment (IB) of thin-film interfaces offers the opportunity to modify the interface properties of thin-film systems without destroying the thin films, e.g., as shown for exchange-bias systems [1].

Samples of Pt 4 nm/Fe 10 nm//MgO(001) were fabricated by sputter deposition and the subsequent IB was performed with 10 keV He^+ ions with a varying ion dose from 10^{15} to 10^{17} ions/cm^2 in a few steps. To analyze the strength of the MPE in Pt, x-ray resonant magnetic reflectivity measurements were performed at the Pt L_3 absorption edge (11.567 keV) at DESY beamline P09 [2].

The fits of the x-ray reflectivity measurements provide a significant difference for the roughness σ of the Pt-Fe interface due to IB while substrate and surface roughnesses as well as layer thicknesses remained nearly unchanged. The resulting maximum Pt moment at the interface for the sample with IB is higher than without IB, due to the increasing intermixing of Pt and Fe atoms at the Pt-Fe interface.

[1] Ehresmann et al., J. Phys. D: Appl. Phys. 38, 801 (2005)
[2] Kuschel et al., Phys. Rev. Lett. 115, 097401 (2015)

MA 5.2 Mon 9:45 POT/0351

Exchange splitting at surfaces: a new paradigm for spin-polarization in antiferromagnets — •William Schaarman and Sophie Weber — Chalmers University of Technology, Göteborg, Sweden

There has been recent interest in combining the robustness and ultrafast dynamics of antiferromagnets with the transport properties of spin-polarized band structures. While antiferromagnetic bands are typically spin-degenerate, exceptions to this rule such as the altermagnets have demonstrated the possibility to obtain spin polarization in bulk antiferromagnets via selective symmetry lowering. Here, we use symmetry analysis and density functional theory to examine a ferromagnetic-like exchange splitting at certain surfaces. Such spin polarization of the surface-projected band structure can occur for surface orientations with a net two-dimensional magnetization which can emerge via symmetry-lowering at the antiferromagnet's surface. By analyzing the band structure of a slab geometry projected onto a single surface, we confirm surface spin polarization in two representative materials, magnetoelectric Cr2O3 and altermagnetic FeF2. We rationalize the magnitudes of exchange splitting on distance surface orientations in these two materials as a complex interplay between the exchange and crystal field splittings of individual magnetic atoms making up the surface. Notably, our analysis shows the effect of surface exchange splitting can in some cases be of the order of eV which has important implications for spintronic devices.

MA 5.3 Mon 10:00 POT/0351

Image-potential states on a 2D Gr-ferromagnet hybrid: enhancing spin and stacking sensing — Maciej Bazarnik[1,2] and •Anika Schlenhoff[1,2] — [1]Institute of Physics, University of Münster, Germany — [2]Department of Physics, University of Hamburg, Germany

With the increasing research interest in 2D materials, image-potential states (IPSs) have regained attention as sensitive probes, e.g. for a charge transfer at buried graphene(Gr)-metal interfaces. For a Gr-ferromagnet hybrid, the question arises how IPSs sense a respective spin transfer laterally varying within the moiré heterostructure.

Here, we present spin-resolved scanning tunneling microscopy and spectroscopy studies on Fe intercalated Gr/Ir(111), that show the IPSs' sensitivity to the spatial variation of the Gr-Fe distance, and of the interfacial charge and spin transfer within the moiré unit cell [1]. A stacking contrast between fcc and hcp sites, indistinguishable in the direct tunneling mode, is provided by the IPSs. We observe a moiré-site- and energy-dependent spin-polarization of the IPSs that can be mapped across the entire moiré unit cell. Unlike the electronic states around the Fermi energy, the lowest IPSs are found to exhibit a high spin-polarization on the on-top sites attributed to their interfacial character at the respective Gr-Fe distance. Since the physisorbed Gr is only weakly spin-polarized on these sites, our work demonstrates that the lowest order IPSs can be used to locally sense the spin density at magnetic interfaces buried by a nonmagnetic passivation layer.

[1] M. Bazarnik and A. Schlenhoff, ACS Nano 19, 25812 (2025).

MA 5.4 Mon 10:15 POT/0351

Theoretical Investigation of Intrinsically Patterned 2D Transition Metal Halides: Defects, Structure, and Magnetic Phenomena — •Neeta Bisht[1], Andreas Görling[1], Feifei Xiang[2], Binbin Da[2], Mohammad Sajjan[2], Sabine Maier[2], and Christian Neiss[1] — [1]Lehrstuhl für Theoretische Chemie, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen

— [2]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen

In the quest for complex structured functional materials, defect engineering and patterning in two-dimensional (2D) systems are critical for tuning material properties and enabling new functionalities. Herein, we report on intrinsically patterned 2D transition metal dihalides (TMDs) on a gold surface, featuring periodic halogen vacancies in the upper and bottom halide layers that result in alternating coordination of the transition metal atoms throughout the film.

We explore the formation pathways leading to periodic halogen vacancies and their role in modifying the electronic and magnetic structure of TMDs. Our calculations also explores the possibility of non-collinear magnetic textures through the magnetic anisotropy calculations. The excellent match between the experimental findings and the DFT calculations, confirms the intrinsic vacancy lattice. By coupling our theoretical results with experimental observations, we provide a comprehensive framework for understanding the structure formation and magnetic properties of 2D materials.

MA 5.5 Mon 10:30 POT/0351

Magnetic domain structure of holmium films at low temperatures — •Patrick Härtl[1], Vijayalaxmi Sankeshwar[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Indian Institute of Science Education and Research(IISER), Pune, Maharashtra 411008, India

Rare-earth metals play a central role in modern magnetism, with their behavior largely governed by the element-specific sign and oscillation period of the RKKY interaction. However, real-space investigations of their complex magnetic domain structures remain scarce. Here, we present a systematic study of the structural and magnetic properties of epitaxial holmium (Ho) films grown on W(110), using low-temperature spin-polarized scanning tunneling microscopy (SP-STM).

Bulk Ho crystallizes in a hexagonal close-packed structure and exhibits an exceptionally large magnetic moment of approximately 10 μ_B, forming a helical spin spiral below T_C = 20 K. In our films, we find predominantly ferromagnetic in-plane domains for thicknesses up to about 50 atomic layers (AL), with domain walls strongly pinned to crystalline defects. For coverages above 50 AL, additional out-of-plane stripe domains emerge, which we attribute to the uncompensated c-axis magnetization of the helical cone state. Domain wall analysis reveals Néel-capped Bloch-type walls with characteristic widths of roughly ≈ 1.2 nm (60°), ≈ 3 nm (120°), and ≈ 4 nm (180°). The stripe domains are suppressed by out-of-plane magnetic fields of $\mu_0 H = \pm 300$ mT.

Published in: P. Härtl et al., Phys. Rev. B **112**, 174402 (2025).

MA 5.6 Mon 10:45 POT/0351

Electronic bounds in magnetic crystals — •Daniel Passos[1] and Ivo Souza[1,2] — [1]Centro de Física de Materiales, Universidad del País Vasco, 20018 San Sebastián, Spain — [2]Ikerbasque Foundation, 48013 Bilbao, Spain

A quantum system in its ground-state must display non-negative optical absorption. This simple statement forms the basis for a string of inequalities between moments of the absorptive conductivity. Through the use of sum rules, these inequalities provide bounds on quantities of physical interest. Recent discoveries include new constraints on the electronic localization length in insulators, and an upper bound on the bandgap of topological insulators. Current research focuses on finding inequalities relating ground-state properties such as the quantum metric to more directly measurable quantities.

We present a systematic study of bound relations between different electronic properties of magnetic crystals: electron density, effective mass, orbital magne-

tization, localization length, Chern invariant, and electric susceptibility. New results include a lower bound on the electric susceptibility of Chern insulators, and an upper bound on the sum-rule part of the orbital magnetization. In addition, bounds involving the Chern invariant are generalized from two dimensions (Chern number) to three (Chern vector). Bound relations are established for metals as well as insulators, and are illustrated for model systems. The manner in which they approach saturation in a model Chern insulator with tunable flat bands is analyzed in terms of the optical absorption spectrum.

15 min break

MA 5.7 Mon 11:15 POT/0351

Hidden Dirac-Like Crossings in a Prototypical Topological Insulator — •Wei-Sheng Chiu[1,2], Ina Marie Verzola[3], Ying-Jiun Chen[1], Rovi Angelo Beloya Villaos[3], Claus Michael Schneider[1,2], Feng-Chuan Chuang[3], and Christian Tusche[1,2] — [1]Forschungszentrum Jülich, Germany — [2]Universität Duisburg-Essen, Germany — [3]National Sun Yat-sen University, Taiwan

The prototypical topological insulator Bi_2Se_3 has been extensively studied for its topological surface state characterized by a $\mathbb{Z}_2$ topological invariant. By using spin-resolving momentum microscopy with an Au passivated Ir(100) imaging spin filter, we simultaneously recorded the spin-resolved momentum maps (k_x, k_y) over entire surface Brillouin zone of Bi_2Se_3. In addition to the well-known Dirac cone near Fermi energy, we observe a sequence of several Dirac-like spin textures and crossings spanning binding energies down to 4 eV at the $\overline{\Gamma}$ point. Moreover, a Dirac-like crossing is also found at a binding energy 2.3 eV at the $\overline{M}$ point. Our first-principles calculations indicate that those overlooked bands are attributed to surface states. The Dirac-like crossing at the $\overline{M}$ point arises from crystalline-symmetry-enforced degeneracy at the high symmetry point, showing that Bi_2Se_3 has a more complex surface electronic structure than previously expected.

MA 5.8 Mon 11:30 POT/0351

Single domain spectroscopic signatures of a magnetic Kagome metal — •Lukasz Plucinski[1], Gustav Bihlmayer[1], Yuriy Mokrousov[1], Yishui Zhou[2], Yixi Su[2], Jonathan Denlinger[3], Aaron Bostwick[3], Christopher Jozwiak[3], Eli Rotenberg[3], Dmitriy Usachov[4], and Claus M. Schneider[1] — [1]FZ Jülich — [2]JCNS/MLZ Garching — [3]ALS/LBNL Berkeley — [4]DIPC San Sebastian

We investigate the magnetic Kagome metal $DyMn_6Sn_6$ using high-resolution micro-focused circular-dichroic angle-resolved photoemission (μ-CD-ARPES) to probe its magnetic and electronic properties. By tuning the kinetic energy to various features of the Dy $4f$ multiplet, we resolve magnetic domains in samples cryo-cooled down to 20 K. Smaller, but clear signatures are detected in the Mn $3p$ levels. The behavior of both Dy $4f$ and Mn $3p$ features are in remarkable agreement with our modeling based on the Hartree-Fock method, revealing ferrimagnetic alignment of Dy and Mn local moments, and further strengthening our interpretation. Adjusting the energy to the Mn $3d$-dominated valence bands reveals signatures which we relate to the orbital magnetization through a comparison to *ab initio* electronic structure calculations. Our study establishes the spectroscopic access to a single magnetic domain in a Kagome metal, paving the way for further research into imaging magnetic phases of novel magnetic materials using μ-CD-ARPES. Preprint is available at https://arxiv.org/abs/2507.12085.

MA 5.9 Mon 11:45 POT/0351

Topologically non-trivial Kondo insulating state in graphene nanoribbons — •Amogh Kinikar[1,2], Guangze Chen[3], Yanwei Gu[4], David Jacob[5,6], Joaquín Fernández-Rossier[7], Gonçalo Catarina[2], António T. Costa[7], Oliver Gröning[2], Carlo Antonio Pignedoli[2], Klaus Müllen[4], Pascal Ruffieux[2], Jose L. Lado[8], Akimitsu Narita[4], and Roman Fasel[2,9] — [1]KIT, Karlsruhe, Germany — [2]Empa, Dübendorf, Switzerland — [3]Chalmers University of Technology, Gothenburg, Sweden — [4]MPIP, Mainz, Germany — [5]UPV/EHU, San Sebastián, Spain — [6]Basque Foundation for Science,Bilbao, Spain — [7]INL, Braga, Portugal — [8]Aalto University, Espoo, Finland — [9]University of Bern, Bern, Switzerland

Metallic rare-earth alloys display characteristic correlated electron phenomena due to interactions between electrons which give rise to a narrow heavy-fermion band near the Fermi level that hybridizes with the metallic band and opens a hybridization gap. When the Fermi level falls within this gap the system forms a Kondo insulator, which can also acquire a topologically non-trivial character. Here we provide evidence for a topological Kondo insulating state in a specific atomically precise graphene nanoribbon synthesized on Au(111) by on surface methods and characterized by scanning probe microscopy. We observe a sharp resonance near the Fermi level and a pronounced zero-bias peak at the ribbon termini. We show that these spectroscopic signatures are a fingerprint of a topological Kondo insulating state in this graphene nanoribbon.

MA 6: Magnetic Imaging Techniques I

Time: Monday 9:30–12:45 Location: POT/0361

MA 6.1 Mon 9:30 POT/0361

Nanoscale Dipolar Fields in Artificial Spin Ice Probed by Scanning NV Magnetometry — •Ephraim Spindler[1], Vinayak Shantaram Bhat[2], Elke Neu[1], Mathias Weiler[1], and M. Benjamin Jungfleisch[2] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU in Kaiserslautern, Germany — [2]Department of Physics & Astronomy, University of Delaware, Newark, USA

Artificial spin ices (ASI) offer a versatile platform to study frustration and collective spin dynamics in engineered magnetic lattices. We employ scanning probe microscopy based on a single nitrogen-vacancy (NV) center in diamond - a non-invasive, nanoscale quantum sensing technique - to study two square-lattice ASI systems with varied inter-element coupling strengths.

We use NV fluorescence quenching for rapid state determination and continuous-wave optically detected magnetic resonance to quantitatively map magnetic stray fields and extract vectorial dipolar field information. We fit the experimentally determined field components to micromagnetic simulations to infer local magnetic configurations in an iterative procedure.

These micromagnetic modeling results demonstrate that our method successfully quantifies the deviation between the expected and detected dipolar coupling field strengths, which we describe using an effective saturation magnetization. We show that the subtle magnetization tilt induced by small external fields is detectable and quantifiable through its impact on the local dipolar stray fields in the ASI.

MA 6.2 Mon 9:45 POT/0361

Probing nanoscale magnetic phenomena with cryogenic scanning NV magnetometry — •Mirko Bacani[1], Clemens Schäfermeier[1], Ankit Sharma[1], Christopher Kelvin von Grundherr[1], Dieter Andres[1], Khaled Karrai[1], Gabriel Puebla-Hellmann[2], Jan Rhensius[2], Andrea Morales[2], and Florian Otto[1] — [1]attocube systems GmbH , Haar, Germany — [2]QZabre AG, Zurich, Switzerland

Emerging technologies increasingly rely on precise control and understanding of magnetic phenomena at the nanoscale and cryogenic temperatures. NV magnetometry offers a unique approach, combining quantum sensing with scanning probe precision to achieve magnetic field mapping at resolutions and sensitivities beyond conventional limits. We present cw-ODMR imaging of materials hosting emergent quantum and topological magnetic phenomena, including Abrikosov vortices in BSCCO and YBCO, interlayer domain textures in twisted bilayer CrSBr, magnetic domains in skyrmions-hosting Ir/Fe/Co/Pt multilayers, and meronic spin textures in synthetic antiferromagnets.

The imaging was performed by the cryogenic scanning NV magnetometer integrated into a closed-cycle cryostat with turnkey operation from 2-300 K. The system reaches the sensitivity of 3 uT/sqrt(Hz) with automated ODMR for quantitative stray-field mapping. These results exemplify the versatility of cryogenic NV magnetometry as a tool for probing superconductivity, correlated magnetism, and emergent spin textures in quantum materials.

MA 6.3 Mon 10:00 POT/0361

Switchable magnetic nanowire probes for differential magnetic force microscopy — Florian Sandbaumhüter[1,2], •Aniruddha Sathyadharma Prasad[1,2], Rachappa Ravishankar[1,2], Volker Neu[1], Bernd Büchner[1,2], and Thomas Mühl[1] — [1]IFW Dresden — [2]TU Dresden

Recent work on magnetic force microscopy (MFM) has highlighted the need to implement a differential MFM technique to better eliminate interfering electrostatic and topographical crosstalk from MFM images. In addition, the use of specialized MFM probes containing iron-filled carbon nanotubes (FeCNTs) as the sensing element has enabled easy quantitative imaging of magnetic fields and field gradients [1]. In this talk, we demonstrate in-situ differential MFM in a reversed tip-sample arrangement. This is based on our switchable magnetic probes which consist of FeCNTs attached to micron-sized electromagnets, i.e. planar microcoils [2]. The large field gradients of these microcoils make sure that there is only a minimal effect on the sample being measured. Furthermore, the highly inhomogeneous fields produced by our microcoils also provide a new playground for studies of domain wall motion in ferromagnetic nanowires.

[1] Freitag, Norbert H., et al. Communications Physics 6, 11 (2023).

[2] Sathyadharma Prasad, Aniruddha, et al. Communications Materials 6, 164 (2025).

MA 6.4 Mon 10:15 POT/0361

Magnetic Vector Tomography of Thick Chiral Magnets — •Polly Mitchell[1], Claire Donnelly[1,3], Luke Turnbull[2], Jeffrey Neethirajan[1], Rikako Yamamoto[1,3], Marina Raboni Ferreira[1], Burkhard Kaulich[2], and Luke Higgins[2] — [1]MPI CPfS, Dresden, Germany — [2]Diamond Light Source, Harwell Campus, Didcot, UK — [3]SKCM[2] Hiroshima University, Hiroshima, Japan

Complex three-dimensional (3D) textures such as Bloch points, chiral bobbers and hopfions form in chiral magnets through the interplay between Dzyaloshinskii-Moriya and exchange interactions. The 3D nature of such structures provides advantages such as higher degrees of freedom, and the potential for volume-based information encoding. However, the investigation of thick samples presents a number of challenges: first, whether the cancellation of opposing magnetic vectors through the sample will hinder the 3D reconstruction, and second, the high absorption of soft x-ray and electron microscopies. Here we address both challenges, obtaining experimental insight into the 3D configuration of thick chiral magnets. By performing numerical simulations of magnetic vector tomography, we find that increased angular sampling mitigates vector cancellation, allowing accurate high-resolution 3D mapping of samples up to 3μm thick. Following this insight, we harness pre-edge phase soft X-ray ptychography to perform magnetic tomography of a 700nm thick $Co_8Zn_9Mn_3$ sample. In this way, we are able to recover the 3D magnetisation vector field of a thick chiral sample, demonstrating magnetic tomography as a robust technique to recover complex configurations in thick magnetic systems.

MA 6.5 Mon 10:30 POT/0361

Self-Consistent Magnetic Force Microscopy Simulator Framework — •Dominik Schramm[1], Claas Abert[2], Jakub Jurczyk[1], and Amalio Fernández-Pacheco[1] — [1]Tu Wien — [2]Universität Wien

With the advancement in 3D nanofabrication techniques such as Focused Electron Beam Induced Deposition (FEBID), manufacturing of complex magnetic nanostructures emanating more complex stray fields becomes feasible. [1] To quantify these fields, the development of a modified Vector- Magnetic Force Microscope (MFM), resolving all three spatial components of the stray field while still maintaining industrial feasibility, is targeted.

To design an optimized MFM tip, the micromagnetic simulation framework Neuralmag is leveraged to simulate an MFM signal. The simulator allows us to self-consistently study the impact of tip geometry, inclination angle, magnetic state as well as additional oscillatory modes not only on the output, but also on the magnetic states of tip and sample themselves. Furthermore, the simulator is employed to simulate MFM along a topographically non-trivial sample surface.

[1] A. Fernández-Pacheco, et al. Nat Commun 8, (2017) 15756.

MA 6.6 Mon 10:45 POT/0361

Toward 3D magnetic force microscopy: Simultaneous torsional cantilever excitation to access a second, orthogonal stray field component — •Jori F. Schmidt[1], Lukas M. Eng[1,2], and Samuel D. Seddon[1] — [1]TU Dresden, Institute of Applied Physics, Nöthnitzer Strasse 61, 01187 Dresden, Germany — [2]ct.qmat: Dresden-Würzburg Cluster of Excellence EXC 2147, TU Dresden, 01062 Dresden, Germany

Magnetic Force Microscopy (MFM) is a technique for recording maps of the magnetic stray field above a sample, as is for instance well documented for skyrmions. The magnetized tip usually couples to the out-of-plane magnetic sample stray field through cantilever oscillations perpendicular to the sample surface. Nevertheless, the stray field has a 3-dimensional distribution, the reconstruction of which has not been widely performed so far due to the uniaxial sensitivity of standard MFM.

Here, we introduce a novel way towards experimentally mapping the full 3D sample stray field, by simultaneously oscillating the MFM cantilever at its vertical (out-of-plane) and lateral (in-plane) fundamental resonance frequencies, thus making it possible to directly compare and quantify the vertical MFM (V-MFM) and the lateral MFM (L-MFM) signals. We have tested this novel setup for its overall performance and signal-to-noise ratio, using a hard disk with known magnetization, where a good agreement was found between experimental results.[1]

[1] J. Schmidt et al., J. Appl. Phys. 136, 113904 (2024): https://doi.org/10.1063/5.0226570

15 min break

MA 6.7 Mon 11:15 POT/0361

Hamiltonian reverse engineering from magnetic skyrmion images via deep learning surrogates — •Moritz Winterott[1,2] and Samir Lounis[3] — [1]Peter Grünberg Institut, Forschungszentrum Jülich & JARA, Germany — [2]Faculty of Physics, University of Duisburg-Essen, Germany — [3]Institut für Physik and Halle-Berlin-Regensburg Cluster of Excellence CCE, Martin-Luther Universität Halle-Wittenberg, Germany

The extraction of physical parameters from experimental observations is a central inverse problem in condensed matter physics. Complex magnetic textures such as skyrmions are imaged via Scanning Tunneling Microscopy (STM), which probes the local density of states (LDOS). Inferring the underlying interactions by matching theoretical models to experimental LDOS is often computationally expensive. In this work, we introduce a deep-learning framework that serves as a fast and accurate surrogate for this modeling process. Our approach employs a novel neural network architecture that integrates modern Transformers[1,2] with Convolutional Neural Networks (CNNs) to extract spatial features from energy-resolved LDOS images and to learn the highly nonlinear mapping to the parameters of an effective tight-binding Hamiltonian. These parameters encode the skyrmion texture, hopping amplitudes, and spin-orbit coupling strengths. Also, on-the-fly noise augmentation during training enhances robustness, enabling the model to maintain high accuracy even for noisy experimental data.

[1] Vaswani et al. NeurIPS '17; [2] Devlin et al. Proc. NAACL-HLT '19.

MA 6.8 Mon 11:30 POT/0361

Can a Quantum Computer Simulate Nuclear Magnetic Resonance Spectra Better than a Classical One? — •Keith R. Fratus, Nicklas Enenkel, Sebastian Zanker, Jan-Michael Reiner, Michael Marthaler, and Peter Schmitteckert — HQS Quantum Simulations GmbH, Karlsruhe, Germany

The simulation of the spectra measured in nuclear magnetic resonance (NMR) spectroscopy experiments is a computationally non-trivial problem, and as such, it represents a problem for which a quantum computer may provide some practical advantage over traditional computing methods. In order to understand the extent to which such problems may provide examples of useful quantum advantage, it is important to understand the limitations of existing classical simulation methods. In this talk, we present our classical solver designed to solve such problems, and benchmark its performance. We find that it performs well, even outside of the more typical experimental regimes, and discuss what implications this may have for future efforts to demonstrate quantum advantage in the context of NMR.

MA 6.9 Mon 11:45 POT/0361

From imaging static magnetic fields to characterization of GHz magnetic noise - multi-method magnetometer comprising NV, MFM and MOKE — •Nele Harnack, Björn Josteinsson, Andrea Morales, Simon Josephy, and Gabriel Puebla-Hellmann — QZabre Ltd., Zürich (Switzerland)

Nanoscale imaging of static and GHz magnetic fields allows the in-depth study of phenomena like skyrmions, spin-waves and antiferromagnets. Experimental techniques include nitrogen-vacancy (NV) magnetometry, magnetic force microscopy (MFM) and magneto-optic Kerr effect (MOKE) [1,2]. In NV magnetometry, a spin defect in diamond serves as an atomic-scale sensor, delivering quantitative results and high resolution [3]. Here, we show how NV centers yield information complementary to MFM and MOKE - stray field and reconstructed magnetization - in a comparative study of BiYIG using the three techniques. The study is performed on a commercial microscope (QSM), enabling fast localization of the sample region when switching between modes. NV imaging provides insight beyond static field imaging [4]. Here we use scanning relaxometry (T1) to image the GHz magnetic noise present in the sample. The combination of methods enables an in-depth study of magnetic textures in BiYIG, with NV extending the capabilities of well-established techniques by measuring the coupling of the NV spin state to spin fluctuations in the material. [1] Kazakova et al; J. Appl. Phys., 2019, 125, 060901. [2] Kimel et al; J. Phys. D: Appl. Phys., 2022, 55, 463003. [3] Degen; Appl. Phys. Lett, 2008, 92, 243111. [4] Finco et al.; Nat. Comm., 2021, 12, 767.

MA 6.10 Mon 12:00 POT/0361

Nanoscale mapping of magnetic orientations with complex x-ray magnetic linear dichroism — •Marina Raboni-Ferreira[1,2], Benedikt J. Daurer[3], Jeffrey Neethirajan[1], Andreas Apseros[4,5], Sandra Ruiz-Gómez[1,6], Burkhard Kaulich[3], Majid Kazemian[3], and Claire Donnelly[1,7] — [1]MPI CPfS, Dresden, Germany — [2]UNICAMP, Campinas, Brazil — [3]DLS, Didcot, UK — [4]ETH, Zurich, Switzerland — [5]PSI, Villigen, Switzerland — [6]ALBA, Barcelona, Spain — [7]WPI-SKCM2, Hiroshima, Japan

Compensated magnets are of increasing interest for both fundamental research and applications, as their net-zero magnetization enables ultrafast dynamics and robust order. To understand and control this order, nanoscale mapping of local domain structures is essential. Here, we combine X-ray magnetic linear dichroism (XMLD), a spectroscopic technique sensitive to the local Néel-vector orientation, with ptychography, a coherent X-ray imaging technique, to obtain high-resolution images of in-plane magnetic orientations in a model sample exhibiting a Landau pattern. By combining these techniques with an unsupervised machine learning approach, we retrieve the full complex XMLD spectrum of the sample, and map its magnetic domains with sub-100-nm resolution. Our results show that phase contrast is significantly stronger than the corresponding absorption contrast, offering higher spatial resolution imaging. This establishes phase contrast as a high-resolution mechanism for mapping magnetic orientations and paves the way toward higher-dimensional X-ray imaging, including Néel-vector orientation tomography of antiferromagnets.

MA 6.11 Mon 12:15 POT/0361

Development of in-house high-yield in-situ TEM chip production with magnetic thin-films — •Sindre Vie Jørgensen[1], Patrick R. B. Thomassen[1], Trond Hauklien[1], Marthe Linnerud[1], Asle Sudbø[1], David Barriet[1,2], and Magnus Nord[1] — [1]IFY, NTNU, Norway — [2]NYB Partner DA

Transmission Electron Microscopy (TEM) is a powerful tool for studying materials at the nanoscale. For future device materials, being able to apply a biasing voltage during TEM imaging is highly advantageous for observing magnetic domain responses at the nanoscale. We have developed a 'frontside-then-backside' method to create in-situ biasing TEM chips for as-deposited thin-film samples. This creates 100+ chips from a 4" Si wafer per production batch, which is highly customisable, allowing for multiple designs, TEM window dimensions, and circuit layouts simultaneously, with little variation in production time. This method has been tested with 20 nm thick, 5 um wide permalloy thin films with two narrow sections, 2,5 um wide, for a local increase in current density. Bias has been applied during magnetic Lorentz TEM (LTEM) to verify in-situ capabilities by shifting magnetic domain walls within the film via thermal excitation. This greatly expands the utility of the TEM for studying device-relevant magnetic materials, as simultaneous in-situ studies of the magnetics, structure and composition become possible.

MA 6.12 Mon 12:30 POT/0361

Scanning Magnetometry of van der Waals magnets under in-situ controlled strain — •Yuchen Zhao[1], José Claudio Corsaletti Filho[1], Chenhui Zhang[2], Yejin Lee[1], Young-Gwan Choi[1], Elina Zhakina[1], Hyunsoo Yang[2], Elena Gati[1], Claire Donnelly[1], and Uri Vool[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]National University of Singapore, Singapore, Singapore

In recent years, van der Waals (vdW) magnets have emerged as one of the promising research directions in the field of condensed matter physics. Due to their thin nature, vdW magnets are mechanically more flexible than their bulk counterparts, allowing them to withstand greater strain. Because strain distorts the lattice, it is expected to modify magnetic properties and may even stabilize new magnetic states. While magnetic imaging of vdW materials has so far been limited to small applied strains, achieving and visualizing magnetic textures under large strain remains a significant challenge. Here, we report a technique that enables large in-situ controlled strain engineering of vdW magnets under scanning probe microscopy at room temperature. We use a piezoelectric actuator-based uniaxial strain cell to strain Fe_3GaTe_2 flakes as a proof-of-principle example of our method. By incorporating this setup into the Magnetic Force Microscope (MFM), we can locally probe the influence of strain on magnetic textures, revealing strain modulation of the magnetic configuration. In the future, this setup will open the investigations of strain-induced magnetic effects in a broad class of vdW systems.

MA 7: Poster Magnetism I

Time: Monday 9:30–12:30 Location: P2

MA 7.1 Mon 9:30 P2

Gapped ground state in a new V(IV) based sawtooth chain — •Ralf Feyerherm[1], Tim Müller[2], and Gündog Yücesan[2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, 14109 Berlin — [2]Heinrich-Heine-Universität Düsseldorf, 40225 Düsseldorf

The sawtooth chain (or delta chain) consists of edge-sharing triangles of magnetic ions carrying Heisenberg spins. Assuming antiferromagnetic interactions between the spins, it is a relatively simple model system for studying the effect of magnetic frustration. Despite extensive theoretical literature, experimental realizations of antiferromagnetic sawtooth chains are very rare. Recently, we (TM and GY) synthesized $[VO(2,2'\text{-bpy})(H_2O)][V(\mu\text{-}O)(C_6H_5PO_3)_2]2H_2O$, a new Vanadyl complex, in which V(IV) ions with $S = 1/2$ form a sawtooth chain. The T dependence of the magnetic susceptibility χ suggests a dimerized state with $J = 18$ K and a gap of 36 K, consistent with heat capacity data. Notably, $\chi(T)$ cannot be well described by the Bleaney-Bowers equation, suggesting that a simple dimer model does not work. The magnetization $M(H)$ at 2 K starts to increase steeply above ≈ 80 kOe and reaches a value of $0.065\mu_B$ per f.u. at 140 kOe. High-field magnetization measurements are under way to search for a possible $M_{sat}/2$ plateau predicted theoretically for a specific range of parameters.

MA 7.2 Mon 9:30 P2

Disorder-driven magnetic duality in ktenasite — •Anton Kulbakov[1], Kaushick Parui[1], Roman Gumeniuk[2], Eduardo Carrillo-Aravena[3,4], María Teresa Fernández-díaz[5], Stanislav Savvin[5,6], Artem Korshunov[7], Sergey Granovsky[1], Thomas Doert[3], Dmytro Inosov[1], and Darren Peets[1] — [1]IFMP, TUD, Dresden, Germany — [2]Institut für Experimentelle Physik, TU Bergakademie Freiberg, 09596 Freiberg, Germany — [3]Fakultät für Chemie und Lebensmittelchemie, TUD — [4]Würzburg-Dresden ct.qmat, TUD, Dresden, Germany — [5]ILL, 71 avenue des Martyrs, CS 20156, 38042 Grenoble CEDEX 9, France — [6]ICMA, Facultad de Ciencias, CSIC Universidad de Zaragoza, 50009 Zaragoza, Spain — [7]DIPC, Paseo Manuel de Lardizábal, 20018 San Sebastián, Spain

Ktenasite is a rare platform where structural disorder tunes the effective dimensionality and stabilizes coexisting ordered and glassy magnetic phases, offering a unique opportunity to explore the interplay of frustration, disorder, and dimensional crossover in quantum magnets. Neutron diffraction reveals significant Cu/Zn mixing at the Cu2 site, which tunes the Cu^{2+} sublattice from a two-dimensional scalene-distorted triangular lattice into a one-dimensional spin-chain network. Magnetic susceptibility, neutron diffraction, ac susceptibility, and specific heat measurements collectively indicate magnetic duality.

MA 7.3 Mon 9:30 P2

Using applied magnetic fields to induce unconventional magnetic order in the frustrated quantum magnet, clinoatacamite, Cu2Cl(OH)3 — •Juliana Avtarovski[1], Kirrily Rule[1,2], Leonie Heinze[3,4], Stefan Sullow[3], Michael Lerch[1], Moeava Tehei[1], and Siobhan Tobin[2] — [1]School of Physics, University of Wollongong, NSW 2522, Australia — [2]Australian Centre for Neutron Scattering, Australian Nuclear Science and Technology Organisation, Lucas Heights, NSW 2234, Australia — [3]Institut für Physik der Kondensierten Materie, Technische Universität Braunschweig, D- 38106 Braunschweig, Germany — [4]Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, 85748 Garching, Germany

The natural mineral clinoatacamite, [Cu2Cl(OH)3], exhibits low-temperature, frustrated magnetic behaviour where competing interactions are responsible for novel magnetic properties. Attempts to establish the magnetic phases in this material have been undertaken and an unconventional applied field (H||b) phase diagram has been revealed. Two critical transition temperatures at zero field have been identified with long range antiferromagnetic (AFM) order for T1 < 6K, and paramagnetic behaviour for T2 >18K. In-field magnetisation data collected between 6-18K reveal three distinct phases for H||b which are not completely understood. Until now, the phase diagram of clinoatacamite has not been probed for H||a* or H||c*. We present neutron scattering of single crystal clinoatacamite in applied fields to map out the phase diagram for H||a*.

MA 7.4 Mon 9:30 P2

Optimization of Neural Quantum States for Frustrated and Chiral Spin Hamiltonians — Andreas Haller, •Stefan Liscak, Vladislav Kuchkin, Andreas Michels, and Thomas Schmidt — University of Luxembourg

Neural quantum states (NQS) offer a versatile variational Ansatz for the study of strongly correlated quantum systems, especially when dimensionality or frustration restricts the use of traditional tensor-network techniques. In order to facilitate effective ground-state searches for such Hamiltonians, we introduce a custom optimization code base. We evaluate the performance of our framework's implementations of the stochastic reconfiguration (SR) and the minimal-step SR (minSR) scheme against well-known NQS optimizers like those available in NetKet. For standard test cases, our results achieve accuracy similar to matrix product state methods (DMRG), demonstrating the competitiveness and robustness of the optimization protocols. Based on these validations, we have investigated an extension of the variational Ansatz that incorporates parameter-dependent local rotations of the computational basis directly into the optimization process. This concept is inspired by earlier findings that, following appropriate local spin rotations, skyrmionic matrix-product states show significant overlap with the simple product states. We studied the effect of adaptive basis rotations in chiral and frustrated systems on sampling requirements and convergence.

MA 7.5 Mon 9:30 P2

Single-crystal growth of intermetallic compounds using the optical floating-zone method — •Moritz Scheffer[1], Florian Kübelbäck[1], Leo Maximov[1], Andreas Bauer[1], and Christian Pfleiderer[1,2,3] — [1]School of Natural Sciences, Technical University of Munich, Garching, Germany — [2]Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München,Garching,Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Technical University of Munich, Garching, Germany

High-quality single crystals are an important prerequisite for major advances in experimental solid-state research. To ensure high degree of structural order with a small crystalline mosaicity, low concentrations of defects and impurities, and the absence of parasitic phases, it is crucial to avoid contaminations in every step

of the preparation process [1]. The central part of our preparation process is the optical floating zone technique. After moving to a new laboratory, we have re-established our ultra-high vacuum compatible preparation chain for intermetallic compounds and demonstrated its potential by preparing samples from several compound, such as the potentially frustrated paramagnet Fe_2Al_5 [2].

[1] A.Bauer Rev. Sc. 87, 113902 (2016) [2] Ji Chi Ph. Rev. B 82, 174419 (2010)

MA 7.6 Mon 9:30 P2

Rare-earth substitution tuning of a proximate quantum spin-ice pyrochlore — •Yinghao Zhu, Jonathan Gustavo Acosta Ramon, and Yixi Su — JCNS-MLZ, Forschungszentrum Jülich GmbH, Garching, Germany

Pyrochlore-structure frustrated magnets with the general formula R2B2O7 (where R represents magnetic 4f rare-earth ions and B is a non-magnetic cation) consist of a three-dimensional network of corner-sharing tetrahedra. This 3D geometry gives rise to a richer landscape of magnetic interactions and spin configurations compared to their 2D counterparts, such as triangular or kagome latices. The nature of the magnetic anisotropy depends on the specific rare-earth ion: for instance, in Nd2Zr2O7, the Nd3+ ions exhibit local (111) Ising anisotropy, leading to an all-in-all-out antiferromagnetic ground state. In contrast, Yb2Ti2O7 hosts XY-like spins with moments confined to planes perpendicular to the local (111) axes. In this work, we introduce partial substitution of Nd3+ into Yb2Ti2O7, aiming to perturb the pure XY anisotropy of Yb3+ with Ising-like contributions from Nd3+. This allows us to explore the interplay between different types of magnetic anisotropy within the geometrically frustrated pyrochlore framework. Building on the high-quality single crystal obtained, future neutron scattering studies on YbNdTi2O7 are expected to provide valuable insights into the anisotropic spin correlations and potential emergent quantum phenomena arising from the interplay of Ising and XY interactions.

MA 7.7 Mon 9:30 P2

Echo pulses of ultrafast terahertz spintronic emitters — •Krishna Rani Sahoo[1], David Stein[2], Jannis Bensmann[1], Robert Schmidt[1], Steffen Michaelis de Vasconcellos[1], Manfred Albrecht[2], and Rudolf Bratschitsch[1] — [1]University of Münster, Institute of Physics, 48149 Münster, Germany — [2]University of Augsburg, Institute of Physics, 86159 Augsburg, Germany

In its simplest form, an ultrafast terahertz (THz) spintronic emitter consists of a ferromagnetic layer (e.g. Fe) and a nonmagnetic layer (e.g. Pt), grown on an insulating substrate (e.g. sapphire). THz time-domain spectroscopy is a powerful tool for investigating the ultrafast dynamics in THz spintronic emitters. The measured THz waveform provides not only access to the amplitude but also to the phase. Interestingly, additional echo pulses are found in the THz emission of spintronic emitters. We show that these delayed THz pulses are due to reflections of either the optical pump pulse or the THz pulse at different interfaces of the spintronic emitter. Our study provides design strategies for novel spintronic THz emitters with tailored pulse sequences.

MA 7.8 Mon 9:30 P2

Narrow Band THz Emission from micropatterned STEs — •Nikos Kanistras[1], Bikash Das-Mohapatra[1], Seth Kurfman[1], Quentin Remy[2], Reza Rouzegar[2], Tobias Kampfrath[2], and Georg Schmidt[1] — [1]Institut für Physik, Martin-Luther Universität Halle Wittenberg, Von-Danckelmann-Platz 3, 06120 Halle, Germany — [2]Department of Physics, Freie Universität Berlin, 14195 Berlin, Germany

It has recently been demonstrated that Spintronic THz Emitters (STEs) made of metallic multilayers can be used to create ultrashort and broad band THz emission. Such STEs show great potential to complement or even replace conventional semi conducting THz sources due to their straightforward and cost-effective fabrication techniques resulting in seamless on-chip integration with modern device technologies[1, 2]. While quite often the broad band emission is highly desirable, in some cases narrow band or even single frequency emission is preferred, for example for spectroscopy applications.

In this work we present devices for narrow band emission of THz radiation in the range of 1-20THz, based on CoFeB/Pt STE. The samples use a striped emitter on a wedge of a material with an index of refraction >1 (e.g. glass). Our results demonstrate a viable and straightforward method to produce controlled emission in a deterministic THz frequency band, supported by a simple model.

[1] Seifert, T. et al. Nature Photon 10, 483-488 (2016).

[2] Georg Schmidt et al. Phys. Rev. Appl., 19:L041001, Apr 2023.

MA 7.9 Mon 9:30 P2

Switching the magnetization of quantum antiferromagnets: Schwinger boson mean-field approximation gauged with exact diagonalization — Florian Johannesmann, •Asliddin Khudoyberdiev, and Götz S. Uhrig — Condensed Matter Theory, TU Dortmund University, Otto-Hahn-Straße 4, 44227 Dortmund, Germany

For operation on the THz scale, antiferromagnets (AFM) are preferable to commonly used ferromagnets. Also, the lack of stray fields allows for much higher densities of bits. Still, efficient switching of the AFM order and the control of its orientation remain one of the main challenges for applications. Recently, we developed a time-dependent Schwinger boson mean-field theory, to study the sublattice magnetization in anisotropic quantum AFMs [1,2]. To corroborate the obtained results, we compare the short-time dynamics of the mean-field approach to exact numerical calculations for small clusters. We obtained a good agreement: The numerical approach corroborates our mean-field findings, with only about 6 % deviations.

[1] K. Bolsmann, A. Khudoyberdiev, and G. S. Uhrig, PRX Quantum 4, 030332 (2023) [2] A. Khudoyberdiev and G. S. Uhrig, Phys. Rev. B 109, 174419 (2024); Phys. Rev. B 111, 064408 (2025); SciPost Phys. 19, 117 (2025)

MA 7.10 Mon 9:30 P2

Ultrafast Magnetization Dynamics of the self-intercalated vdW ferromagnet Cr_xTe_y — •Maximilian Staabs[1], Tim Titze[1], Pia Henning[2], G.S.Matthijs Jansen[1], Stefan Mathias[1], Jasnamol Palakkal[2], and Daniel Steil[1] — [1]I. Physikalisches Institut, University of Goettingen — [2]Institute for materials physics, University of Goettingen

The groundbreaking discovery of ferromagnetic ordering in layered two-dimensional $CrTe_2$ at ambient temperature [1] has sparked the research interest in chromium-tellurides over the last several years, establishing Cr_xTe_y as a premier platform for next generation spintronics or skyrmionic devices [2].

While the role of intercalation on the magnetic ordering in a static setting is well understood, its impact on ultrafast dynamics remains unclear. Here we use time-resolved MOKE and transient reflectivity measurements to identify the role of intercalation on the ultrafast dynamics in thin films of $CrTe_2$ and Cr_2Te_3 fabricated by hybrid pulsed laser deposition [3]. The pump-probe experiments reveal several significant differences in the ultrafast magnetization dynamics, including the appearance of heavily damped magnon modes at lower temperatures of Cr_2Te_3, as well as significantly stronger coherent phonon modes in $CrTe_2$.

[1] Freitas *et al.*, *J. Phys.: Condens. Matter* **27** 176002 (2015).

[2] Zhang *et al.*, *Adv. Mater.* **35**, 2205967 (2023).

[3] Henning *et al.*, Preprint 10.21203/rs.3.rs-4861088 (2024).

MA 7.11 Mon 9:30 P2

Coupled Magnon-Phonon Dynamics: From Ab Initio Boltzmann Transport to the Three-Temperature Model — •Philipp Rieger, Markus Weissenhofer, and Peter M. Oppeneer — Uppsala University, Uppsala, Sweden

The ultrafast transfer of angular momentum and heat between spin and lattice subsystems is key to spintronics, recently demonstrated to occur on sub-picosecond timescales [1]. While the Three-Temperature Model (3TM) remains a cornerstone for describing this ultrafast demagnetization, its crucial spin-lattice coupling parameter, G_{sl}, typically relies on empirical fitting [2]. To address this, we developed an atomistic framework [3,4] that solves the coupled magnon-phonon Boltzmann transport equation based solely on ab initio inputs. Applied to bcc Fe and fcc Ni, we resolve real-time mode-level dynamics, transport properties, and quasiparticle lifetimes. Crucially, we demonstrate for the first time that the macroscopic 3TM spin-lattice coupling emerges as a valid linear approximation of the underlying non-thermal microscopic dynamics. Consequently, we derive a first-principles G_{sl} that reproduces the seminal results of Beaurepaire et al. [2], unifying the microscopic and phenomenological descriptions of ultrafast spin-lattice dynamics.

[1] S. R. Tauchert et al., Nature **602**, 73–77 (2022)

[2] E. Beaurepaire et al., PRL **76**, 4250 (1996)

[3] S. Mankovsky et al., PRL **129**, 067202 (2022)

[4] M. Weissenhofer, P. Rieger et al., PRL **135**, 216701 (2025)

MA 7.12 Mon 9:30 P2

Fluence dependency of ultrafast-demagnetization in Gadolinium and Terbium — •Timo Dully, Christian Strüber, and Martin Weinelt — Freie Universität Berlin

The magnetic moment in rare-earth metals is primarily determined by the 4f orbitals. Upon optical pumping, the 4f spin polarization decays on markedly different timescales in Gd and Tb of 14 ps and 0.4 ps, respectively. Earlier studies attributed this difference to the stronger magnetocrystalline anisotropy of Tb relative to Gd [1].

Optical excitation of the 5d6s electrons transfers energy to the phonon system; the 4f orbitals are strongly localized and tightly coupled to the lattice. Recent measurements, however, have revealed direct 5d - 4f electron scattering upon optical excitation of Tb, offering an alternative explanation for the differing response times. The first 4f multiplet excitation in Tb requires 0.26 eV, whereas the corresponding excitation energy in Gd is 4.1 eV. Thus hot electrons in the 5d6s valence bands excite 4f electrons via inelastic electron-electron scattering in Tb but not in Gd [2] This should lead to an ultrafast equilibration of 5d and 4f electron temperatures in Tb.

Motivated by these findings, we investigate the fluence dependence of the valence-electron temperature. Using a tr-ARPES setup with 1300 nm pump and XUV probe pulses, we determine the electron-temperature dependence on pump fluence.

[1] B. Frietsch et al., *Sci. Adv.* **6**, eabb1601 (2020)

[2] N. Thielemann-Kühn et al.,*Sci. Adv.* **10**, eadk9522 (2024)

MA 7.13 Mon 9:30 P2

Magnetic properties of Mn_3Sn layer systems — •Paul Marschall[1], Wolfgang Hoppe[1], Prajwal Rigvedi[2], Banabir Pal[2], Georg Woltersdorf[1], and Stuart Parkin[2] — [1]Martin Luther University Halle-Wittenberg, Institute of Physics, Halle (Saale), Germany — [2]Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

Illuminating a nanometer thin metallic bilayer consisting of a ferromagnetic (FM) and a non-magnetic layer (NM) with an intense femtosecond laser pulse launches an ultrafast spin current from the FM into the NM layer where it is subsequently converted into a charge current pulse via the inverse spin Hall effect. This system is established as a so called spintronic terahertz emitter (STE) usable either as a source for THz radiation [1] or for on-chip ultrafast current pulses [2]. The polarity of radiation or current can be fully inverted by switching the magnetization of the FM layer. In this study we focus on the magnetic cluster moment of the non-collinear antiferromagnet Mn_3Sn [3] replacing the FM layer of the canonical STE. The on-chip ultrafast current pulses generated by single Mn_3Sn layers or Mn_3Sn|Pt layer systems are measured with the help of a fast sampling oscilloscope and coplanar microwave probe tip [2]. The conducted experiments allow to analyze the reorietation of the in-plane magnetic cluster moment due to external magnetic fields.

[1] T. Seifert et al., Nat. Photon. 10, 483-488 (2016)
[2] W. Hoppe et al., ACS Appl. Nano Mater. 4, 7454-7460 (2021)
[3] B. Pal et al., Sci. Adv. 8, eabo5930 (2022)

MA 7.14 Mon 9:30 P2

Femtosecond spin dynamics in Ni and Fe probed by transient x-ray magnetic circular dichroism — •L. Endler[1], M. Elhanoty[2], T. Lojewski[3], L. Le Guyader[4], G. Mercurio[4], B. van Kuiken[4], J. Tasto[5], L. Kämmerer[5], A. Delin[6], O. Eriksson[2], O. Granas[2], U. Bovensiepen[5], H. Wende[5], K. Ollefs[1], and A. Eschenlohr[5] — [1]Univ. Heidelberg — [2]Uppsala Univ. — [3]Univ. of Tokyo — [4]European XFEL — [5]Univ. Duisburg-Essen — [6]KTH Sweden

Despite their simple compositions, elemental Fe, Ni and their alloys still spark questions with regard to ultrafast demagnetization dynamics after photoexcitation. By combining ultrafast X-ray absorption, circular dichroism spectroscopy (XMCD) and *ab intio* theory we aim to entangle the underlying processes in elemental Fe and Ni. Electronic correlations have been found to influence the dynamics at ultrafast timescales in elemental Ni [1]. We observed XMCD peak shifts toward lower photon energies at <1 ps timescales, followed by a shift towards higher energies at a few ps. Fe XMCD spectra showed an increase in L_3 and decrease in L_2 edge spectral area at ≈ 100 fs.

We acknowledge the financial support through the DFG within the framework of the CRC1242.

[1] T. Lojewski et al., Mater. Res. Lett., **11**, 655 (2023)

MA 7.15 Mon 9:30 P2

Development of a Laboratory Soft X-Ray Reflectometer for Ultrafast Magnetisation Studies — •Pierre Gautier[1], Clemens von Korff Schmising[1], and Stefan Eisebitt[1,2] — [1]Max Born Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Berlin, Germany — [2]Technische Universität Berlin, Institut für Optik und Atomare Physik, Berlin, Germany

Ultrafast spectroscopy in the extreme ultraviolet (XUV) range is a powerful experimental tool for investigating ultrafast magnetisation dynamics, providing element-specific information and access to the non-equilibrium electronic density of states. Using reflection geometry, experimental observables also allow direct access to depth-dependent dynamics. In this study, we present the initial findings from a recently developed experimental setup optimised for broadband reflectometry of magnetic materials. Soft X-ray radiation is generated through highharmonic generation using 100 kHz, sub-10 femtosecond laser pulses produced by a fibre laser with a two-stage pulse compression scheme. A high-resolution spectrometer optimised for photon energies between 45 eV and 180 eV is mounted on a goniometer arm, allowing access to angles of incidence ranging from $\theta = 0^{\circ}$ to 80°. The goal of this research is to resolve the ultrafast dynamics of spatial magnetisation profiles, spin currents, and spin accumulation within functional heterostructures.

MA 7.16 Mon 9:30 P2

Ultrafast Rearrangement of Antiferromagnetic Spin order Probed with Femtosecond X-ray Diffraction — •Yoav William Windsor[1,2], Sang-Eun Lee[1], Daniela Zahn[1], Kristin Kliemt[3], Christian Schüssler-Langeheine[4], Niko Pontius[4], Denis Vyalikh[5], Urs Staub[6], Cornelius Krellner[3], and Laurenz Rettig[1] — [1]Fritz Haber Institute der MPG, DE — [2]TU Berlin, DE — [3]Goethe-Universität Frankfurt, DE — [4]Helmholtz-Zentrum Berlin, DE — [5]DIPC, San Sebastián, ES — [6]Paul Scherrer Institut, Villigen, CH

Ultrafast spin manipulation carries great potential for future information technology. In particular, antiferromagnets offer the prospect of faster and more efficient spin dynamics, as well as exploitable magnetic properties that are unavailable in ferromagnets. One example is the internal arrangement of spins. Controlling this can alter how the antiferromagnet stores data, interacts with neighboring materials, etc.

Here we demonstrate manipulation of the spin structure in $LnRh_2Si_2$ (Ln = Ho, Dy; see also [1-3]) by means of femtosecond optical excitation. We probe the transient spin arrangement using femtosecond resonant X-ray diffraction tuned to the Ln ions' $M_{4,5}$ edges ("soft X-rays"). By probing the azimuthal dependence of the transient magnetic Bragg intensity, we disentangle the ultrafast rearrangement of the spin order from ultrafast demagnetization.

1. Windsor et al., Communications Physics 3, 139 (2020)
2. Windsor et al., Nature Materials 21, 514-517 (2022)
3. Lee et al., Phys. Rev. Research 6, 043019 (2024)

MA 7.17 Mon 9:30 P2

Miniaturized Multipoles for Ultrafast Electron Microscopy — •Johannes Schultz[1], Max Herzog[1], and Axel Lubk[1,2] — [1]IFF, IFW Dresden, Helmholtzstraße 20, 01069 Dresden — [2]IFMP, TU Dresden, Haeckelstraße 3, 01069 Dresden

Ultrafast Electron Microscopy (UEM) is an emerging technique developed in the last decades. By combining the high spatial resolution of EMs with a temporal resolution down to fs, it provides insights into dynamic processes in the field of nanophotonics, magnetodynamics, and lattice motion among others. Most UEM setups use pumped electron sources, which provide the highest time resolution but suffer from a limited repetition rate (≈10 MHz), are expensive and technically complex and hence difficult to (retro)fit into EMs. We therefore propose an alternative technique based on easy-to-retrofit, miniaturized (for fast switching) magnetic multipoles chopping the beam to short pulses. They consist of planar copper electrodes with permalloy pole pieces on top (≈ 50 μm size), which are structured by lithography on a silicon wafer. The devices are supplied with radio-frequency electrical signals via a custom made holder compatible with standard ports of our EM (FEI Titan^3), which allows for easy device integration into the central part (C2 aperture plane) of the condenser system. In the lower part of the EM, the beam is chopped by a small aperture (C3 aperture). Considering the magnification of the condenser system, the optical power of the devices (100 μrad deflection at 3 GHz and 300 keV electron energy) and the diameter of the chopping aperture (150 nm), a time resolution of ≈ 1 ps at repetition rates ≫ 10 MHz can be achieved.

MA 7.18 Mon 9:30 P2

Magnetization-dependent electronic structure and ultrafast electron dynamics in CrGeTe3 — •Tulio de Castro[1], Samuel Beaulieu[1], Shuo Dong[1], Maciej Dendzik[1], Tommaso Pincelli[2], Lawson Lloyd Lloyd[2], Ralph Ernstorfer[2], Martin Wolf[1], and Laurenz Rettig[1] — [1]Fritz-Harber-Institut der Max-Planck-Gesellschaft, Berlin — [2]I0AP, Technische Universität Berlin, Berlin.

Magnetic 2D van-der-Waals materials offer novel opportunities for spin-based nanodevices, with advantages over charge-based technologies. One promising material is the semiconductor CrGeTe3 (CGT), which exhibits ferromagnetic order below the Curie temperature(TC=63 K). Here, we investigate bulk CGT using femtosecond time and angle-resolved photoemission spectroscopy(trARPES), to elucidate how magnetic order modifies the electronic structure, and to directly measure the ultrafast dynamics of exchange splitting and demagnetization. We observe a temperature-dependent shift in band energies below TC, associated with magnetic order. Upon femtosecond optical excitation, we observe an ultrafast renormalization of band energies, which we discuss in terms of transiently modified exchange splitting and superexchange pathways. Our results provide a direct ultrafast timescale for electron redistribution in magnetically ordered CGT, and give insight into the pathways of spin-electron interactions in CGT.

MA 7.19 Mon 9:30 P2

Time-resolved resonant magnetic small-angle scattering with a laser-driven soft-X-ray plasma source — •Pascal Wernicke[1], Maximilian Mattern[1], Johannes Tümmler[1], Stefan Eisebitt[1,2], and Daniel Schick[1] — [1]Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Berlin, Germany — [2]Institut für Physik & Astronomie, TU Berlin, Germany

Resonant soft-X-ray scattering methods provide unique possibilities to study nanometer-scale magnetization states with element selectivity. Employing ultrashort pulsed X-ray sources accesses the laser-induced dynamics on ultrafast timescales beyond a spatially-averaged insight. Based on a laser-driven plasma X-ray source, we have developed a novel instrument to carry out time-resolved magnetic small-angle X-ray scattering (SAXS) experiments in the soft-X-ray range between 500 and 1500 eV with sub-10 ps temporal resolution. Due to the flexibility of our laboratory-scale setup, we can further vary the sample environment, e.g., by applying external magnetic fields as well as cryogenic temperatures, and hence investigate ground-state-dependent dynamics of emergent textures such as magnetic domains. Specifically, we aim at following laser-driven dynamics of spatially heterogenous phase transitions, e.g. during the prototypical magneto-structural antiferromagnetic (AFM) to ferromagnetic (FM) transition in FeRh. Here, resonant magnetic SAXS can resolve the relevant time and length scales on which FM domains emerge during this first-order transition.

MA 7.20 Mon 9:30 P2

Impact of crystallographic cuts on the magnetoelectric switching of Cr_2O_3. — •Anuvrat Tripathi, Igor Veremchuk, Oleksandr V. Pylypovskyi, Pavlo Makushko, and Denys Makarov — Helmholtz-Zentrum Dresden-Rossendorf e.V., Bautzner Landstrasse 400, 01328 Dresden, Germany

The phenomenon of magnetoelectric (ME) switching in Cr_2O_3 has been demonstrated to facilitate the control of magnetism by an electric field, a property that renders it a subject of considerable interest for applications in low-power spintronics and memory devices [1]. However, the dependence of switching efficiency on crystallographic orientation remains poorly understood [2]. A systematic study of magnetic switching in bulk Cr_2O_3 single crystals with different crystallographic cuts and epitaxial Cr_2O_3 thin films grown on Al_2O_3 substrates with varying orientations has been conducted. By applying fields over a transition from the paramagnetic to the magnetically ordered state, we are able to modify the distribution of the antiferromagnetic (AFM) domains in Cr_2O_3 and identify this change via magnetotransport. A comparison between single crystals and thin films reveal the role of crystal-cut symmetry and epitaxial grown in governing the switching process. The results of this study make it possible to optimize controlled magnetism in spintronic devices based on Cr_2O_3.

[1] P. Rickhaus, O. V. Pylypovskyi et al., Nano Letters 24, 13172 (2024).

[2] O. Pylypovskyi et al., Phys. Rev. Lett. 132, 226702 (2024).

MA 7.21 Mon 9:30 P2

Ferromagnetic Cellulose Nanocomposite for Coating and Filament Production toward Flexible Electronic Materials — •Andrei Chumakov[1], K. Gordeyeva[2], C.J. Brett[1,2], D. Menzel[3], A.V. Riazanova[2], M. Schwartzkopf[1], and D. Soederberg[2] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]KTH Royal Institute of Technology, Stockholm, Sweden — [3]Technische Universität Braunschweig, Braunschweig, Germany

Nanocellulose is a renewable, lightweight, and robust platform for sustainable flexible electronics. Imparting stable ferromagnetism enables thin, patternable, biodegradable components for sensing, tagging, and memory. We report a ferromagnetic nanocomposite via electrostatic co-assembly of negatively charged cellulose nanofibrils (-1360 μmol g^{-1}) with positively charged strontium hexaferrite nanoplatelets. Opposite charges ensure homogeneous dispersion and high coercivity retention of the final composite. Spray-coated films (10-100 nm) on silicon show uniform loading, in-plane nanoplatelet alignment (SEM/SAXS/WAXS), and coercive fields matching hard-magnetic particles. In parallel, we produce magnetic filaments by (i) co-extruding aligned CNFs with ferrites via gelation and (ii) coating CNF yarns with ferrite sheaths. These fibers retain nanocellulose's high specific modulus (60 GPa·cm^3/g) and >1000 MPa strength while gaining magnetic functionality. Together, these coatings and fibers offer a scalable, water-based techniques to magnetically active, biodegradable media.

MA 7.22 Mon 9:30 P2

Copper- and zinc-substituted nanocrystalline ferrites for biomedical applications — •Todor R. Karadimov, Milena T. Georgieva, and Petar A. Georgiev — Faculty of Physics, Sofia University St. Kliment Ohridski, Department of Condensed Matter Physics and Microelectronics, Sofia, 1164, Bulgaria

Worlwide concern of antibiotic resistance has prompted the research of novel, inorganic nanomaterials, effective against pathogens. Nanocrystalline copper- and copper/zinc-substituted ferrites were prepared under solvothermal synthesis conditions at temperatures up to 200°C. The samples' crystalline phases, particle shape and size, and magnetic properties at ambient temperatures, were determined by powder x-ray diffraction, electron microscopies, and vibrating sample magnetometry, respectively. These revealed that the resultant Cu-modified ferrites consisted of agglomerates of nanocrystalline iron ferrite, Fe_3O_4, with metallic copper inclusions. In the zinc-substituted samples the resultant precipitate consisted of agglomerates of a superparamagnetic spinel phase, e.g. $Zn_{0.6}Fe_{0.4}Fe_2O_4$, with nano-crystalline copper particles spread within them. The zinc-substituted samples showed a maximum magnetization of 30 emu/g, which is significant for practical applications. Antimicrobial agar well tests against Gram-positive and Gram-negative bacteria Escherichia coli ATCC 25922 and Staphylococcus aureus ATCC 25923 showed moderate activity of all investigated materials, correlating with the copper content and particle size. However, *Daphnia magna* toxicity tests indicated strong ecotoxicity, suggesting uncontrolled release in the environment should be avoided.

MA 7.23 Mon 9:30 P2

Machine Learning assisted 3D Tracking, Evaluation and Analysis of near-substrate transported Superparamagnetic Microparticles for Intelligent Experimentation and Sensing Applications — •Nikolai Weidt[1,2], Nikita Popkov[2,3], Yahya Shubbak[1,2], Rico Huhnstock[1,2], Kristina Dingel[2,3], Bernhard Sick[2,3], and Arno Ehresmann[1,2] — [1]Institute for Physics and CINSaT, University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany — [2]AIM-ED, Joint Lab of Helmholtzzentrum für Materialien und Energie, Berlin (HZB) and University of Kassel, Hahn-Meitner-Platz 1, 14109, Berlin, Germany — [3]Intelligent Embedded Systems, University of Kassel, Wilhelmshöher Allee 71-73, 34121, Kassel, Germany

We present a framework for intelligent control and analysis of superparamagnetic microparticles transported above magnetic domain-patterned samples. Particles are actuated by tailored magnetic stray field landscapes and external field pulse sequences, enabling remote-controlled, near-surface motion. Implementing the open-source TANGO Controls system, the setup supports modular hardware integration, synchronized operation and live data evaluation. Real-time 3D particle trajectory reconstruction can be achieved by combining deep-learning-based tracking with an automated focus-sweep calibration. This closed-loop approach paves the way for rapid evaluation of particle interaction events and supports adaptive experiments, advancing lab-on-a-chip biosensing and machine-learning-assisted diagnostics.

MA 7.24 Mon 9:30 P2

Enhancement of Magnetic and Photocatalytic properties of MnZn/CdZn core/shell structures via lattice matching. — •Ahmed Faramawy, Hesham El-Sayed, Adel Abdel-Sattar, and Romany Nessem — Ain Shams University, Cairo, Egypt

Core/shell nanostructures of ferrite as shell (Mn0.7Zn0.3Fe2O4/CdxZn1-xFe2O4 (x = 0-0.)) were successfully synthesized via a hydrothermal route to explore the role of lattice matching on their structural, magnetic, optical, and photodegradation properties. X-ray diffraction and Rietveld refinement confirmed the formation of single-phase spinel structures with coherent core/shell interfaces. TEM and EDX mapping verified uniform shell growth and compositional gradients, indicating true core/shell formation. Moreover, the saturation magnetization showed a 14% enhancement at x = 0.3 due to optimal lattice coherence and minimal interfacial strain. Optical analysis showed that the direct bandgap decreased. The observed bandgap narrowing and high Urbach energy at moderate Cd2+ levels indicate improved electronic mobility and reduced activation energy for charge transport. Furthermore, Photocatalytic activity studies confirm that the synthesized Mn0.7Zn0.3Fe2O4/CdxZn1-xFe2O4 core-shell nanocomposites have excellent photodegradation behaviour to methylene blue (MB) compared to the bare core.

MA 7.25 Mon 9:30 P2

Magnetic relaxation and structural characterization of single-core FeOx nanoparticle dispersions in solvents of varying viscosity — •Amala Thuruthiyil Jose[1,2], Sascha Ehlert[3], Artem Feoktystov[4], Andreas Stadler[3,2], Martin Dulle[3], and Oleg Petracic[1,5] — [1]Jülich Centre for Neutron Science JCNS-2, Forschungszentrum Jülich GmbH, Germany — [2]RWTH Aachen University, Landoltweg 2, 52056 Aachen, Germany — [3]Jülich Centre for Neutron Science JCNS-1, Forschungszentrum Jülich GmbH, Germany — [4]Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS) at MLZ, Lichtenbergstrasse 1, Garching, Germany — [5]Heinrich Heine University Düsseldorf, Faculty of Mathematics and Natural Sciences, Düsseldorf

We have investigated the structural and magnetic properties of monodisperse single-core iron-oxide nanoparticles dispersed in solvents of systematically varied viscosity. The particles were synthesized via thermal decomposition. Magnetic measurements were performed using SQUID magnetometry, employing zero-field-cooled (ZFC) and field-cooled (FC) curves to probe changes in blocking behavior and relaxation dynamics. To examine the influence of the solvent environment on particle stability, SAXS measurements were carried out. We observe clear viscosity-dependent shifts in the nanoparticle solvent system, reflecting the gradual emergence of Brownian relaxation as solvent mobility increases. The observed viscosity and phase-dependent magnetic signatures demonstrate how solvent dynamics can be used to tune and separate Néel and Brownian relaxation.

MA 7.26 Mon 9:30 P2

Coexistence of ferromagnetism and spin-glass behaviour in CeNiSb3 — •Haribrahma Singh[1], Prabuddha Kant Mishra[1], Gaurav Kumar[2], Aarti Gautam[1], Rie Y. Umetsu[3], Ratnamala Chatterjee[2], and Ashok Kumar Ganguli[1,4] — [1]Department of Chemistry, Indian Institute of Technology Delhi, 110016, India — [2]Department of Physics, Indian Institute of Technology Delhi, New Delhi 110016, India — [3]Institute for Materials Research, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan — [4]Department of Chemical Sciences, Indian Institute of Science Education and Research, Berhampur, Odisha 760003, India

We present a comprehensive investigation of the structural and magnetic properties of of CeNiSb3. DC magnetization measurements confirm long-range ferromagnetic ordering below the Curie temperature TC = 7.2 K accompanied by marked magnetic irreversibility. In the ordered phase, CeNiSb3 exhibits strong magnetic anisotropy. Additionally, a field-induced spin-reorientation transition is observed along the b-axis at TC = 6.8 K. Non-equilibrium spin-dynamics measurements reveal a clear memory effect, and thermoremanent magnetization relaxations follow a stretched-exponential form with β=0.30, indicative of spin-glass like behaviour. This is corroborated by AC susceptibility, Power-law analysis yields a characteristic relaxation time of 10^-10s. Under an applied DC magnetic field, the AC susceptibility evolves from a single cusp to a double-peak structure, providing strong evidence for the coexistence of reentrant spin-glass and ferromagnetic ordering below TC in CeNiSb3.

MA 7.27 Mon 9:30 P2

Magnetic phase transitions in Z-type magneto-electric hexaferrites — •Borislava Georgieva[1], Petya Peneva[1], Svetoslav Kolev[1,2], Kiril Krezhov[1], Chavdar Ghelev[1], Lan Maria Tran[3], Michał Babij[3], Benedicte Vertruyen[4], Peter Tzvetkov[5], Daniela Kovacheva[5], and Tatyana Koutzarova[1] — [1]Institute of Electronics, Bulgarian Academy of Sciences, Sofia, Bulgaria — [2]Neofit Rilski South-Western University, Blagoevgrad, Bulgaria — [3]Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Wroclaw, Poland — [4]CESAM, GREENMAT, Chemistry Institute, University of Liège, Liège, Belgium — [5]Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, Sofia, Bulgaria

The difference is well known in the occurrence of strong magnetoelectric effects in single magnetoelectric materials (ferrites), depending on their physical state. The single-crystal Z-type hexaferrite Sr3Co2Fe24O41 exhibits a magnetoelectric effect at room temperature. We report studies on the structural and magnetic properties of Sr3Co2Fe24O41 in powder and bulk samples, focusing on the influence of the synthesis conditions. The precursor powders were prepared by sol-gel auto combustion and synthesized at 1200-1250 °C. XRD spectra showed characteristic peaks corresponding to the Z-type hexaferrite structure as a main phase. SEM images of the powder sample showed agglomerated particles forming clusters of different sizes and shapes, while in the bulk sample we observed large regions of hexagonal particles. Magnetic phase transitions between 4.2 and 300 K were observed.

MA 7.28 Mon 9:30 P2

Investigating magnetoelastic effects in multiferroic $CoCr_2O_4$ — •Abdelrahman Elsaid[1], Ryan Morrow[1], Robert Kluge[1], Sabine Wurmehl[1], Bernd Büchner[1,2], and Vilmos Kocsis[1] — [1]IFW-Dresden — [2]TU-Dresden

In a previous study based on optical spectroscopy, chromium-based spinels were found to exhibit significant magnetoelasticity if the magnetic A-site ion was occupied by a Jahn-Teller active ion. While the sentiment of this finding is true, optical spectroscopy is mostly sensitive to symmetry lowerings, and magnetoelasticity - meaning any sort of lattice deformation - may remain unnoticed in optics. Moreover, one of the chromium spinels with orbital singlet ions, $CoCr_2O_4$ is a known multiferroic, where the magnetoelectric interactions are originating from the conical spin order. It is an interesting question whether the polar distortion accompanying the spin order has a noticeable effect on the size of the unit cell, namely: can a piezo-magnetoelectric effect appear in $CoCr_2O_4$?

This motivated us to investigate $CoCr_2O_4$ using high-sensitivity capacitance dilatometry, a method not just sensitive to symmetry lowerings, but also to delicate changes in the size of the unit cell. We have found that, in line with the optical spectroscopy measurements, the unit cell shows zero change in size upon the appearance of the magnetic order. However, the application of magnetic field still reveals a significant magnetostriction in the magnetoelectric conical phase, which suggests the presence of piezo-magnetoelectric interactions.

MA 7.29 Mon 9:30 P2

Equilibrium control of quantum magnets via cavity magneto-electric coupling — •Nicolas Schmölz[1], Beatriz Pérez González[2], Mónica Benito[2], Marcus Kollar[1], and Francesco Piazza[1] — [1]Theoretische Physik III, University of Augsburg — [2]Quanteninformation und Quantencomputing, University of Augsburg

We investigate the possibility of exploiting a cavity magneto-electric coupling mechanism, whereby spin excitations carry an electric dipole moment, in order to enhance the interactions between photons and correlated (quantum) magnets.

The free-energy of the material is modified by the hybridization between collective spin excitations and cavity photons. We provide estimates for the change in free energy for specific materials which are solely based on experimental input via the measurement of the optical conductivity and the magnetoelectric response.

Our results should guide future experimental realizations by identifying optimal magnetic materials and cavity designs, aiming at a non-invasive equilibrium control of material's phases and functionalities.

MA 7.30 Mon 9:30 P2

Magnetic phase transitions and spin-driven multiferroicity in BaHoFeO4 — •Filip Kadlec[1], Christelle Kadlec[1], Toan Dang[2], Denis Kozlenko[3], T.P. Hoang[2], Sergei Kichanov[3], LTP Thao[4], TL Phan[5], N Tran[2], Tomáš Kmječ[6], Jaroslav Kohout[6], Vojtěch Chlan[6], and Manh-Huong Phan[7] — [1]Institute of Physics CAS, Prague, Czechia — [2]Duy Tan Univ., Danang, Vietnam — [3]Dubna, Russia — [4]Univ. of Danang, Vietnam — [5]VNU Hanoi, Vietnam — [6]Fac.of Mathematics and Physics, Charles Univ., Prague — [7]Univ.of South Florida, Tampa, USA

Magnetic and multiferroic properties of $BaHoFeO_4$ originate in geometrical frustration and in interactions between Fe and Ho sublattices. The magnetic phase transitions remind of the parent compound $BaYFeO_4$ which exhibits an AFM order below the Néel temperature of 48 K. Below 3K, in magnetic field above 1.5 T, specific changes in the magnetic configuration lead to a spin- and H-induced ferroelectric polarization. As magnetic field increases, the ferroelectric polarization peaks, and it disappears above 5 T. Such an unusual ferroelectric behavior is likely related to H-induced metamagnetic phase transitions. We studied polycrystalline BaHoFeO4 using THz time-domain spectroscopy, X-ray diffraction, neutron powder diffraction, Mössbauer spectroscopy and magnetization measurements. Three different AFM structures were observed on cooling, as well as two metamagnetic phase transitions induced by magnetic field of up to 7 T. In view of the proven robustness of the sublattice of Fe spins, these changes of magnetic configurations are attributed to the frustrated Ho-spin sublattice.

MA 7.31 Mon 9:30 P2

Ab initio approaches to the dynamical magnetoelectric effect — •Torsten Geirsson[1], Davide Sangalli[2], and Alejandro Molina-Sánchez[1] — [1]ICMUV, University of Valencia, Spain — [2]ISM-CNR, Rome, Italy

The magnetoelectric (ME) tensor quantifies how an electric field induces magnetization and is key to understanding the coupling between electric and magnetic degrees of freedom. While most studies address the static ME response, its finite-frequency generalization reveals how electric fields drive magnetic excitations on ultrafast timescales. At optical frequencies, the ME effect can be resonantly enhanced by interband or excitonic transitions, giving rise to measurable nonreciprocal magneto-optical signals, as observed for Cr2O3.

We present a first-principles framework to compute the dynamical ME tensor in magnetic insulators, separating spin and orbital contributions and focusing on the electronic response. Approaches based on linear-response theory and real-time simulations are combined to access both equilibrium and transient ME dynamics. Using Cr_2O_3 as a prototypical example, we show how real-time propagation captures non-equilibrium ME effects induced by ultrafast electric-field pulses. Our work establishes a route for connecting ab initio ME response calculations with emerging ultrafast magneto-optical experiments.

MA 7.32 Mon 9:30 P2

High-resolution optical imaging of multiferroic domain topology in $ErMnO_3$ — •Andy Disheng An[1], Andrin Caviezel[1], Erik de Vos[1], Thomas Lottermoser[1], Jan Gerrit Horstmann[1,2], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zürich, Switzerland — [2]Institute of Physical and Theoretical Chemistry, University of Würzburg, Germany

We present a study of the multiferroic domain structure in $ErMnO_3$ using scanning second-harmonic generation (SHG) microscopy. As SHG can couple to both magnetic and ferroelectric orders simultaneously, this confocal technique allows for artefact-free, high-resolution imaging of multiferroic order. In the ferroelectric phase of the type-I multiferroic $ErMnO_3$, topological defects arise as vortices at the meeting point of their six domain states, giving rise to their characteristic six-fold cloverleaf domain pattern. Below the Néel temperature, new topological defects form at the intersection between the cloverleaf domain structure and the antiferromagnetic domain walls. We show for the first time that the SHG intensity is strongly suppressed at the vortex cores. Furthermore, recent theoretical calculations predict attractive interactions between the magnetic domain walls in hexagonal manganites [1], whereby our low-temperature scanning SHG setup is a capable and practical method for the experimental verification of these predictions.

[1] Müller A., et al., arXiv:2510.13020, (2025).

MA 7.33 Mon 9:30 P2

Magnetic Phases in ErFeO3 — •Leo Maximov[1,3], Thomas Reyher[1], Florian Kübelbäck[1,3], Johanna Jochum[2], Andreas Bauer[1,3], and Christian Pfleiderer[1,2,3] — [1]School of Natural Science, Physik-Department, Technical University of Munich, Garching, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich, Garching, Germany — [3]Zentrum für QuantumEngineering (ZQE), Technical University of Munich, Garching, Germany

Rare-earth orthoferrites (RFeO3) have been extensively studied for their multiferroic properties [1,2]. Most recently, in ErFeO3, a central motivation has been the observation of Dicke cooperativity in magnetic interactions [3], suggesting that collective coupling between localized moments and excitations can strongly alter spin dynamics. Such cooperative effects may influence magnon dispersion near crystal-field levels. Neutron studies provided Fe3+ spin-wave dispersions [4], and revealed hybrid spin-wave and crystal-field excitations [5]. However, a systematic mapping of the full spin-wave dispersion, as well as possible cooperative effects, remains lacking. We report single-crystal growth of ErFeO3 using the optical floating-zone method. Structural quality was verified by single-crystal Laue and powder X-ray diffraction. Measurements of the magnetization and the heat capacity allow us to establish the anisotropic magnetic phase diagram as a prerequisite for further studies. [1] Y.Ke, et al., Sci. Rep. 6, 19775 (2016). [2] R.L. White, JAP 40, 1061 (1969). [3] Li, Xinwei, et al. Science 361.6404 (2018). [4] Shapiro Physical Review B 10.5 (1974). [5] Zic, et al., J. Appl. Phys. 130, 014102 (2021).

MA 7.34 Mon 9:30 P2

Exploring Quantum Geometry in the Dual Topological Insulator BiTe — •Maksim Povolotskiy[1], Renjith Mathew Roy[1], Ji Eun Lee[1], Yanpeng Qi[2], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]School of Physical Science and Technology, Shanghai Tech University, Shanghai 201210, China

We present an optical spectroscopy study of the dual topological insulator bismuth telluride (BiTe) over a broad infrared range (from 5 meV to 2.5 eV), supported by transport measurements and ab initio calculations. BiTe, a member of the $(Bi_2)_m(Bi_2Te_3)_n$ homologous series, hosts both weak topological insulator (WTI) and topological crystalline insulator (TCI) surface states [1]. High pressure, low temperatures, and directional magnetic fields are applied to access and probe distinct electronic states located on different crystal facets. By systematically varying the measurement geometry and external conditions, the optical response aims to distinguish bulk contributions from surface states protected by different symmetries: time-reversal symmetry in the WTI and crystalline symmetry in the TCI [2]. Additionally, the analysis focuses on signatures of quantum geometric effects on electron-phonon coupling, which are expected to manifest as anomalies in the infrared-active phonon modes and reflect nontrivial Berry curvature in the electronic bands [3]. The results offer perspectives on the interplay between topology, lattice vibrations, and quantum geometry in BiTe. [1] Nat Commun 8, 14976 (2017) [2] Nat. Mater. 19, 610 (2020) [3] arXiv:2410.09677 (2024)

MA 7.35 Mon 9:30 P2

Design and Implementation of Voltage Gating in Weyl Semimetals — •Kamila Szczurek[1], Dola Chakrabartty[1], Lilian Prodan[1], István Kézsmárki[1], Kai Litzius[1], and Felix Büttner[1,2] — [1]Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

Weyl semimetals are promising candidates for next generation spintronic devices due to their exotic electronic properties, expected to lead to low power magnetic switching. These promising properties were predicted by theoretical work but have yet to be verified. This research presents the design and implementation of an experimental setup aimed at enabling voltage gating studies of Weyl semimetals using magneto-optical Kerr effect (MOKE) techniques. A polar laser MOKE system in combination with a full-field Kerr microscope was developed and tested, with particular focus on the alignment of the components during operation in a shared setup. A small lamella of the ferromagnetic Weyl semimetal Fe_3Sn_2 was used as the initial sample due to the material's large anomalous Hall response and tunable Berry curvature effect, making it particularly attractive for voltage-control studies using MOKE. However, the limited size and geometry of a lamella introduced challenges in obtaining a clear MOKE signal, highlighting the neccessity for combined full-field and laser MOKE measurements. Despite practical challenges, the setup was successfully commissioned, laying the groundwork for future measurements under applied gate voltages.

MA 7.36 Mon 9:30 P2

Imaging Magnetic Orders in Topological Kagome Ferro- and Antiferromagnets using Single-Spin Magnetometry — •Anusree Vannada Puleri, Yuchen Zhao, Claire Donnelly, Uri Vool, Claudia Felser, and Edouard Lesne — Max-Planck-Institute für Chemische Physik fester Stoffe, Dresden, Germany

Kagome magnets are promising candidates for next-generation memory applications due to their high ordering temperatures and untapped unconventional magnetic ground states and topological properties. These include large anomalous Hall and spin Hall responses arising from sizeable accumulations of Berry curvature in momentum space.

In this study, we focus on the Kagome ferromagnet (FM) Fe_3Sn_2 which exhibits massive Dirac fermions and noncollinear FM order [1], and the Kagome antiferromagnet Mn_3Sn, which displays non-collinear anti-ferromagnetism and Weyl fermions [2]. We present how high-quality epitaxial thin films of Fe_3Sn_2 and Mn_3Sn, can be grown using magnetron sputtering, with controlled tuning of thicknesses and strain. We perform detailed structural characterizations, and resort to a combination of magnetic force microscopy, and nitrogen vacancy (NV)-based magnetometry to image FM and AF domains in these intriguing Kagome magnets.

[1] L. Ye et al., Nature 555, 638-642 (2018).
[2] S. Nakatsuji et al., Nature 527, 212-215 (2015).

MA 7.37 Mon 9:30 P2

Synthesis, characterization and magnetic properties of selected Shandites compounds — •Mervenur Keles, Ahmad Omar, Christian G. F. Blum, Dmitriy Efremov, Bernd Büchner, and Sabine Wurmehl — Leibniz Institute for Solid State and Materials Research, Helmholtzstraße 20, Dresden, 01069, Germany

Shandite-type Co3M2X2 (M: In, Sn, Pb, Tl; X: S, Se), with a unique Kagome lattice structure, serves as a model system for studying the interaction between structure, magnetism, topology, and electronic correlation. Some shandite compounds are magnetic Weyl semimetals that exhibit unconventional transport phenomena. However, the physical properties are strongly dependent on the stoichiometry and sample quality, which are rather difficult to achieve as-desired along with high reproducibility. To address this, we investigate multiple synthesis and crystal-growth routes for selected Co3M2X2 compounds, performing comprehensive structural, chemical, transport, and magnetic characterization. We present correlations between the synthesis route, resulting structure/stoichiometry, and observed physical properties. Through DFT calculations and ARPES measurements done in collaboration, we further investigate the band structure of these potential Co3M2X2 Kagome semimetals, with the aim to establish key parameters for topological band formation and magnetic order, and thus validate a Weyl Type III semimetal.

MA 7.38 Mon 9:30 P2

Investigating Magnetic Material Parameters — •Kübra Kalkan[1], Ross Knapman[1,2], Atreya Majumdar[1], and Karin Everschor-Sitte[1] — [1]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany — [2]Institute of Mechanics, University of Duisburg-Essen, Germany

Ideal magnetic materials would significantly enhance the performance and energy efficiency of modern technological devices [1]. In practice, however, real magnetic samples inevitably contain spatial inhomogeneities that weaken magnetic properties and thus, limit device capabilities. Understanding how these imperfections influence magnetization dynamics is therefore essential for both fundamental insight and material optimization. In this study, we investigate how spatial variations in exchange stiffness and uniaxial anisotropy affect high-temperature magnetization dynamics in thin films. Using physically inspired latent-inference methods [2, 3] applied to micromagnetic simulations, we develop a physics-informed, data-driven framework for quantifying the role of inhomogeneities. This approach enables the inference of material parameters directly from highly fluctuating magnetization behavior, offering a route toward deeper understanding and the design of more energy-efficient magnetic materials.

[1] O. Gutfleisch et al., Adv. Mater., 23, 821-842 (2011).
[2] D. R. Rodriges et al., iScience, 24, 3 (2021).
[3] I. Horenko et al., Comm. App. Math. And Comp. Sci., 16, 2 (2021).

MA 7.39 Mon 9:30 P2

Atomistic spin dynamics with quantum coloured noise — •Fried-Conrad Weber[1,2], Felix Hartman[2], Matias Bargheer[1,2], Janet Anders[2,3], and Richard Evans[4] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH — [2]University of Potsdam, Institute of Physics and Astronomy — [3]Department of Physics and Astronomy, University of Exeter — [4]School of Physics, Engineering and Technology, University of York

Predicting temperature-dependent magnetisation is a challenge to classical atomistic spin dynamics (ASD) due to the absence of quantum statistics. Here, we present a novel implementation of an open-system Landau-Lifshitz-Gilbert equation within the VAMPIRE package that incorporates quantum coloured noise and non-Markovian memory effects. This approach models the quantum nature of the thermal bath and its self-consistent interaction with magnetic moments. Our results show excellent quantitative agreement with experimental magnetisation curves for nickel and gadolinium across the full temperature range, significantly enhancing the predictive capabilities of ASD beyond standard classical methods.

MA 7.40 Mon 9:30 P2

Differentiable Micromagnetics for Inverse Parameter Extraction — •Moritz Kamm[1,2], Kai Litzius[2], and Felix Büttner[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Center for Electronic Correlations and Magnetism, University of Augsburg

Extracting intrinsic micromagnetic parameters from imaging data usually involves extensive trial-and-error and often remains ambiguous. We address this challenge with a differentiable inversion method that recovers material parameters directly from a single magnetic domain image. Unlike recent neural-network approaches, the method is fully analytical and physics-driven. Because the entire pipeline is differentiable, it integrates naturally with modern optimization and gradient-based design workflows. From an experimentally accessible magnetization image, we perform a deterministic Néel-type reconstruction of the full vector field and infer material constants by enforcing fixed-point consistency under the Landau-Lifshitz-Gilbert relaxation operator. The recovery of the wall-width-determining ratio $\rho = A/K_u$ is enabled by our autograd-compatible micromagnetic solver and consistently achieves relative errors below 1%, providing physically meaningful parameters for downstream micromagnetic modeling or the identification of candidate exotic spin textures. While demonstrated here for Néel walls, the framework is general and extensible to richer energy models, alternative lifting strategies, and other magnetic imaging modalities, establishing a foundation for differentiable inverse micromagnetics.

MA 7.41 Mon 9:30 P2

jaxFMM: Fast and Accurate Stray Field Evaluation for FEM Micromagnetics — •Robert Kraft[1,2], Florian Bruckner[3], Dieter Suess[1,3], and Claas Abert[1,3] — [1]Research Platform MMM Mathematics-Magnetism-Materials, University of Vienna, Vienna, Austria — [2]Vienna Doctoral School in Physics, University of Vienna, Vienna, Austria — [3]Physics of Functional Materials, University of Vienna, Vienna, Austria

Micromagnetic simulations provide invaluable insight for the design of novel magnetic devices and materials. The size and complexity of simulated geometries is ever-increasing, quickly reaching limits in terms of computational cost. Here, the long-ranged stray or demagnetizing field proves to be particularly challenging since its complexity scales quadratically with the system size. Therefore, highly efficient and parallel routines for the evaluation of the stray field are a crucial component in any micromagnetic simulation code. We introduce jaxFMM, an open-source Fast Multipole Method (FMM) implementation written in JAX with a focus on stray field evaluation for Finite-Element simulation codes. Linear complexity scaling, efficient parallel execution on GPUs and precise control over the approximation error enable dynamic simulations of very large and complicated geometries. Additionally, the code is easy to use, extremely concise and ready for machine-learning or inverse-design tasks with automatic differentiation.

MA 7.42 Mon 9:30 P2

Theoretical study of the electronic and magnetic properties of Cd1-xMnxTe quantum wire under the combined effects of the applied magnetic field, spin orbit coupling and exchange effects — •Diana dahliah, Mohammad Elsaid, and Asaad Shandi — physics department, An Najah National University

This poster presents a study for the electronic and magnetic properties of Cd1-xMnxTe quantum wire (QW). The Hamiltonian for an electron confined in a quantum wire, in the presence of an external magnetic field and Rashba spin orbit interaction, had been solved. The obtained energy dispersion relation had been used to calculate the electronic structure and display the Landau levels and density of states for different physical Hamiltonian s parameters. The density of states function shows a significant dependence on spin, Rashba, exchange effect and magnetic field. The dependence of the magnetic properties like magnetization and magnetic susceptibility on the magnetic field strength, quantum wire radius, and exchange and Rashba strength parameters have been examined. The computed results show that the material can display a phase transition between Paramagnetic and Diamagnetic types. In addition, an oscillatory behavior in the magnetic susceptibility as a function of magnetic field has been observed. This oscillating behavior is a result of Landau levels crossing in the quantum wire energy spectra.

MA 7.43 Mon 9:30 P2

Workflow for Robust Code and Data Management exemplified for the numerical calculation of the Hopf index — •Jonas Nothhelfer, Ross Knapman, and Karin Everschor-Sitte — Universität Duisburg-Essen

Structured workflows for code and data management are essential in scientific projects to ensure reproducibility, transparency, and high-quality results. In this work, we examine such workflows from the perspective of a system administrator, focusing on the infrastructure and tools required to support scientific computing. Using a recent project as a case study, we illustrate a workflow designed to make the projects numerical methods for calculating the three-dimensional topological Hopf index accessible to the research community [1]. The workflow not only provides Python scripts but also includes extensions for the established micromagnetic simulation software Mumax3 [2]. Code development and version control are managed via GitLab, ensuring that the most up-to-date source code is available [3], while Zenodo is employed to assign persistent identifiers to released versions, thereby facilitating long-term accessibility and citation [4].

[1] R. Knapman, et al., Phys. Rev. B 111, 134408 (2025).
[2] A. Vansteenkiste, et al., AIP Adv. 4, 107133 (2014).
[3] https://git.uni-due.de/twist-external/numericalhopfindexcalculation.
[4] https://zenodo.org/records/14007386, https://zenodo.org/records/14006428.

MA 7.44 Mon 9:30 P2

Overcoming quadratic complexity in time for fast-moving textures in micromagnetics: A moving window approach — •Michael Karl Steinbauer[1,2,3], Florian Bruckner[1,2], and Claas Abert[1,2] — [1]University of Vienna — [2]Research Platform MMM — [3]Vienna Doctoral School in Physics

From domain walls and skyrmion race track memory to magnon wave guides: A lot of recent interest in the field of magnetism has focused on fast-moving magnetic textures in otherwise homogeneously magnetized media. Micromagnetic modeling of these phenomena presents a significant computational challenge however, as the displacement of the texture typically requires the simulation volume to increase proportional to time t, leading to an overall simulation complexity of $O(t^2)$.

We introduce a general-purpose simulation methodology that achieves linear scaling $O(t)$ instead. This is accomplished by employing a moving simulation window that encompasses only a small region around the magnetic feature and is continuously re-centered as the feature moves, leveraging that the magnetization ahead of and behind the feature is often highly uniform. To mitigate finite-size effects, we implement a compensation of surface charges. Furthermore, this approach readily accommodates the introduction of location-dependent material parameters, such as material defects or grain structures. The method was implemented for the python library magnum.np [1], where it was successfully used to reduce computational times of a domain wall simulation from multiple weeks to less than a day.

[1] F. Bruckner et al., Sci. Rep. 13, 12054 (2023).

MA 7.45 Mon 9:30 P2

Ferroelectric-controllable spin-orbit torque in two-dimensional magnetic heterostructures — •Weiyi Pan, Gusthavo Brizolla, and Jaroslav Fabian — Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany

The spin-orbit torque (SOT) in two-dimensional (2D) van der Waals magnets plays a crucial role in next-generation spintronic devices. However, achieving nonvolatile control of SOT in 2D systems remains challenging. In this work, we theoretically demonstrate that placing Fe_3GeTe_2, a promising 2D magnet exhibiting experimentally observable SOT effects, on a ferroelectric In_2Se_3 substrate, enables nonvolatile manipulation of the SOT through ferroelectric polarization reversal. Further analysis reveals that the polarization switching mainly affect the intra-band contribution to the SOT. Our results provide an effective strategy for controlling SOT in realistic 2D heterostructures, paving the way for tunable and energy-efficient spintronic devices in the future. This research has been supported by 2D SPIN-TECH.

MA 7.46 Mon 9:30 P2

Unidirectional Rashba-Edelstein Magnetoresistance in Topological Insulator-based magnetic Heterostructures — •Steffen Kober[1], Ruslan Salikhov[2], Jan Deinert[2], Igor Ilyakov[2], Alexey Ponomaryov[2], Atiqa Arshad[2], Thales Oliveira[2], Kang Jin[2], Gulloo Prajapati[2], Patrik Pilch[1], Anneke Reinold[1], Sergio Valenzuela[3], Carmen Gómez Carbonell[3], Zhe Wang[1], and Sergey Kovalev[1] — [1]TU Dortmund, Department of Physics, Dortmund, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]Catalan Institute of Nanoscience and Nanotechnology

Our recent experimental study of transition metal-based heterostructures has demonstrated that the unidirectional spin-Hall magnetoresistance remains active even at picosecond timescales. Here, we report on experimental investigations of the unidirectional Rashba-Edelstein magnetoresistance in topological insulator (TI)-based magnetic heterostructures, in particular, on the nonlinear terahertz (THz) responses in TI/Al/NiFe/Al thin films. The Rashba-Edelstein effect lifts the spin degeneracy due to inversion symmetry breaking at the interface of the TI, enhancing spin-dependency in the momentum space. We use anisotropic THz second harmonic generation to characterize the Rashba-Edelstein magnetoresistance. To separate this from other possible contributions, such as the thermally driven spin-Seebeck effect, we study samples with varying aluminum layer thicknesses between the TI and the ferromagnetic NiFe, which modifies spin propagation and proximity effects between the ferromagnet and the TI's spin texture.

MA 7.47 Mon 9:30 P2

X-ray Absorption Spectroscopy and X-ray Magnetic Circular Dichroism investigation of magnetic properties in monolayer van-der-Waals 3d transition metal diiodides — •Lorenzo Grilli[1], Amina Kimouche[2], Awsaf Chowdhury[1], Jendrik Gördes[1], Chen Luo[3], Florin Radu[3], Sangeeta Thakur[1], Marcel Walter[1], and Wolfgang Kuch[1] — [1]Freie Universität Berlin, Germany — [2]Universität Potsdam, Germany — [3]Helmholtz-Zentrum Berlin for Materials and Energy, Germany

Numerous theoretical works [e.g. A. S. Botana, Phys. Rev. Materials 3, 044001 (2019)] predict that robust magnetic order can persist down to the monolayer limit in 3d transition-metal dihalides. Here we investigate the epitaxial growth and electronic properties of ultrathin MnI_2 and CoI_2 films on heavy-metal and van-der-Waals substrates, using thermal evaporation from stoichiometric sources. Structural properties are characterized in-situ by LEED and XPS. Motivated by STM results [Daniel Rothhardt et al., ACS Nano 19, 2261 (2025)] showing that iodine reacts with Ag before forming MnI_2 islands, we use XPS to quantify stoichiometry and interface chemistry for MnI_2 grown on Ag(111) and on graphene, directly comparing a reactive metal substrate with an inert van-der-Waals one. In parallel, we explore growth of CoI_2 on similar substrates. The magnetic response of these epitaxial films is probed by XAS and XMCD at the VEKMAG end station of BESSY II, providing element-specific sensitivity to spin and orbital moments in the ultrathin limit. We discuss how the substrate influences the magnetic behaviour of MnI_2 and CoI_2 monolayers.

MA 7.48 Mon 9:30 P2

Strong Magnetic Anisotropy in CrSBr Revealed by Magnetotransport Measurements — •Paul Nufer[1,2], Monika Scheufele[1,2], Matthias Grammer[1,2], Julian Herrschmann[2,4], Florian Dirnberger[2,3,4], Matthias Althammer[1,2], and Stephan Geprägs[1] — [1]Walther-Meißner-Institut, BAdW, Garching, Germany — [2]TUM School of Natural Sciences, Physics Department, TUM, Garching, Germany — [3]Munich Center for Quantum Science and Technology, Munich, Germany — [4]Zentrum für Quantum Engineering (ZQE), TUM, Garching, Germany

The antiferromagnetic two-dimensional van-der-Waals material CrSBr exhibits unique electronic properties, as its conductivity is strongly dependent on the direction of the current flow with respect to its orthorhombic crystalline symmetry as well as on the anisotropic magnetic properties. In our work, we investigate the interplay of the magnetic and electronic anisotropies by magnetotransport measurements. Therefore, exfoliated CrSBr multilayers are patterned into Hall-bar structures via lift-off processes using electron-beam lithography and sputter deposition. The magnetotransport measurements are conducted in cryogenic conditions between 10 K and 200 K. By measuring the field- and angle-dependent magnetoresistance in different rotation planes of the magnetic field, we characterize the temperature- and field-dependent magnetic phase transitions of CrSBr and find an anisotropic magnetoresistance of up to 40%. We extract the anisotropy and critical magnetic fields by using free-energy simulations and demonstrate the good agreement between simulation and experimental data.

MA 7.49 Mon 9:30 P2

High-frequency spin eigenstates of an altermagnetic domain wall — •Oksana Peschanska[1] and Volodymyr Kravchuk[1,2] — [1]Bogolyubov Institute for Theoretical Physics of the National Academy of Sciences of Ukraine, 03143 Kyiv, Ukraine — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung, Helmholtzstraße 20, D-01069 Dresden, Germany

We have considered the scattering of spin waves by a domain wall (DW) in an easy-axis d-wave altermagnet (e.g. CoF2, MnF2). Similar to the conventional antiferromagnet, the scattering problem is reduced to the Schröedinger equation with $sech^2$ potential. However, due to altermagnetism, the amplitude of the scattering potential depends on the energy of the magnons. The latter has a number of physical consequences: (i) the scattering process is different for the clockwise and counterclockwise polarized magnons; (ii) the transmission coefficient is a nonmeromorphic function of the complex-valued wave vector, so a modification of Levinson's theorem is required; (iii) new high-frequency bound (localized) eigenstates appear and propagate along DW. The number of new eigenstates, their eigenfrequencies, and eigenfunctions depend on the altermagnetic strength, wave vector q along DW, and orientation of the DW relative to the crystallographic axes. With the increase of q, the size of the localization region of the bound state can increase as well as decrease, depending on the eigenstate polarization, the sign of the altermagnetic parameter, and the DW orientation.

MA 7.50 Mon 9:30 P2

Mössbauer Spectroscopy on the Candidate Altermagnet Material $FeNb_4S_8$ — •Jan Friedrichsen[1], Felix Seewald[1], Lilian Prodan[2], Joachim Deisenhofer[2], István Kézsmárki[2], and Hans-Henning Klauss[1] — [1]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [2]Experimental Physics V, Institute of Physics, University of Augsburg, Augsburg, Germany

$FeNb_4S_8$ is a proposed altermagnet and a member of the layered intercalated transition metal dichalcogenides. The crystal structure consists of stacked layers of $NbSe_2$, with sandwich layers of intercalated Fe atoms in hexagonal order[1]. Magnetic order is reported below the transition temperature $T_C = 150$ K.[2] Mössbauer spectra at room temperature show the presence of a finite electric field gradient (EFG) of $V_{zz} = -6.50(74)$ V/Å^2. At 4.2 K however the absolute value of the electric field gradient is considerably larger with a value of $V_{zz} = -66.45(13)$ V/Å^2. Mössbauer data proof predominantly colinear arrangement of the local iron spins along the c-axis and is consistend with the proposed altermagnetic state. First measurements indicate a strong magnetostriction as a likely source of the strong temperature dependence of V_{zz}. The hyperfine field that is reached at 4.2K is 15.52(14) T. We will discuss the implications of the mössbauer results on the electronic and magnetic structure and dynamics.

[1]Regmi, Resham Babu, et al. "Altermagnetism in the layered intercalated transition metal dichalcogenide CoNb4Se8.". [2]Lawrence, Erick A., et al. "Fe site order and magnetic properties of Fe1/4NbS2."

MA 7.51 Mon 9:30 P2

Altermagnetism on hyperbolic lattices — •Eric Petermann[1,2], Kristian Maeland[1,2], Haye Hinrichsen[1,2], and Björn Trauzettel[1,2] — [1]Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, D-97074 Würzburg, Germany

Altermagnets are a novel class of magnetic systems characterized by their momentum-dependent spin splitting without net magnetization. In this work, we extend established Euclidean tight-binding models of altermagnets to hyperbolic lattices defined on a discretized Poincaré disk. Using hyperbolic crystallography and hyperbolic band theory, we derive and analyze the band structure in these lattices. We discover particular properties of altermagnetism in hyperbolic space, for instance, higher angular momentum spin splitting in two-dimensional real space models. We find that orbital ordering or nonmagnetic sites are not essential to see spin-splitting in hyperbolic lattices, unlike Euclidean space.

MA 7.52 Mon 9:30 P2

Magnetic aftereffect and Barkhausen steps in thin Mn_5Si_3 films — •Gregor Skobjin[1], Javier Rial[2], Sebastian Beckert[3,4], Helena Reichlová[3,5], Vincent Baltz[2], Lisa Michez[6], Richard Schlitz[1], Michaela Lammel[1], and Sebastian Goennenwein[1] — [1]Department of Physics, University of Konstanz, Germany — [2]Univ. Grenoble Alpes, CNRS, CEA, Gren. INP, IRIG-SPINTEC, France — [3]IFMP and Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, Germany — [4]DCN, TU Dresden, Germany — [5]Institute of Physics ASCR, Czech Republic — [6]Aix Marseille Université, CNRS, CINAM, AMUTECH, France

Altermagnets are an intriguing novel class of magnetic materials. We exploit the anomalous Hall effect response of micropatterned Mn_5Si_3 thin films to investigate their magnetization relaxation behavior. In experiments at T < 200 K i.e., in the altermagnetic phase, and for magnetic fields for which the samples exhibit large magnetic susceptibility, we observe a strong magnetic aftereffect as well as Barkhausen-like steps in the time-dependent Hall voltage evolution. More specifically, we recorded the evolution of the Hall voltage in micropatterned Hall bars with widths of 10 μm down to 0.1 μm at a series of different magnetic field magnitudes to gain insights into potential domain effects in the altermagnetic phase of Mn_5Si_3 at micron and submicron length scales. We critically analyze our experimental results and discuss implications for the micromagnetic structures in altermagnetic thin films.

MA 7.53 Mon 9:30 P2

Magnon-Driven Propulsion of Domain Walls in Altermagnets — •Nils Keller, Ricardo Zarzuela, Rodrigo Jaeschke-Ubiergo, and Jairo Sinova — Institut für Physik, Johannes Gutenberg Universität Mainz, D-55099 Mainz, Germany

Altermagnets form a recently identified class of collinear magnets whose compensated order coexists with time-reversal symmetry breaking and a spin-split electronic band structure with characteristic d-, g- and i-wave symmetry. Domain-wall propulsion by magnons is a central mechanism for spin-based information processing, but in antiferromagnets it relies on angular-momentum transfer because the domain-wall potential itself is reflectionless. In contrast, we show that altermagnetic domain walls can be propelled directly by magnons through linear-momentum transfer, without requiring the wall to acquire internal angular momentum first. This arises from the characteristic symmetry of the altermagnet, which generates a direction-dependent modification of the spin-wave scattering potential. As a result, both redshift and partial reflection of magnons become possible, lowering the energy cost for domain-wall motion and enabling direction-selective propulsion. These anisotropies suggest new strategies for logic and memory concepts based on steering domain walls along symmetry-selected channels. We identify the low-velocity regime and clarify the distinct scattering mechanisms responsible for the propulsion.

MA 7.54 Mon 9:30 P2

Current-induced Spin-Orbit Torque effects in RuO_2 thin films — •Niklas Schmolka, Florian Knossalla, Maik Gärner, Karsten Rott, and Günter Reiss — Bielefeld University, Germany

Current-induced manipulation of the antiferromagnetic order offers a promising route toward ultrafast and energy-efficient spintronic memory devices [1]. Results that are consistent with Néel vector switching could be a hint for antiferromagnetism in RuO_2 [2].

Here, we use eight-terminal devices to investigate Spin-Orbit Torque effects in RuO_2 thin films. We study bilayers consisting of RuO_2|Pt and RuO_2|W where Pt and W act as heavy-metal layers generating Spin-Orbit Torques. We observe signatures of reversible Néel vector reorientation through Hall measurements, with the two sample systems showing opposite responses consistent with the opposite Spin Hall Angles of Pt and W [3].

Additionally we measure pure RuO_2 films and examine the temperature dependence of the switching mechanism to further identify magnetic contributions and disentangle possible non-magnetic effects [4].

[1] T. Jungwirth et al., Nature Nanotechnology 11, 231-241 (2016)
[2] Y. Zhang et al., Nature Communications 16, 5646 (2025)
[3] L. Liu et al., Appl. Phys. Lett. 101 122404 (2012)
[4] T. Matalla-Wagner et al., Phys. Rev. Research 2, 033077 (2020)

MA 7.55 Mon 9:30 P2

Tuning Anomalous Hall Effect in a d-wave Altermagnet — •Sergio Rodríguez Fernández, Rodrigo Jaeschke Ubiergo, and Jairo Sinova — Johannes Gutenberg-Universität Mainz, Deutschland

Altermagnets are a novel class of collinear magnets that, despite being magnetically compensated, break time-reversal symmetry. Their electronic band struc-

ture shows spin splitting with characteristic d-, g-, or i-wave symmetry. Owing to their broken time-reversal symmetry, they have been shown, both theoretically and experimentally, to exhibit an Anomalous Hall Effect (AHE) that depends strongly on the orientation of the Néel order.

In this poster, we discuss the AHE in d-wave altermagnets. Using minimal models, symmetry analysis, and the Kubo response formalism, we show how the AHE emerges from different orientations of the Néel vector. We build our minimal models with focus on the tunnability of these responses, and we apply our approach to realistic candidate materials. Our work deepens the understanding of transport properties in altermagnets, contributing to their growing relevance in spintronics research.

MA 7.56 Mon 9:30 P2

Growth of $MnSe_2$ Single Crystals as a Candidate for Supercell Altermagnets — •Mayra Handel, Franziska Walther, Sarah Krebber, Cornelius Krellner, and Kristin Kliemt — Physikalisches Institut, Goethe Universität Frankfurt, 60438 Frankfurt am Main

$MnSe_2$ is predicted to be a supercell altermagnet with d-wave order [1] at a temperature below T_N=49K [2]. $MnSe_2$ crystallizes in a cubic structure and shows a commensurate magnetic structure. Supercell altermagnets are characterized by a magnetic unit cell that is an integer multiple of the crystallographic unit cell. The enlarged magnetic unit cell introduces additional degrees of freedom in supercell altermagnets, enabling control over the spatial orientation of the order parameter. We report on the current progress in the growth of $MnSe_2$ single crystals by means of chemical vapor transport, employing various stoichiometries and transport agents. In addition, we present the chemical and structural characterization of polycrystalline samples of $MnSe_2$.

[1] R. Jaeschke-Ubiergo et al., Phys. Rev. B 109, 094425 (2024)
[2] T. Chattopadhyay et al., Solid State Communications 63, 65 (1987)

MA 7.57 Mon 9:30 P2

Possibility for altermagnetic to antiferromagnetic phase transition in $LaTiO_3$ — •Igor Maznichenko and Samir Lounis — Institute of Physics, Martin Luther University Halle-Wittenberg, D-06099 Halle, Germany

Here we investigate and compare the electronic band structure of altermagnetic and antiferromagnetic phases in Mott insulator $LaTiO_3$ [1]. Using *abinitio* calculations, we have found a stable altermagnetic phase with the *G*-type arrangement. In $LaTiO_3$, triple-degenerated cubic Ti t_{2g} orbitals are occupied by only one electron, the semiconducting band gap separates the occupied Ti $t_{2g}^1 e_g^0$ subband from the unoccupied conduction band edge, while the *f* states of La appear at much higher energies. The key structural factor of *Pbnm*-$LaTiO_3$, which determines its band gap and zero magnetization, is optimally rotated TiO_6. Using simulations of disorder for these Ti t_{2g} orbitals, we demonstrate the fragility of the altermagnetic phase with multiorbital effects.

[1] I.V.Maznichenko *etal*, Phys. Rev. Materials 8, 064403 (2024).

MA 7.58 Mon 9:30 P2

Electrical control of the exchange bias effect at model ferromagnet-altermagnet junctions — •Gaspar De la Barrera and Alvaro Nunez — Universidad de Chile, Santiago, Chile

This work analyzes the behavior of the interface between a ferromagnetic material and an altermagnet. We use a well-established line of arguments based on electronic mean-field calculations to show that new surface phenomena that lead to altermagnetic materials induce an exchange bias effect on the nearby ferromagnet. We reveal the physical mechanisms behind this phenomenon that lead to quantitative control over its strength. Interestingly, we predict exotic electric-field-induced phenomena. This is an analogy to the relationship between exchange bias and the injection of spin currents in spin-transfer-dominated scenarios, which has been reported earlier in the traditional antiferromagnetic/ferromagnetic junction.

MA 7.59 Mon 9:30 P2

NEGF Quantum Transport Simulations in Altermagnetic Systems — •Tim Kalsberger[1], Erik Schroedter[1], Nicola Lo Gullo[2], Jan-Philip Joost[1], and Michael Bonitz[1] — [1]CAU Kiel, Germany — [2]Università della Calabria, Italy

Altermagnets have the potential to open a broad landscape of new applications. Promising examples include the fields of spintronics and ultrafast photomagnetism, which combine the special properties of altermagnets with ultrafast dynamics and quantum transport. One of these properties is the emergence of spin-polarized currents under an applied bias due to the spin-anisotropic Fermi surface, despite having zero net magnetization [1]. Accurate simulations of spin-resolved dynamics in large, strongly correlated systems are challenging and, with most methods, often impossible for long time scales due to the large basis size and complexity, even for simple lattice models. In this work, we use the quantum fluctuations approach based on non-equilibrium Green functions (NEGF) [2, 3] to simulate correlated, time-resolved, large altermagnetic systems out of equilibrium in scenarios aligned with realistic experimental setups.

[1] Šmejkal *et al.*, Emerging Research Landscape of Altermagnetism. Phys. Rev. X 12, 040501 (2022).
[2] E. Schroedter *et al.*, Quantum fluctuations approach to the nonequilibrium GW approximation, Condens. Matter Phys. 25, 23401 (2022).
[3] E. Schroedter *et al.*, "Nonequilibrium Green Functions Simulations for Large Systems", subm. for publication

MA 7.60 Mon 9:30 P2

Chirality dependent orbital magnetism and anomalous transport in twisted antiferromagnetic bilayers — •Zhiyuan He — Weinberg 2, 06120 Halle (Saale), Germany

Twisted magnetic van der Waals heterostructures have emerged as a fertile ground for exploring the interplay between lattice geometry and magnetism. While the twist angle magnitude governs the moiré potential scale, the physical consequences of the twist angle sign (chirality) remain unexplored due to the inherent mirror symmetry in conventional bilayer systems. In largely this work, we theoretically investigate the electronic structure and orbital transport properties of twisted A-type antiferromagnetic bilayers using a tight-binding model that incorporates lattice anisotropy and interface-induced symmetry breaking. We researched that the interference between the rotating lattice anisotropy and a fixed symmetry-breaking field lifts texture the degeneracy between positive ($+\theta$) and negative ($-\theta$) twist configurations. This symmetry breaking manifests significantly in the momentum-space distribution of the Orbital Magnetic Moment (OMM). on the twist chirality, leading to non-reciprocal Berry curvature distributions. These findings suggest that the twist sign can serve as a switchable degree of freedom to manipulate orbital-driven transport phenomena, such as the topological Hall effect and magneto-optical responses, in altermagnetic moiré systems.

MA 7.61 Mon 9:30 P2

EMCD on Altermagnets — Hitoshi Makino[1], Sebastian Schneider[1], Sebastian Beckert[1], Rikako Yamamoto[2,3], Claire Donnelly[2,3], and •Pohl Darius[1] — [1]DCN, TUD Dresden University of Technology, Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]WPI-SKCM Hiroshima University, Hiroshima, Japan

Altermagnets represent a recently discovered class of magnetic materials featuring unique symmetry properties and compensated magnetic structures, which set them apart from conventional ferromagnets and antiferromagnets. Their novel electronic and magnetic characteristics are interesting for both fundamental research and advanced technological applications, particularly in spintronics. It has recently been shown that X-ray Magnetic Circular Dichroism is sensitive to time-reversal symmetry breaking in altermagnets. A similar behavior is expected for electron energy loss magnetic chiral dichroism (EMCD), the electron wave analogue to XMCD, a method providing element-specific sensitivity and high spatial resolution spectroscopic and imaging capabilities in an electron microscope. We will present first proof-of-principle EMCD experiments on MnTe and Fe_2O_3 and its comparison to structural TEM investigations and XMCD measurements to demonstrate the versatility of our approach and its application to probe altermagnetic materials at the nanoscale.

MA 7.62 Mon 9:30 P2

Growth and properties of altermagnetic MnTe thin films — •Lukas Stroh, Maik Gaerner, Judith Bünte, Karsten Rott, Jan Schmalhorst, Andreas Hütten, and Günter Reiss — Bielefeld University, Germany

In recent years, a new unconventional magnetic phase, named altermagnetism, has emerged [1]. Such altermagnetic materials combine anisotropic time-reversal symmetry breaking with the vanishing net-magnetization of antiferromagnets. One of the materials in which altermagnetism has been observed in is manganese telluride (MnTe) [2,3]. Here, we systematically investigate the growth of MnTe thin films on SrF_2(111) via magnetron co-sputtering. We analyze how the growth-conditions influence structural and electronic properties, including the spontaneous anomalous Hall effect.

[1] Šmejkal et al., Phys. Rev. X, 12:040501 (2022).
[2] Krempaský et al., Nature, 626:517 522 (2024).
[3] Betancourt et al., Phys. Rev. Lett., 130:036702 (2023).

MA 7.63 Mon 9:30 P2

Seed-layer assisted epitaxial growth of Mn_5Si_3 thin films on Al_2O_3 — •Maximilian Koll[1], Maik Gaerner[1], Judith Bünte[1], Finn Peters[1], Andreas Hütten[1], Karsten Rott[1], Jan Schmalhorst[1], Martin Wortmann[2], and Günter Reiss[1] — [1]Bielefeld University, Faculty of Physics, 33615 Bielefeld, Germany — [2]Bielefeld University of Applied Sciences and Arts, Faculty of Engineering and Mathematics, 33619 Bielefeld, Germany

Mn_5Si_3 thin films are a prominent platform in which signatures of altermagnetism, such as the anomalous Hall effect [1] or the anomalous Nernst effect [2,3], have been observed. These responses are consistent with a theoretically predicted d-wave altermagnetic state that breaks time-reversal symmetry while exhibiting zero net magnetization as well as THz spin-current dynamics [4].

Here, we report on the growth of epitaxial Mn_5Si_3(0001) on Al_2O_3(0001) via magnetron sputtering and molecular beam epitaxy. We demonstrate that a high-temperature Mn_5Si_3 seed layer significantly enhances the crystallinity of the thin

films while maintaining a smooth surface morphology. Finally, we show that the emergence of a spontaneous anomalous Hall effect in the Mn_5Si_3 thin films is highly sensitive to the Mn content as well as the annealing procedure.

[1] H. Reichlova et al., Nat. Commun. 15, 4961 (2024)
[2] A. Badura et al., Nat. Commun. 16, 7111 (2025)
[3] L. Han et al., Phys. Rev. Applied 23, 044066 (2025)
[4] L. Šmejkal et al., Phys. Rev. X 12, 04051 (2022)

MA 7.64 Mon 9:30 P2

Ab-initio investigation of altermagnetic splitting in the NiAs-type solid solutions (Cr,Mn)-(Sb,Te) — •Karel Knížek and Kyohoon Ahn — Institute of Physics, Czech Academy of Sciences, Prague, Czechia

CrSb is a layered collinear antiferromagnet with perpendicular magnetic anisotropy in the hexagonal structure of NiAs-type, which holds particular interest for AFM spintronics since it belongs to a few compounds which have both high ordering temperature (T_N = 705 K) and substantial altermagnetic spin splitting. Phase diagrams of solid solutions between antiferromagnetic CrSb and ferromagnetic MnSb and CrTe are rich in many various magnetic arrangements [1,2,3]. The observed evolution of the magnetic order as a function of composition for both phase diagrams is consistent with the assumption of the dominance of the M-X-M (M=Cr,Mn, X=Sb,Te) superexchange interaction. The strength of this interaction depends on the M-X-M angle, which is correlated with trigonal distortion of the MX_6 octahedra. Within these phase diagrams, we have performed electronic structure calculation to investigate the evolution of magnetic ordering, with focus on the altermagnetic spin splitting in case of antiferromagnetic ordering, as a function of structural parameters, namely the trigonal distortion and cell volume. In particular we have studied the effect of uniaxial pressure.

[1] F.K.Lotgering et al., J. Phys. Chem. Solids 3, 238 (1957).
[2] W.J.Takei et al., J. Appl. Phys. 37, 973 (1966).
[3] W Reimers et al., J. Phys. C: Solid State Phys. 15 3597 (1982).

MA 7.65 Mon 9:30 P2

Correlation of in-situ Hall measurements with LTEM on Fe/Gd multilayers — •Sebastian Beckert[1], Sebastian Schneider[1], Joe Sunny[2], Manfred Albrecht[2], Bernd Rellinghaus[1], and Darius Pohl[1] — [1]DCN, cfaed, TU Dresden, Dresden, Germany — [2]Institute of Physics, University of Augsburg, Augsburg, Germany

Topologically protected skyrmions are promising information carriers for next generation memory devices, because they can be electrically manipulated and detected, e.g., through their Hall signatures. Sputtered Fe/Gd multilayers host skyrmions at room temperature, making them an ideal model system for exploring the correlation between skyrmion formation and the topological Hall effect (THE) [1].

Building on prior in-situ correlations of Hall responses and Lorentz transmission electron microscopy (LTEM) imaging in antiskyrmion hosting materials [2], we combine simultaneous Hall-voltage measurements with LTEM imaging of the magnetic state of sputtered Fe/Gd multilayers. These experiments aim to disentangle the relationship between skyrmion presence and the Hall signal, which are typically probed independently.

[1] M. Heigl *et al.*, Nat. Commun. **12**, 2611 (2021)
[2] A. Thomas *et al.*, Small Methods **9**, 2401875 (2025)

MA 7.66 Mon 9:30 P2

Effects of chiral polypeptides on skyrmion stability and skyrmion diffusion — Fabian Kammerbauer[1], Yael Kapon[2], •Theo Balland[1], Shira Yochelis[2], Yossi Paltiel[2], and Mathias Kläui[1] — [1]Institut für Physik, Johannes Gutenberg Universität Mainz, 55099 Mainz, Germany — [2]Institute of Applied Physics, Faculty of Sciences, The Hebrew university of Jerusalem, Jerusalem 9190401, Israel

CISS, chirality-induced spin selectivity is a phenomenon that has raised significant interest due to the large spin polarizations generated by organic molecules and other effects such as magnetic switching of ferromagnets impacted by chiral molecules [1]. In hybrid systems, these chiral molecules have been observed to influence magnetic properties such as changes in the magnetization [2]. In this study, we investigate how chiral molecules of α-helix polyalanine interact with chiral spin structures, namely magnetic skyrmions, which are stabilized in ferromagnetic/heavy metal multilayers due to Dzyaloshinskii-Moriya interaction [3]. Using magneto-optic Kerr effect imaging, we show that chiral polypeptides can influence the stability of skyrmions by modifying the ranges of temperature and applied magnetic field in which they are stable. We also show that the chiral molecules affect the skyrmion dynamics, in particular the thermal diffusion of the skyrmions [4].

[1] R. Naaman et al. Nat. Rev. Chem. 3, 250 (2019)
[2] Y. Kapon et al. J. Chem. Phys. 159, 064701 (2023)
[3] K. Everschor-Sitte et al. J. Appl. Phys. 124, 240901 (2018)
[4] Y. Kapon et al. Nano Lett. 25, 306-312 (2025)

MA 7.67 Mon 9:30 P2

Coupled and decoupled topological textures in van der Waals heterostructure — •Sourav Chowdhury[1], Daniel Metternich[2], Simon Gaebel[2], Chithra Sharma[3], Jayjit Dey[1], Victor Deinhart[2], Tim Butcher[2], Michael Schneider[2], Josefin Fuchs[2], Bastian Pfau[2], and Moritz Hoesch[1] — [1]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — [2]Max-Born-Institut (MBI), Berlin, Germany — [3]University of Hamburg, Hamburg, Germany

Topological nanodomain spin textures in two-dimensional (2D) van der Waals (vdW) magnets are attracting increasing interest for next-generation spintronic technologies, offering pathways to ultradense data storage, energy-efficient operation, and unconventional data processing architectures [1]. Using element-specific X-ray imaging, we visualize a variety of topological spin textures in an Fe3GeTe2/CrGeTe3 heterostructure and directly resolve their interlayer behavior. We find that nanodomains in the two layers are strongly coupled under certain conditions, while within a specific magnetic-field window, the domains become decoupled and evolve independently. This transition from coupled to decoupled topological textures can be understood in terms of distinct magnetic anisotropy contributions in the two layers, arising from interlayer interactions rather than solely from the properties of the individual materials. [1] K. Chang et al., Science 2016, 353, 274.

MA 7.68 Mon 9:30 P2

Anisotropic skyrmion liquid phase — •Daniel Schick[1], Tim Matthies[2], Thomas Mutschler[1], Levente Rózsa[3,4], and Ulrich Nowak[1] — [1]University of Konstanz, Konstanz, Germany — [2]University of Hamburg, Hamburg, Germany — [3]Wigner Research Centre for Physics, Budapest, Hungary — [4]Budapest University of Technology and Economics, Budapest, Hungary

Melting transitions in two-dimensional systems of particles have attracted much attention in research since the development of the Kosterlitz-Thouless-Harperlin-Nelson-Young theory, particularly because of an intermediate phase with long-ranged orientational but short-ranged translational order, called the hexatic phase.

Magnetic skyrmions are topological quasiparticles in thin magnetic films and, due to their two-dimensional nature, are subject to KTHNY theory. Recently, the hexatic phase was identified experimentally in skyrmion lattices [1]. Here, we use a molecular dynamics simulation to study the phase transitions in skyrmion ensembles. Taking into account the anisotropic interaction of skyrmions in the $(Pt_{0.95}Ir_{0.05})$/Fe/Pd(111) system, we show how this anisotropy influences the phase of the skyrmion system. Instead of an intermediate hexatic phase between solid and liquid phase, one observes a direct solid-liquid transition, with a global orientational order even in the liquid phase.

[1] R.Gruber et. al. Nat. Nanotechnol. **20**, 1405-1411 (2025)

MA 7.69 Mon 9:30 P2

Rotating Skyrmion Lattice by Circularly Polarized Light — •Reza Doostani and Achim Rosch — University of Cologne, Cologne, Germany

Previously, it has been studied that shining a circularly polarized light on a skyrmion crystal (SkX) induces rotation in the lattice. This is due to Inverse Faraday Effect where spins experience local magnetic field. The magnitude of rotation depends on the fluence of light and its polarization. There exist a fluence threahold under which the SkX does not rotate. Further, one can start and stop the rotation by doing double pulse laser experiment and changing the separation time between two pulses. These results has been theoretically described where coherent oscillation of rotation amplitude as a function of pulse separation matches the experimental observation. However the theoretical value for rotation amplitude (for clean system) is orders of magnitude smaller than experimental value. Previously, the only source of rotation was due to Gilbert damping, however this cannot describe the rotation alone. In this work, we investigate other source of rotation in this system, namely we induce disorder and analyze its effect.

MA 7.70 Mon 9:30 P2

Noise measurements on magnetic skyrmions in magnetic multilayers — •Arthur Schmidt[1], Bereket Ghebretinsae[1], Joe Sunny[2], Manfred Albrecht[2], and Jens Müller[1] — [1]Institute of Physics, Goethe University Frankfurt, 60438 Frankfurt am Main, Germany — [2]Institute of Physics, University of Augsburg, Universitätsstraße 1, 86135 Augsburg, Germany

Magnetic skyrmions are topologically protected spin textures which usually appear in materials with broken inversion symmetry and strong spin-orbit coupling due to emergent Dzyaloshinskii-Moriya interaction (DMI). While in bulk materials skyrmions exist mostly at low temperatures, in magnetic multilayers (MM) they can be stabilized at room temperature [1], which, in combination with their small size, stability and fast and energy efficient movement, make them promising for spintronics applications e.g. in unconventional computing and high-density magnetic storage. Here we present first results on low-frequency resistance noise spectroscopy measurements on Pt-Co-Ta-based MM systems which host Néel-type skyrmions at room temperature. The intention is to utilize low-frequency noise as an effective probe for the electrical characterization of

fundamental skyrmion properties such as the skyrmion lattice constant or their mean velocity and to investigate their current-induced dynamics [2-4].
[1] Hassan *et al.*, Nat. Phys. **20**, 615 (2024)
[2] Sato *et al.*, Phys. Rev. B **100**, 094410 (2019)
[3] Wang *et al.*, Phys. Rev. B **108**, 094431 (2023)
[4] Diaz *et al.*, Phys. Rev. B **96**, 085106 (2017)

MA 7.71 Mon 9:30 P2

Parameter-Dependent Stability of Magnetic Hopfions — •Niklas Oettgen, Sandra C. Shaju, Maria Azhar, and Karin Everschor-Sitte — Faculty of Physics, University of Duisburg-Essen, Duisburg, Germany

Hopfions are three-dimensional topologically protected magnetic textures that can be considered as closed loops of twisted skyrmion strings. We implement a model of spatially varying Dzyaloshinskii-Moriya interactions in micromagnetic simulations to explore Hopfion stability across a range of external magnetic fields and uniaxial anisotropies. Our simulations identify a clear regime in which the Hopfion remains metastable, and give insight into the conditions required for their formation and robustness.

MA 7.72 Mon 9:30 P2

Stability and Internal Structure of Skyrmioniums — •Finn Feldkamp[1,2], Alessandro Pignedoli[1], Ross Knapman[1], Maria Azhar[1], and Karin Everschor-Sitte[1] — [1]Faculty of Physics and Center for Nanointegration Duisburg-Essen, Duisburg, Germany — [2]Faculty of Physics and Earth System Sciences Leipzig University, Leipzig, Germany

Skyrmioniums are magnetic textures that can emerge in thin-film magnets under suitable conditions, potentially coexisting with other configurations such as domain walls and skyrmions. They can be understood as two nested skyrmions with opposite topological charge, giving rise to a ring-like, non-topological structure rather than the single-core profile characteristic of skyrmions. In this work, we investigate the stability and internal structure of skyrmioniums in thin films, examining the influence of crystalline anisotropy, external magnetic fields, and the demagnetization field. We present a comparative analysis with skyrmions, highlighting key similarities and differences in their stability regimes and structural responses to material and field parameters.

MA 7.73 Mon 9:30 P2

Investigation of the hyperfine coupling constants of the endohedral fullerene N@C_{60} — •Rebecca Löffler, Marco Sommer, and Johann Klare — Inst. of Physics, Univ. Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

Endohedral fullerenes such as N@C_{60} are considered promising systems for spin-based quantum bits and quantum sensors on a nanoscale due to their exceptional spin stability and long coherence times, even at room temperature. In this work, the temperature-dependent hyperfine coupling constant of N@C_{60} in various solvents was investigated using EPR spectroscopy. To understand the influence of the chemical environment, crystalline N@C_{60} was introduced into organic solvents (toluene, CS_2) and into an aqueous host*guest complex with two γ-cyclodextrin molecules and then compared. The results show that a vibration model to Waiblinger (PhD thesis, Univ. Konstanz, 2001) reliably describes the behavior of N@C_{60} in crystalline form and in organic solvents, but cannot be applied to the γ-cyclodextrin complex. For crystalline N@C_{60}, a vibrational energy of E = (14,7 ± 0,2) meV was determined. Phase transitions could be detected in toluene and in the γ-cyclodextrin complex by changes in the hyperfine coupling constants. The results show that the hyperfine coupling constant has great potential for use in quantum sensor technology, especially for precise measurements of phase transitions, such as the freezing of water.

MA 7.74 Mon 9:30 P2

Electron paramagnetic resonance and magnetization studies on tetrahedral Co^{II} complexes — •Matthias Heinrich[1], Jan Arneth[1], Amit Gharu[2], Kuduva Vignesh[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]Department of Chemical Sciences, IISER Mohali, India

We report the static and dynamic magnetic properties of a series of five cobalt complexes of the type $Co^{II}_4Co^{II}$ with four octahedrally coordinated Co^{III} centers in the low-spin $S = 0$ state and a magnetically isolated Co^{II} ion ($S = 3/2$) in distorted tetrahedral coordination. The tetrahedral distortion differs across the series due to variations in bond lengths and bond angles. Our static and dynamic magnetization measurements of all compounds reveal field-induced magnetic relaxation as well as pronounced magnetic anisotropy. For one representative complex, high-field EPR-studies are presented which allow to determine the anisotropic g-factor as well as the easy-plane anisotropy. The effect of tetrahedral distortion on the magnetic anisotropy is quantitatively evaluated and discussed.

MA 7.75 Mon 9:30 P2

Investigating the Magnetic 3d-3d and 3d-4f Interaction in Triangular $Cr^{III}_3Ln^{III}$ Complexes — •Rui Yang[1], Jan Arneth[1], Muthu Thangavel[2], Christopher Anson[2], Annie Powell[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]Institute for Inorganic Chemistry, Karlsruhe Institute of Technology, Germany

The interplay between the highly localized 4f electrons of the lanthanide ions and the more diffuse transition-metal 3d electrons leads to complex and often weak coupling mechanisms that are difficult to predict and quantify. Here, we report the static and dynamic magnetic properties of a series of isostrucural triangular $Cr^{III}_3Ln^{III}$ (Ln^{III} = Y, Gd, Tb, Dy, Ho, Er, Yb) complexes studied by means of dc/ac magnetization and high-field EPR. In particular, we investigate the bare 3d-magnetism of the Cr^{III}-triangle which is realized for diamagnetic Ln=Y and systematically study the 3d-4f interaction in the series of paramagnetic Ln.

MA 7.76 Mon 9:30 P2

Optimization of metal-doped M0.2Fe2.8O4/PEG nanocomposite for enhanced magnetic and relaxometric performance in MRI applications — •Mennatallah Abouhasswa[1], Ahmed Al Shahawy[2], Samaa El Dek[2], Messaoud Harfouche[3], Nagwa Okasha[1], Giuliana Aquilanti[4], Neama Imam[5], and Jan Ingo Flege[5] — [1]Physics Department, Ain Shams University, Egypt — [2]Faculty of Postgraduate Studies for Advanced Sciences, BeniSuef University, Egypt — [3]SESAME Synchrotron, Jordan — [4]Elettra,Sincrotrone Trieste, Italy — [5]Brandenburg University of Technology Cottbus, Senftenberg, Germany

Magnetic spinel ferrites are promising magnetic resonance imaging (MRI) contrast agents owing to their tunable structure, magnetic anisotropy, and biocompatibility. M0.2Fe2.8O4 nanoparticles (M = Fe2+, Mn2+, Cu2+) coated Polyethylene glycol (30%PEG-6000) were synthesized to correlate cation substitution with structural, magnetic, and relaxometric behavior. XRD, HRTEM, FTIR, XPS, synchrotron-based XAFS spectroscopy, and Vibrating Sample Magnetometer (VSM) confirmed single-phase nanocrystals (8-13 nm) with mixed Fe2+/Fe3+ states and preserved spinel geometry upon PEG coating. Mn-doping enhanced saturation magnetization and transverse relaxivity, providing the strongest T2 weighted MRI contrast. The results demonstrate that combining controlled B-site substitution with hydrophilic PEG capping enables concurrent optimization of magnetic response and colloidal stability, highlighting Mn0.2Fe2.8O4/PEG as a high-performance and biocompatible MRI nanocontrast agent.

MA 7.77 Mon 9:30 P2

Height Calibration of Nitrogen Vacancy Diamond Tips Using Current-Carrying Wires — Robin Abram, •Ricarda Reuter, Alexander Fernández Scarioni, Sibylle Sievers, and Hans Werner Schumacher — Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

Scanning Nitrogen Vacancy Microscopy (SNVM) is a measurement technique capable of resolving the spatial distribution of magnetic stray fields with nanometer and microtesla resolution, respectively. It combines optical field detection with a scanning probe-like approach, where the key component is a diamond scanning tip containing a single NV center. While magnetic field measurements are quantum-calibrated with respect to the position of the NV center, precise knowledge of the distance to the sample is required to also consider the height dependence. The latter can currently only be estimated with an uncertainty of up to several nanometers, most commonly by calibration with a known stray field, e.g. using ferromagnetic microstructures. We established an improved height calibration based on SNVM studies of the current-induced Oersted field in Pt wires by Lee et al.. The out of plane field component is extracted from the raw data taken along the NV spin axis, following the approach first introduced by Schendel et al. and later applied to SNVM by Dovzhenko et al., and fitted to an analytical model. Using this approach, we realized a height calibration with an uncertainty of 10 nanometers for both 100 and 111 cut diamond tips. We also found that the nominally expected NV height underestimates the calibration result by about 30 nanometers.

MA 7.78 Mon 9:30 P2

Influence of Reference Sample and Scan Parameters on Magnetic Force Microscopy Calibrations — •Christopher Habenschaden[1], Baha Sakar[2], Sibylle Sievers[1], and Hans Werner Schumacher[1] — [1]Physikalisch-Technische Bundesanstalt (PTB), 38116 Braunschweig, Germany — [2]Felix Bloch Institute for Solid State Physics, University of Leipzig, Linnéstraße 5, 04103 Leipzig

Magnetic force microscopy (MFM) is a technique that enables the precise characterization of magnetic stray field distributions with high sensitivity and spatial resolution. By employing an appropriate calibration procedure, MFM can also provide quantitative values for magnetic fields. This calibration typically involves measuring a reference sample to identify the stray field or stray field gradient of the tip at the sample's surface. This distribution is known as the tip transfer function (TTF), which is obtained through regularized deconvolution in Fourier space. The performance of this process is heavily influenced by the reference sample's properties, scan parameters, and the detection system's noise characteristics, which can restrict its applicability. Our findings indicate that achieving a strong overlap of frequency components between the reference sample and the sample under test is more crucial for accurately reconstructing the stray field than simply obtaining a precise real-space representation of the tip's stray field distribution.

MA 7.79 Mon 9:30 P2

Accessing in-plane stray field components with torsional resonance mode magnetic force microscopy — •Jorge Marqués-Marchán[1], José Claudio Corsaletti Filho[1], Pamela Morales-Fernández[1], and Claire Donnelly[1,2] — [1]MPI CPfS, Dresden, Germany — [2]WPI-SKCM2, Hiroshima, Japan

In recent years, the emergence of 3D nanomagnetism and topological configurations has highlighted the importance of mapping the 3D vector field components in these systems. A lab-based technique that could provide such contrast is torsional resonance mode magnetic force microscopy (TR-MFM), where the MFM probe oscillates laterally with respect to the sample surface. Although MFM is a well-established technique, the use of TR-MFM has only been validated on standard samples [1,2]. Here, we use TR-MFM in combination with standard MFM to map both the in-plane and out-of-plane stray field components of different samples, aiding the understanding of different 3D magnetic configurations.

[1] A. Kaidatzis and J. M. García-Martín, Nanotechnology 24, 165704 (2013)
[2] J. F. Schmidt et al., J. Appl. Phys. 136, 113904 (2024)

MA 7.80 Mon 9:30 P2

Lensless magneto-optical imaging — •Volker Neu[1], Giancarlo Pedrini[2], Ivan Soldatov[1], Stephan Reichelt[2], and Rudolf Schäfer[1] — [1]IFW Dresden, Helmholtzstr. 20, 01069 Dresden — [2]Institut für Technische Optik (ITO), Univ. Stuttgart, Pfaffenwaldring 9, 70569 Stuttgart

Magneto-optical methods, which utilize the interaction of polarized light with the magnetization state of the sample in reflection (magneto-optical Kerr effect) or in transmission (Faraday effect) present the most prominent classical microscopy techniques to investigate magnetic microstructures down to a few hundred nanometers.

In a first proof-of-principle study [1] we verified the feasibility of lensless magnetic imaging in the optical regime and explored the various contrast mechanisms that can be applied in such an approach. We demonstrate that the reconstructed intensity is in full qualitative agreement with the intensity contrast expected from conventional lens-based Faraday microscopy. This holds for the usual application of linearly polarized light with an almost crossed analyzer, but also for the less common combination of linearly polarized light with fully crossed analyzer. The additional phase information, not accessible with conventional microscopy, offers direct access to domain information in the latter case. This initial verification of lensless magneto-optical imaging will enable the various established advantages of lensless microscopy to be utilized for the examination of magnetic materials in the future.

[1] V. Neu, G. Pedrini, I. Soldatov, S. Reichelt, R. Schäfer, "Lensless magneto-optical imaging", Scientific Reports 15, 28277 (2025).

MA 7.81 Mon 9:30 P2

Soft X-ray ptychography with SOPHIE — Tim A Butcher[1,2], Simone Finizio[1], Lars Heller[1], Nicholas W Phillips[1,3], Blagoj Sarafimov[1], Carlos A F Vaz[1], Armin Kleibert[1], Benjamin Watts[1], Mirko Holler[1], and •Jörg Raabe[1] — [1]Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — [2]Max Born Institut, 12489 Berlin, Germany — [3]CSIRO, 3168 Clayton, Australia

Soft X-ray ptychography is rapidly becoming one of the key synchrotron-based magnetic imaging techniques, thanks to the possibility of combining high spatial resolutions over large scan areas with strong contrast mechanisms such as X-ray circular and linear dichroisms. To meet the demands of the user community for ptychography imaging, the SOft X-ray Ptychography Highly Integrated Endstation (SOPHIE) was developed at the Swiss Light Source. In this presentation, we give an overview of the design and performance of the endstation during its commissioning at the SoftiMAX beamline of MaxIV, together with an example of its imaging capabilites, where sub 10nm resolution at the Fe L_3 edge was demonstrated in routine conditions.

MA 7.82 Mon 9:30 P2

High resolution imaging of ultrathin PMA films for racetrack applications — •Anindit Das[1], Sebastian Schneider[1], Jae-Chun Jeon[2], and Bernd Rellinghaus[1] — [1]DCN, cfaed, TU Dresden, Dresden, Germany — [2]Max Planck Institute for Microstructure Physics, D-06120 Halle (Saale), Germany

The realization of domain wall (DW)-based racetrack memory requires Perpendicular Magnetic Anisotropy (PMA) thin films with finely tuned magnetic properties. This work combines direct imaging via Lorentz Transmission Electron Microscopy (LTEM) with micromagnetic simulations to establish design principles for such materials. Our simulations systematically vary key parameters—including saturation magnetization (M_s), uniaxial anisotropy (K_u), exchange stiffness (A_{ex}), and the Dzyaloshinskii-Moriya interaction (DMI)—to understand their impact on DW structure and dynamics. We identify that an optimal balance is critical: a high K_u ensures thermal stability, while a moderate M_s and tailored DMI are essential for efficient, fast DW motion. However, significant challenges arise from conflicting requirements; for instance, a high A_{ex} is necessary for robust DWs but can also increase the depinning field, and excessive DMI can compromise DW integrity. This study provides a crucial map of the material parameter space, highlighting the trade-offs between stability, speed, and fabricability to guide the development of viable PMA films for racetrack memory.

Financial support by the DFG through TRR 404, project no. 528378584, is gratefully acknowledged.

MA 7.83 Mon 9:30 P2

Theory of transport properties of coplanar spin spirals — •Ilja Turek — Institute of Physics of Materials, Czech Acad. Sci., Brno, Czech Rep.

Coplanar spin spirals are compensated magnetic systems related closely to the recently introduced p-wave magnets [1]. Their special magnetic order leads to the absence of space-inversion symmetry, which is a necessary prerequisite for a nonzero Edelstein effect (change of magnetization due to an external electric field). Here, we consider simple tight-binding models of nonrelativistic coplanar spin spirals and study their transport properties within the Kubo linear response theory and the conserving selfconsistent Born approximation [2]. We reveal that depending on the model details, both the electric conductivity and the coefficient of the Edelstein effect contain not only a coherent (quadratic in the averaged one-particle propagators) term, but also a nonnegligible incoherent term due to the disorder-induced vertex corrections. Consequences for reliable evaluation of the transport properties of real spin-spiral systems are discussed briefly as well. [1] A. Chakraborty et al., Nat. Commun. 16 (2025) 7270. [2] I. Turek, Phys. Rev. B 93 (2016) 245114.

MA 7.84 Mon 9:30 P2

Emergent non-coplanar magnetism and colossal transverse magnetoresponse in strongly correlated nodal-line half-metal — •Jyotirmoy Sau[1,2], Sourav Chakraborty[1], and Manoranjan Kumar[1] — [1]S. N. Bose National Centre for Basic Sciences, Kolkata 700106, India — [2]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

Understanding the interplay of strong correlation and temperature in nodal-line semimetals can unlock new pathways for spin current control. Here, we consider the $3d$-$5d$ double-perovskite Ba_2CoWO_6, which features mirror-symmetry-protected nodal lines, strong Co-site interactions, and spin-orbit coupling at W sites. Our first-principles and exact diagonalization results reveal a half-metallic ground state with high-spin Co and topologically non-trivial bands. Finite spin-orbit coupling gaps out nodal points and induces band inversion. The ensuing non-trivial Berry curvature generates an anomalous Hall response and stabilizes a non-coplanar magnetic order. Our semi-classical Monte Carlo finite-temperature simulation of the five-orbital Hubbard model confirms the non-coplanar magnetic order and uncovers colossal transverse magnetoresponse. We predict the temperature and magnetic field scales for the tunability of the magnetoresponse.

MA 7.85 Mon 9:30 P2

Exploring the tunability of magnetism and charge density waves states in VSe2 — •Javier Corral Sertal[1,2], Adolfo O. Fumega[3], S. Blanco-Canosa[4], and Victor Pardo[2,5] — [1]CiQUS, Centro Singular de Investigacion en Quimica Biolóxica e Materiais Moleculares, Universidade de Santiago de Compostela, Santiago de Compostela, Spain — [2]Departamento de Física Aplicada, Universidade de Santiago de Compostela, Santiago de Compostela, Spain — [3]Department of Applied Physics, Aalto University, 02150 Espoo, Finland — [4]Donostia International Physics Center (DIPC), San Sebastián, Spain — [5]Instituto de Materiais iMATUS, Universidade de Santiago de Compostela, Santiago de Compostela, Spain

Transition metal dichalcogenides (TMDs, MX_2 : M = Nb, Ti, V..., X = S, Se, Te...) are a familiy of two-dimensional (2D) layered materials that attract great attention because of their large landscape of collective phenomena that differ from the bulk ones. Among them, magnetism in low dimensions has been argued for decades, being rejected by the Mermin-Wagner theorem but found as Ising-type ferromagnets in purely 2D-materials VSe_2 is a TMDs where ferromagnetism is present in its normal state (NS) bulk phase, but becomes supressed when the charge density wave (CDW) phase $4 \times 4 \times 3$ appears or it is reduced to the monolayer limit. Here, we present a computational study of several heterostructure packaging of VSe_2 with other TMDs materials in order to elucidate if the formation of the CDW can be supressed by different stacking arrangements, and if with these stackings we are able to retain magnetism in the system.

MA 7.86 Mon 9:30 P2

Temperature dependence of the spin-wave dispersion in the spin-polarized homogeneous electron gas — •Michael Neugum, Noah Spiegelberg, and Arno Schindlmayr — Universität Paderborn, Department Physik, 33095 Paderborn, Germany

Spin waves are an important class of elementary excitations in magnetically ordered materials. Due to the absence of an energy gap, they are easily thermally excited and, consequently, influence technological applications like spintronics or magnetic data storage. The impact of temperature is twofold: First, the occupation numbers of the bosonic spin-wave modes increase with the temperature. Second, the dispersion itself changes, leading to lowered spin-wave energies and hence to an accelerated population. The latter effect is largely ignored in cur-

rent ab initio calculations, which are typically performed at 0 K and often lack proper temperature-dependent functional expressions. Here we calculate the spin-wave dispersion of the spin-polarized homogeneous electron gas at finite temperature within time-dependent density-functional theory, taking only the exchange functional into account. The temperature dependence of the exchange kernel is fully included. Our results demonstrate that the spin-wave energies are indeed systematically lowered as the temperature increases. As an important observation, the spin-wave stiffness also decreases, so that there is a nonnegligible effect on long-wavelength modes and on thermodynamic quantities, such as the specific heat capacity, even at low temperature.

MA 8: Altermagnets II

Time: Monday 15:00–18:30 Location: HSZ/0002

MA 8.1 Mon 15:00 HSZ/0002

Odd-parity spin splitting and anomalous Hall effect in spiral magnets — •Shun Okumura[1,2], Moritz M. Hirschmann[2], and Yukitoshi Motome[3] — [1]Quantum-Phase Electronics Center, The University of Tokyo, Tokyo, Japan — [2]RIKEN Center for Emergent Matter Science, Wako, Japan — [3]Department of Applied Physics, The University of Tokyo, Tokyo, Japan

Altermagnetism with collinear antiferromagnetic order has recently attracted considerable interest for a spontaneous anomalous Hall effect (AHE) mediated by spin-orbit coupling (SOC). In contrast, non-coplanar magnetic textures such as skyrmions exhibit a topological Hall effect by imprinting a Berry phase on itinerant electrons even in the absence of SOC. However, in the case of spiral magnetism, a prototypical example of a non-collinear and coplanar magnetic structure, the conditions required to realize AHE have yet to be thoroughly explored.

In this study, we investigate the AHE in metallic systems coupled to commensurate spiral magnetic textures. The electronic bands exhibit odd-parity spin splitting with spin polarization perpendicular to the helical plane. In the presence of SOC and finite magnetization, the Berry curvature concentrated along the spin-nodal lines leads to a characteristic AHE in the spin spiral state. This spiral-induced AHE depends sensitively on the SOC type, helical plane, and magnetization direction. We also demonstrate that a "p-wave" magnet with a commensurate spin spiral, recently identified in an f-electron material, can host this enormous AHE.

MA 8.2 Mon 15:15 HSZ/0002

Pines' Demons in d-Wave Altermagnets: From Hidden Modes to Fano-Demon States — •Habib Rostami[1] and Johannes Hofmann[2] — [1]Department of Physics, University of Bath, United Kingdom — [2]Department of Physics, Gothenburg University, Sweden

We develop a Fermi-liquid description of d-wave altermagnets and analyze their charge and spin collective excitations [1]. In addition to the conventional undamped plasmon, where both spin components oscillate in phase, we find an acoustic plasmon (demon) mode with out-of-phase spin dynamics. Using the dynamical structure factor, we show that the demon frequency and spectral weight depend sensitively on the Landau parameters and on the propagation direction. As a function of angle, the acoustic mode evolves from a hidden state with vanishing spectral weight in the density response, to a weakly damped propagating demon, and, below a critical interaction parameter, to a Fano-demon mixed state that strongly hybridizes with particle-hole excitations and exhibits an asymmetric line shape. We briefly discuss possible implications for probing and exploiting collective electron spin oscillations in altermagnetic materials.

[1] H. Rostami and J. Hofmann, Fermi liquid theory of d-wave altermagnets: demon modes and Fano-demon states, arXiv:2505.07083, to appear in Physical Review Letters.

MA 8.3 Mon 15:30 HSZ/0002

Studying altermagnetism with muon-spin spectroscopy — •Thomas Hicken[1], Jonas Kreiger[1], Jennifer Graham[1], Zurab Guguchia[1], Franziska Walther[2], Kristin Kliemt[2], Cornelius Krellner[2], Helena Reichlova[3], Klára Uhlířová[4], Juraj Krempaský[1], Nirmal Ghimire[5], and Hubertus Luetkens[1] — [1]PSI, Switzerland — [2]Goethe-Universität Frankfurt, Germany — [3]Czech Academy of Science, Czech Republic — [4]École Polytechnique Fédérale de Lausanne, Switzerland — [5]University of Notre Dame, USA

With properties of both ferro- and antiferro-magnets, altermagnetism is of interest for fundamental physics and spintronic applications. Understanding the magnetic structure, and hence magnetic symmetries, is of utmost importance. Further, it has been suggested that altermagnets may have unique dynamic fluctuations. To answer these questions, muon spin spectroscopy (μSR) measurements provide information that is complementary to, and unique from, other probes. I will discuss how we are using μSR to probe a number of materials, including $Co_{1/4}NbSe_2$ [1], a proposed g-wave altermagnet, Ce_4Sb_3, which shows promise as an altermagnet with $4f$ moments, and MnTe [2], which is perhaps the best studied altermagnet so far. Our measurements, combined with muon stopping site calculations, reveal the sometimes unexpected magnetic structure of candidate altermagnetic materials, and test some of the key predictions of altermagnetism.

[1] J. N. Graham, T. J. Hicken et al., arXiv:2503.09193 (2025).
[2] T. J. Hicken et al., arXiv:2507.14710 (2025).

MA 8.4 Mon 15:45 HSZ/0002

Broadband nonlinear Hall response and multiple wave mixing in a room temperature altermagnet — •Berthold Jaeck — HKUST, Department of Physics, Clear Water Bay, Kowloong, Hong Kong

Altermagnets are characterized by magnetic crystal order that manifests in a non-relativistic spin-splitting of the electronic bands. Their electric material properties should thus be determined by the underlying symmetries. We report the discovery of a broadband third-order nonlinear anomalous Hall effect in altermagnetic CrSb at room temperature that exhibits a distinct spatial anisotropy [1]. The comparison of our experimental observations with symmetry analyses and model calculations shows that this nonlinear Hall response is induced by the nonlinear electric susceptibility of a Berry curvature quadrupole. This quadrupole precisely reflects the magnetic and crystalline symmetries encoded in the altermagnetic g-wave order parameter. We then utilize the nonlinear electric susceptibility of CrSb to realize a multiple wave mixing device with pronounced four wave mixing output. Our study provides a generalized understanding of the impact of magnetic crystal order on the electric material properties of altermagnets and significantly expands their technological scope to include high-frequency applications up to the THz regime.

We acknowledge funding by the Hong Kong RGC (Grant Nos.26304221, 16302422, 16302624, and C6033-22G) and the Croucher Foundation (Grant No.CIA22SC02).

[1] S. Sankar et al., arXiv:2511.10471 [cond-mat.mes-hall] (2025)

MA 8.5 Mon 16:00 HSZ/0002

Ce_4Sb_3: A Kondo metal as candidate for d-wave altermagnetism — •Franziska Walther[1], Thomas J. Hicken[2], Venkata Krishna Bharadwaj[3], Julian Kaiser[4], Bin Shen[4], Jan Priessnitz[5], Rahel Ohlendorf[6], Michelle Ocker[1], Alexander Fedorov[7], Anton Jesche[4], Hubertus Luetkens[2], Philipp Gegenwart[4], Elena Gati[7], Denis Vyalikh[8], Libor Šmejkal[5], Jairo Sinova[3], Cornelius Krellner[1], and Kristin Kliemt[1] — [1]Uni Frankfurt, Germany — [2]PSI, Switzerland — [3]Uni Mainz, Germany — [4]Uni Augsburg, Germany — [5]MPI PKS Dresden, Germany — [6]MPI CPfS Dresden, Germany — [7]HZB Berlin, Germany — [8]DIPC Donostia, Spain

The study of altermagnetic materials has been focused so far on magnetic d-systems. Here, we present Ce_4Sb_3 as a lanthanoid-based altermagnetic candidate to study the altermagnetism arising from local $4f$ moments, where magnetism is mediated indirectly by the RKKY interaction. Below 4 K, the cubic compound Ce_4Sb_3 orders magnetically and d-wave altermagnetism is theoretically predicted. Furthermore, the material shows Kondo behaviour, enabling it to be a promising candidate to study pressure-induced quantum critical phenomena in systems with altermagnetic spin fluctuations. Here, we report on the single crystal growth by the Czochralski method in a quasi-crucible free high pressure setup, the physical characterization of the magnetic ground state and a first study by angle-resolved photoemission and muon spin spectroscopy.

MA 8.6 Mon 16:15 HSZ/0002

Optical Kerr Signatures in d-wave and g-wave Altermagnets — •Luca Felipe Haag[1], Paul Herrgen[1], Jairo Sinova[2], Benjamin Stadtmüller[3], Martin Aeschlimann[1], and Hans Christian Schneider[1] — [1]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, Germany — [2]Institut für Physik, Johannes Gutenberg University, Mainz — [3]Experimentalphysik II, Institute of Physics, University of Augsburg, Germany

The non-relativistic spin splitting in the electronic states of altermagnets makes them promising candidates for next-generation spintronic materials [1,2], but the identification and characterization of these materials is difficult. In a previous study, we demonstrated that altermagnets show intriguing time-dependent magneto-optical properties when probed by ultrashort pulses, which are linked to their particular spin symmetries [3]. In this contribution we analyze the pump-induced Kerr response of different candidate materials in detail. To this end, we theoretically investigate the probe response due to the pump induced birefringence and explain how to distinguish between anisotropic charge carrier distributions and magnetic signatures. Our results suggest that pump-probe Kerr microscopy is a viable tool to image the domain structure of specific altermagnets.

[1] Šmejkal et al., Phys. Rev. X 12, 040501 (2022) [2] Šmejkal et al., Phys. Rev. X 12, 031042 (2022) [3] Weber et al., arXiv:2408.05187 (2024)

MA 8.7 Mon 16:30 HSZ/0002

Ferroelectricity-driven altermagnetism in two-dimensional van der Waals multiferroics — •Bo Zhao[1], Fu Li[1], Wei Ren[2], Hao Wang[1], and Hongbin Zhang[1] — [1]Theory of Magnetic Materials, Institute of Materials Science, Technical University of Darmstadt, 64287 Darmstadt, Germany — [2]Institute for Quantum Science and Technology, State Key Laboratory of Advanced Refractories, Materials Genome Institute, Physics Department, Shanghai University, Shanghai 200444, China

Altermagnets (AMs) are an unconventional class of collinear compensated antiferromagnets that exhibit momentum-dependent spin splitting despite zero net magnetization. Using spin space group (SSG) symmetry analysis and first-principles calculations, we show that altermagnetism in two-dimensional multiferroics can be efficiently controlled by ferroelectric polarization and interlayer sliding. As a material platform, monolayer and bilayer $FeCuP_2S_6$ display finite spin splitting when ferroelectric sublattices are linked by nonsymmorphic screw-axis operations instead of pure translation or inversion. Interlayer sliding allows reversible switching or suppression of this spin splitting through SSG modifications. We further find that the anomalous Hall response directly probes these spin-split states. These results highlight 2D van der Waals multiferroics as promising systems for electrically tunable altermagnetism and next-generation spintronic applications.

[1] B. Zhao et al. arXiv:2511.00712.

15 min break

MA 8.8 Mon 17:00 HSZ/0002

Elastocaloric probing and tuning of multipolar order in the altermagnet MnF_2 — •Rahel Ohlendorf[1,2], Luca Buiarelli[3], Hilary M. L. Noad[1], Andrew P. Mackenzie[1,4], Rafael M. Fernandes[5], Turan Birol[3], Jörg Schmalian[6], and Elena Gati[1,2,7] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Technische Universität, Dresden, Germany — [3]University of Minnesota, Minneapolis, USA — [4]University of St Andrews, UK — [5]University of Illinois Urbana-Champain, Urbana, USA — [6]Karlsruhe Institute of Technology, Karlsruhe, Germany — [7]Goethe Universität, Frankfurt, Germany

Altermagnets break time-reversal symmetry without net magnetization [1], with the order parameter described by the ferroic ordering of multipoles rather than dipoles. In *d*-wave altermagnets, the predicted ferrooctupolar order couples to magnetic field and strain. In this talk, we demonstrate that elastocaloric experiments under strain and magnetic field are a powerful thermodynamic and symmetry-sensitive probe of the finite-temperature ferrooctupolar critical point. We resolve elastocaloric signatures of altermagnetic crossover lines and entropy accumulation. By combining our experiments with DFT calculations, we provide a microsopic explanation for the size of the observed thermodynamic effects. As a result, we outline the route to stronger thermodynamic responses in insulating and metallic altermagnets (both *d*-wave and *g*-wave), establishing elastocaloric measurements as a key probe of altermagnetic criticality.

[1] L. Šmejkal et al., Phys. Rev. X 12, 031042 (2022)

MA 8.9 Mon 17:15 HSZ/0002

Optical phonons as a testing ground for spin group symmetries — Felix Schilberth[1], Mark Kondákor[4], Denis Ukulov[2], Lilian Prodan[1], Alexander Tsirlin[3], Peter Lemmens[2], Karlo Penc[4], Istvan Kézsmárki[1], and •Joachim Deisenhofer[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, D-86159 Augsburg, Germany — [2]Institute of Condensed Matter Physics, TU Braunschweig, Mendelssohnstr. 3, 38106 Braunschweig, Germany — [3]Felix Bloch Institute for Solid-State Physics, Leipzig University, 04103 Leipzig, Germany — [4]Institute for Solid State Physics and Optics, HUN-REN Wigner Research Centre for Physics, H-1525 Budapest, P.O.B. 49, Hungary

We present a detailed study of the infrared- and Raman-active modes in the collinear antiferromagnet and altermagnet candidate $Co_2Mo_3O_8$. Comparing to *ab initio* calculations accurately capturing the eigenfrequencies, we identify all expected phonon modes at room temperature and deduce their selection rules with the magnetic point group and the spin group. We observe the change of selection rules upon antiferromagnetic ordering, agreeing with the relativistic symmetry approach, while the spin group formalism predicts no changes. Therefore, optical phonons sensing the symmetry of the magnetic order can reveal if relevant magnon-phonon coupling is compatible with the spin-group approach or not.

MA 8.10 Mon 17:30 HSZ/0002

Optical properties of altermagnetic candidate MnTe — •Ece Uykur[1], Marcus Schmidt[2], Stephan Winnerl[1], and Alexander A. Tsirlin[3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01067 Dresden, Germany — [3]Felix Bloch Institute for Solid-State Physics, University of Leipzig, 04103 Leipzig, Germany

MnTe is one of the promising altermagnetic candidates, where the band splitting, which is a key feature of altermagnetic materials, are confirmed via angle-resolved photoemission spectroscopy (ARPES) [1] and inelastic neutron scattering [2] experiments. In the next step, control of this unique property is desired. Given that in the spin configuration level the compound is antiferromagnetic, light control is a promising route in this regard.

Here, we present optical characterization of MnTe. Broadband infrared spectroscopy (down to the THz regime) and Raman spectroscopy of the compound are reported. Relevant phonon and magnon responses are identified. Results suggest that unusual optical activity is present in MnTe and provide a promising route for light-matter interactions.

[1] J. Krempaský et al., Nature 626, 517 (2024)
[2] Z. Liu et al., Phys. Rev. Lett. 133, 156702 (2024)

MA 8.11 Mon 17:45 HSZ/0002

First-principles study on piezomagnetism in altermagnet CoF_2 — •Hiroshi Katsumoto[1,2], Kunihiko Yamauchi[2], and Tamio Oguchi[2] — [1]Division of Materials and Manufacturing Science, Graduate School of Engineering, The University of Osaka, Suita, Japan — [2]Center for Spintronics Research Network, The University of Osaka, Toyonaka, Japan

Altermagnetic materials have recently attracted considerable interest due to their characteristic spin splitting in the absence of spin–orbit coupling (SOC). Among them, CoF_2 is notable not only for its altermagnetic band structure but also for its longstanding classification as a piezomagnetic material with large piezomagnetic coefficients [1]. Nevertheless, the microscopic link between its electronic structure and mechanical response has not been fully clarified. In this study, we investigate the origin of piezomagnetism in CoF_2 by means of first-principles calculations. We identify two distinct mechanisms: one driven by SOC-induced anisotropic spin–lattice coupling, and the other emerging from the SOC-independent spin splitting inherent to altermagnetism. By examining how strain influences the electronic states through these mechanisms, we gain new microscopic insights into piezomagnetism in CoF_2 and discuss implications for designing functional antiferromagnets with tailored magnetoelastic properties. This presentation was supported by JSPS KAKENHI Grand Number JP23H05457.

[1] M. Komuro *et al.*, Phys. Rev. B **111**, 214445 (2025).

MA 8.12 Mon 18:00 HSZ/0002

Influencing altermagnetic transitions by strain and layering — •Marnin Di Nunzio, Frank Lechermann, and Ilya Eremin — Institut für Theoretische Physik III, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Altermagnets are collinearly ordered magnets, that break time-reversal symmetry, with a zero magnetization, and a spin-split band structure. By employing the minimal tight-binding Hubbard-like model within mean-field and rotationally invariant slave boson (RISB) approximation we explore the effect of uniaxial strain and electronic correlations on altermagnetism in mono- and bilayer systems. We single out two configurations of bilayer stackings and examine the altermagnetic transition and the effect of doping respectively. Following the application of uniaxial strain and doping in the monolayer, we uncover a fully spin-polarized Fermi surface. In the bilayer system doping itself is sufficient to achieve a complete metallic spin-polarization.

MA 8.13 Mon 18:15 HSZ/0002

Relativistically Distinct Altermagnetic States in α-Fe_2O_3 by X-ray Spectromicroscopy — •Rikako Yamamoto[1,2], Sina Mayr[3,4], Atsushi Hariki[5], Simone Finizio[3], Eugen Weschke[6], Markus Weigand[6], Libor Šmejkal[7], Jan Kuneš[8], Claire Donnelly[1,2], and Sebastian Wintz[6] — [1]MPI-CPfS, Dresden Germany — [2]WPI-SKCM[2] Hiroshima University, Hiroshima, Japan — [3]PSI, Villigen, Switzerland — [4]ETH, Zürich, Switzerland — [5]Osaka Metropolitan University, Osaka, Japan — [6]HZB, Berlin, Germany — [7]MPI-PKS, Dresden, Germany — [8]Masaryk University, Kotlářská, Czech Republic

In this study, we demonstrate the altermagnetic nature of α-Fe_2O_3 using x-ray magnetic linear and circular dichroism (XMLD and XMCD) spectroscopy and imaging. We observed an oscillatory XMCD signal for the x-ray beam along the *c*-axis, perpendicular to the net magnetization due to canting, which originates purely from altermagnetism.

Although the XMCD signal vanishes below the Morin reorientation transition as dictated by symmetry, we show that the x-ray absorption (XAS) alone provides sufficient contrast allowing to distinguish in- and out-of-plane orientations of the Néel vector. By combining the XMCD, XMLD and XAS contrast, we map out the continuous three-dimensional variation of the Néel vector in our samples. This approach can be broadly applied to a wide range of other materials.

MA 9: Magnonics I

Time: Monday 15:00–18:30 Location: HSZ/0004

MA 9.1 Mon 15:00 HSZ/0004

Non-reciprocal phonon propagation along skyrmion strings — •Riccardo Ciola[1], Naofumi Matsuyama[2], Markus Garst[1], Lars Franke[1], Yoshimitsu Kohama[2], Toshihiro Nomura[3], Sergei Zherlitsyn[4], and Shinichiro Seki[2] — [1]Karlsruhe Institute of Technology (KIT), Germany — [2]University of Tokyo, Japan — [3]Shizuoka University, Japan — [4]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany

Non-centrosymmetric cubic chiral magnets host two-dimensional skyrmion textures that extend in the third direction, forming strings. In this work, we investigate the influence of magneto-elastic coupling on the collective excitations of the incommensurate skyrmion lattice phase. Within a microscopic theoretical framework that combines a Ginzburg-Landau description of the chiral magnet with a coupling to the underlying atomic crystal, we predict that magneto-elastic interactions give rise to a pronounced nonreciprocity in the propagation of acoustic phonons along the skyrmion strings. This directional asymmetry stems from the hybridisation between skyrmion lattice magnon modes and acoustic phonons, resulting in hybridized quasiparticles with strongly modified dispersions. Furthermore, our theory predicts the emergence of a phason gap, i.e., a gap of the translational Goldstone mode of the skyrmion lattice induced by a distortion of the atomic crystal. Altogether, our findings establish skyrmion-based topological superlattices as a theoretical platform for engineering chimeric magnon-phonon excitations, opening new directions in quasiparticle design and emergent material functionalities.

MA 9.2 Mon 15:15 HSZ/0004

Magnetically controllable phononic crystals experimentally investigated by combined μSNS-MOKE and μBLS — •Philipp Knaus, Maximilian Alexander Thiel, and Mathias Weiler — Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU Kaiserslautern, Germany

Phononic crystals (PnCs) enable tailored elastic wave propagation and bandgap formation in the GHz range [1]. We present a pillar-type PnC made of gold on a $LiNbO_3$ substrate for controlling Rayleigh surface acoustic waves (SAWs). Using broadband interdigital transducers and nanoscale patterning, we demonstrate a phononic bandgap of 50 MHz at 1.6 GHz. The dispersion relation and spatially resolved SAW fields are measured with a combined micro-focused Super-Nyquist-Sampling Magneto-Optic Kerr Effect (μSNS-MOKE) [2,3] and micro-focused Brillouin Light Scattering (μBLS) setup, providing frequency-, phase-, time-, and space-resolved detection. Measurements reveal clear suppression of SAW propagation within the bandgap and allow direct reconstruction of the dispersion relation. We additionally study the impact of magnetic field on the bandstructrue of PnCs fabricated from CoFe pillars. Paving the way for reconfigurable SAW waveguides, tunable filters, and active phononic devices.

[1] M. Sledzinska et. al, Adv. Funct. Mater. 8, 30 (2020)
[2] G. I. Stegeman, J. Appl. Phys. 49, 5624-5637 (1978)
[3] R. Dreyer, PhD Thesis, Uni Halle (2021)

MA 9.3 Mon 15:30 HSZ/0004

Coherent Magnetoelastic Phonon Generation in CMOS-Compatible Ni/Si Microstructures — •Mohammad Javad Kamali Ashtiani[1], Johan Sebastian Ramirez Amado[2], Abbas Koujok[1], Hanadi Mortada[1,2], Björn Heinz[1], Asma Mouhoub[2], Thibaut Devolder[2], Philipp Pirro[1], and Alexandre Abbass Hamadeh[2] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]Center de Nanosciences et de Nanotechnologies, CNRS, Universite Paris-Saclay, 91120, Palaiseau, France

We investigate coherent phonon generation in a CMOS-compatible device using Ni micro-striplines fabricated on Si. Due to the coherent precession of the magnetization in Ni and its significant magnetostriction, the free energy oscillates at the drive frequency. Under appropriate conditions, this leads to oscillation of elastic forces on the Si substrate, which launches a propagating surface acoustic wave (SAW). By sweeping the excitation frequency and external magnetic field, we identify resonant conditions for magnon excitation in Ni stripes, which leads to coherent phonon generation.

Under this resonant excitation (e.g., 2.35 GHz, 10 mT), we observe strong phonon emission by micro-focused Brillouin light scattering. These results demonstrate that Ni/Si microstructures provide an efficient platform for studying field-tunable magnon-phonon interactions and magnetoelastic phonon generation in non-piezoelectric media. This research was supported by ANR-25-CE24-6700-01 (SAWSiX) and the DFG through TRR-173/3-268565370 Spin+X (Project-B01).

MA 9.4 Mon 15:45 HSZ/0004

Phase-resolved imaging of coherent phonon-magnon coupling — •Yannik Kunz[1], Florian Kraft[1], Kevin Künstle[1], Matthias Küss[2], Stephan Glamsch[2], Manfred Albrecht[2], and Mathias Weiler[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU in Kaiserslautern, Germany — [2]Institute of Physics, University of Augsburg, Augsburg, Germany

The interaction between surface acoustic waves (SAWs) and spin waves (SWs) has become a major focus in magnetoacoustic research, as numerous studies have demonstrated the efficiency of SAW-driven SW excitation [1,2]. However, the coherence of the underlying magnetoelastic driving mechanism has so far only been inferred indirectly from microfocused Brillouin light scattering measurements [3].

We employ spatially resolved polarization-modulating optical detection [4] to directly visualize the resonant SAW-to-SW conversion with phase sensitivity. Hereby, $LiTaO_3$ provides a platform to excite shear-horizontal SAW modes in a magnetostrictive $Co_{40}Fe_{40}B_{20}$(5 nm) layer. Our technique enables direct imaging of the coherent driving of spin waves by surface acoustic waves, providing advanced insights into the dynamics of phonon-magnon coupling.

[1] Küß et al., Frontiers in Physics 10, 981257 (2022)
[2] Kunz et al., Phys. Rev. Appl. 24, 014043 (2025)
[3] Kunz et al., Appl. Phys. Lett. 124, 152403 (2024)
[4] Liensberger et al. IEEE Magn. Lett. 10, 5503905 (2019)

MA 9.5 Mon 16:00 HSZ/0004

Magnon-polaron control in a surface magnetoacoustic wave resonator — •Kevin Künstle[1], Yannik Kunz[1], Tarek Moussa[1], Katharina Lasinger[1,2], Kei Yamamoto[3], Philipp Pirro[1], John F. Gregg[2], Akashdeep Kamra[1], and Mathias Weiler[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, Kaiserslautern, 67663, Germany — [2]Clarendon Laboratory, Department of Physics, University of Oxford, Parks Road, Oxford, OX1 3PU, United Kingdom — [3]Advanced Science Research Center, Japan Atomic Energy Agency, Tokai, 319-1195, Japan

We demonstrate strong coupling between confined phonons and finite-wavelength magnons, forming a magnon-polaron cavity with field-tunable coupling strength [1]. Our platform combines a low-loss YIG film with a ZnO-based surface acoustic wave (SAW) resonator, enabling exceptionally low magnon-polaron dissipation rates below $\kappa/2\pi < 1.5$ MHz. The observed hybridization is accurately captured by a phenomenological model including the spatial mode profiles of SAWs and spin waves. We further observe Rabi-like oscillations in the coupled SAW spin-wave system, revealing time-domain magnon-polaron formation and establishing a platform for engineered hybrid spin-acoustic excitations.

[1] K. Künstle et al., Nat. Commun. 16, 10116 (2025)

MA 9.6 Mon 16:15 HSZ/0004

Understanding change in the sound wave frequency in a ferromagnet under magnetic field influence (Simon effect) in the low-field regime — •Ievgeniia Korniienko[1], Pablo Nieves[2], and Dominik Legut[1] — [1]IT4Innovations, VSB-TU Ostrava, Ostrava, Czech Republic — [2]University of Oviedo, Oviedo, Spain

The Simon effect exhibits itself as the dependence of the ultrasonic wave velocity in a ferromagnetic crystal under applied magnetic field and it was explained using linear theory of magnetoelasticity in 1958. However, the recent research in the interaction of surface acoustic waves with spin waves in ferromagnetic films, as well as widespread use of the pulse echo technique for the study of various materials, has renewed interest in better understanding of the Simon effect. In our work, based on the example of bcc Fe, we propose a refined formula to describe the Simon effect, which contains terms related to dispersion effects associated with the exchange stiffness. We compare our analytical solutions with other alternative computational approaches and show that dispersion effects can be significant and cannot be neglected in the low field regime. As a result, we propose a more accurate analytical formula [1], which, due to its relative simplicity, can become a convenient tool to estimate the magnitude of the magnetic field effect on the sound wave speed propagation in a cubic ferromagnetic crystal, as well as it explains observed deviations from analytically expected results in Simon effect at low magnetic field.

[1] I. Korniienko, et al.: Results in Physics, **73**, 108264 (2025).

MA 9.7 Mon 16:30 HSZ/0004

Magnon-phonon interaction in non-Bravais lattices — •Meritxell Valls Boix[1,2] and Alexander Mook[1,2] — [1]Münster University — [2]Johannes-Gutenberg Universität, Mainz

Non-Bravais lattices with a multi-band magnon spectrum can host a variety of geometrical and topological effects, such as Dirac magnons and nonzero Chern numbers. In this project, we re-examine the magnon-phonon interaction in such systems. In particular, we investigate how the quantum geometry of the magnon bands enters in the theory of magnon-phonon interactions.

15 min break

MA 9.8 Mon 17:00 HSZ/0004

All-YIG based functional magnonic crystals — •Rouven Dreyer, Bikash Das Mohapatra, Seth Kurfman, Georg Schmidt, and Georg Woltersdorf — Martin Luther University Halle-Wittenberg, Institute of Physics, 06120 Halle, Germany

For novel magnon-based applications, such as neuromorphic or reservoir computing, so far metallic ferromagnets with large saturation magnetization and high magnonic damping are the material of choice in order to locally manipulate the amplitude and phase of a propagating spin wave in an Yttrium-Iron-Garnet (YIG) layer underneath. Such YIG-metal heterostructures allow for sufficient control of band gaps in spin-wave dispersion in magnon-based Fabry-Perot-resonators or magnonic crystals [1]. In this work, we demonstrate an all-YIG based heterostructure, which imprints phase shifts and amplitude suppression on propagating waves due to the coupling of the device to the chiral spin wave. Thus, the YIG structure acts as a chiral magnonic resonator (CMR). These CMRs can be combined to realize magnonic crystals and allow for active control of individual gaps. To achieve this, the micron-sized YIG CMRs may be initialized in a different field state with respect to the YIG layer. In particular, an antiparallel magnetization alignment allows for sufficient suppression of a propagating Damon-Eshbach spin wave, as demonstrated by using spatially- and frequency-resolved SNS-MOKE [2].

[1] H. Qin et al., Nat. Commun. 12, 2293 (2021)
[2] R. Dreyer et al., PRM 5, 064411 (2021)

MA 9.9 Mon 17:15 HSZ/0004

Exchange-dominated spin waves in Ga:YIG nanowaveguides — •Andrey Voronov[1], Khrystyna Levchenko[1], Roman Verba[2], Kristyna Davidkova[1,3], Carsten Dubs[4], Michal Urbanek[5], Qi Wang[6], Dieter Suess[1], Claas Abert[1], and Andrii Chumak[1] — [1]Faculty of Physics, University of Vienna, Vienna, Austria — [2]V.G. Baryakhtar Institute of Magnetism of the NAS of Ukraine, Kyiv, Ukraine — [3]Vienna Doctoral School of Physics, University of Vienna, Vienna, Austria — [4]INNOVENT e.V. Technologieentwicklung, Jena, Germany — [5]CEITEC BUT, Brno University of Technology, Brno, Czech Republic — [6]Huazhong University of Science and Technology, Wuhan, China

Spin-wave computing offers a path beyond CMOS scaling, but miniaturization to the 100 nm regime limits long-distance spin-wave transport. Gallium-substituted YIG (Ga:YIG) addresses this challenge through its reduced saturation magnetization, enabling excitation of exchange-dominated spin waves with superior transport properties. We report a combined experimental and theoretical study of spin-wave propagation in Ga:YIG waveguides down to 145 nm width and 73 nm thickness. Using micro-focused Brillouin light scattering, TetraX sim- ulations, and analytical dispersion modeling, we show that Ga:YIG supports spin waves with group velocities up to 600 m/s, largely independent of waveguide width, resulting in enhanced propagation lengths compared to pure YIG. These results demonstrate that gallium substitution enables faster and longer-lived spin waves, establishing Ga:YIG as a promising platform for nanoscale magnonic devices.

MA 9.10 Mon 17:30 HSZ/0004

Spin Hall micro-bars: Near zero effective magnetization for low oscillation-onset thresholds — •Abbas Koujok[1], Hidekazu Kurebayashi[2], kei Yamamoto[3], Björn Heinz[1], Abbass Hamadeh[4], Takeshi Seki[5], and Philipp Pirro[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, Kaiserslautern, Germany — [2]London Centre for Nanotechnology, University College London, London, United Kingdom — [3]Advanced Science Research Center, Japan Atomic Energy Agency, Tokai, Japan — [4]Centre de Nanosciences et de Nanotechnologies, CNRS, Université Paris-Saclay, Palaiseau, France — [5]Institute for Materials Research, Tohoku University, Sendai, Japan

Spin Hall devices, being promising building blocks in magnonic circuitry, are progressively being researched in the context of lowering required driving charge currents. Here, the impact of near zero effective magnetization on reducing oscillation-onset threshold in magnetic spin Hall micro-bars is studied using micro-focused Brillouin light scattering spectroscopy. We show that a threshold current density reduction of more than two orders of magnitude can be achieved in comparison to the lowest reported values from other studies in this regard. This reduction shows that controlling the effective magnetization can pave the way to employ spin Hall based devices as energy efficient elements in magnonic circuitry.

MA 9.11 Mon 17:45 HSZ/0004

Pinch points in the dynamical spin structure factor of dipolar ferromagnets — Michal Stekiel[1], Christoph Resch[2], •Konrad Scharff[3], Markus Garst[3], and Christian Pfleiderer[2] — [1]Jülich Center for Neutron Science at MLZ, Jülich, Germany — [2]School of Natural Sciences, Technical University Munich, Garching, Germany — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany

The long-range dipolar interaction gives rise to a pinch-point non-analyticity in the dynamical spin structure factor of a ferromagnet [1]. Its experimental observation is challenging because the strength of the pinch-point singularity at zero magnetic field scales both with the magnetic moment and the size of the easy-plane anisotropy. We demonstrate that suitable materials for its detection are the rare-earth diborides, ErB2 and HoB2, as they possess a large magnetic moment on the order of 10 Bohr magneton and a pronounced easy-plane anisotropy two orders of magnitude larger than their direct exchange. In both materials, we were able to resolve pinch-point singularities in energy-momentum space using inelastic neutron scattering. The experimental signatures are quantitatively reproduced by a Heisenberg model with exchange, anisotropy and dipolar interaction.

[1] Jensen, J. and Mackintosh, A.R. Rare Earth Magnetism. Clarendon Press - Oxford (1991)

MA 9.12 Mon 18:00 HSZ/0004

Spin-wave emission with current-controlled frequency by a PMA-based spin-Hall oscillator — •Moritz Bechberger[1], David Breitbach[1], Abbas Koujok[1], Björn Heinz[1], Carsten Dubs[2], Abbass Hamadeh[3], and Philipp Pirro[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, D-67663 Kaiserslautern, Germany — [2]INNOVENT e.V. Technologieentwicklung, D-07745 Jena, Germany — [3]Université Paris-Saclay, Centre de Nanosciences et de Nanotechnologies, CNRS, 91120, Palaiseau, France

Spin-Hall oscillators (SHOs) are of particular interest for neuromorphic computing, as they are able to synchronize via spin waves. We demonstrate a SHO based on low-damping gallium-substituted yttrium-iron-garnet (Ga:YIG) with perpendicular magnetic anisotropy (PMA). In-plane magnetized Ga:YIG allows for the operation at a high efficiency level while also enabling resonant spin-wave emission by exploiting the positive nonlinear frequency shift. Via micro-focused Brillouin light scattering spectroscopy, we investigate the properties of auto-oscillation and emission. Multiple modes are excited and compete internally, with two emitted modes detected up to distances larger than 10 μm. Their frequencies combine to an extended bandwidth of approximately 1.6 GHz. The observed two-mode system and its transition to a single mode at higher currents are reproduced via micromagnetic simulations, which account for spatial variation of the PMA arising due to the microstructures on Ga:YIG. Our results propose a promising platform for SHOs with long-range coupling via spin waves.

MA 9.13 Mon 18:15 HSZ/0004

Dispersion-tunable low-loss implanted spin-wave waveguides — •Jannis Bensmann[1], Robert Schmidt[1], Kirill O. Nikolaev[3], Dmitrii Raskhodchikov[1,2], Shraddha Choudhary[1], Richa Bhardwaj[1], Shabnam Teheriniya[1,2,4], Akhil Varri[1,2], Sven Niehues[1], Ahmad El Kadri[1], Johannes Kern[1], Wolfram H. P. Pernice[1,2,4], Sergej O. Demokritov[3], Vladislav E. Demidov[3], Steffen Michaelis de Vasconcellos[1], and Rudolf Bratschitsch[1] — [1]University of Münster, Institute of Physics and Center for Nanotechnology, Münster, Germany — [2]University of Münster, Center for Soft Nanoscience, Münster, Germany — [3]University of Münster, Institute of Applied Physics, Münster, Germany — [4]Heidelberg University, Kirchhoff-Institute for Physics, Heidelberg, Germany

Spin waves offer a promising pathway toward energy-efficient information processing. Here, we present an etchless fabrication method for low-loss spin-wave waveguides in thin yttrium iron garnet (YIG) films using maskless silicon ion implantation. Focused Si-ion irradiation locally amorphizes YIG to create a low-magnetization cladding, effectively confining spin waves while preserving the pristine magnetic properties of the waveguide core. Spin-wave propagation is directly imaged via Faraday rotation microscopy, revealing decay lengths exceeding 100 μm even for submicron waveguides. By tuning the implantation dose and waveguide width, we achieve precise dispersion control. Our approach enables large spin-wave networks, offering a promising route toward magnonic integrated circuits.

MA 10: INNOMAG e.V. Prizes 2026 (Diplom-/Master and Ph.D. Thesis)

Die Arbeitsgemeinschaft Magnetismus der DPG hat einen Dissertationspreis und einen Diplom-/Masterpreis ausgeschrieben, welche auf der Tagung der DPG 2026 in Dresden vergeben werden. Ziel der Preise ist die Anerkennung herausragender Forschung im Rahmen einer Diplom-/Masterarbeit beziehungsweise einer Promotion und deren exzellente Vermittlung in Wort und Schrift. Im Rahmen dieser Sitzung tragen die besten der für ihre an der Hochschule eines Mitgliedslands der European Physical Society durchgeführten Diplom-/Masterarbeit beziehungsweise Dissertation Nominierten vor. Im direkten Anschluss entscheidet das Preiskomitee über den Gewinner bzw. die Gewinnerin des INNOMAG e.V. Diplom/Master-Preises und des Dissertationspreises 2026. Talks will be given in English!

Time: Monday 15:00–18:05 Location: POT/0112

Invited Talk MA 10.1 Mon 15:00 POT/0112

Multi-field analysis of magnetic materials: Phase-field based simulations of magnetic domains and phase transition — •Mobina Alaeddini, Jörg Schröder, and Maximilian Vorwerk — Institut für Mechanik, Universität Duisburg-Essen, Essen, Deutschland

Rising global temperatures have triggered research into novel, efficient, and sustainable alternatives to conventional cooling technologies to tackle the rapidly increasing demand for air conditioning and the resulting strain on energy resources. Among these, novel cooling technologies exploit the magnetocaloric effect, in which the application of magnetic fields induces reversible thermal responses suitable for cooling. Despite its technological relevance, a comprehensive description of the coupled magnetocaloric behavior requires advanced modeling approaches. Current research focuses on understanding and optimizing the magnetocaloric response of materials such as Heusler alloys, which are among the most promising candidates for solid-state cooling. To investigate these effects in a controlled and quantitative manner, a multi-field variational phase-field framework based on finite elements is employed. The formulation relies on the time-dependent Ginzburg-Landau equation and incorporates magnetic, mechanical, and thermal contributions within a unified free-energy description governing the transformation from paramagnetic austenite to ferromagnetic martensite. This approach enables a detailed analysis of the coupled magnetic and structural evolution and provides a predictive framework for magnetocaloric material design.

Invited Talk MA 10.2 Mon 15:20 POT/0112

Realistic Modelling of Finite Temperature Electron Transport Properties in Ferromagnets — •Fabian Engelke and Christian Heiliger — Justus Liebig University Giessen, Germany

The quantitative description of the electrical resistivity of a magnetic material remains challenging to this day. While prior publications reached good agreement with experiment in the so-called supercell or direct approach for non-magnetic materials where the spin-disorder contribution to the resistivity is negligible, an accurate, purely theoretical description of magnetic materials remains elusive. This shortcoming can be attributed to the missing accuracy in the description of the temperature-dependent spin-disorder itself. Considering the example of bcc-Fe, we demonstrate that the inclusion of quantum mechanical effects by semiclassical local quantization of the Heisenberg model significantly improves the description of the spin-disorder component to the electrical resistivity. Compared to previous approaches, this model includes the description of magnetic short-range order effects, enabling us to study temperature effects around and above the Curie temperature, where prior mean-field theory-based approaches inevitably predicted a constant contribution. Furthermore, by analyzing the spin-resolved conductivity tensor, we extend our investigation beyond resistivity to determine the spin-flip diffusion length in bcc-iron.

15 min break

Invited Talk MA 10.3 Mon 15:55 POT/0112

Exploring magneto- and multicaloric materials for room and cryogenic temperature applications — •Benedikt Beckmann — Institute of Materials Science, Technical University of Darmstadt, Darmstadt, Germany

A sustainable future requires energy-efficient and environmentally friendly cooling technologies. This thesis investigates Ni(-Co)-Mn-Ti Heusler alloys [1,2,3], Fe_2AlB_2-type MAB phases [4], $La(Fe,Si)_{13}$-type compounds [5], and $Co_4(OH)_6(SO_4)_2[enH_2]$ [6] for magneto- and multicaloric cooling at room and cryogenic temperatures. At room temperature, optimized Ni(-Co)-Mn-Ti Heusler alloys show large isothermal entropy and adiabatic temperature changes but are limited by hysteresis [1,2], motivating the work on hysteresis-free, low-cost MAB phases [4]. At cryogenic temperatures, universal hysteresis limitations of first-order phase transition materials are revealed for caloric hydrogen liquefaction [3,5], driving follow-up studies [7]. Following these discoveries, the novel second-order material $Co_4(OH)_6(SO_4)_2[enH_2]$ shows record performance among rare-earth-free materials [6], highlighting the potential of transition-metal-based hydrogen liquefaction.

[1] A. Taubel, **B. Beckmann** *et al.*, Acta Mater. 201 (2021), [2] **B. Beckmann** *et al.*, Acta Mater. 282 (2025), [3] **B. Beckmann** *et al.*, Acta Mater. 246 (2023), [4] **B. Beckmann** *et al.*, J. Appl. Phys. 133 (2023), [5] **B. Beckmann** *et al.*, ACS Appl. Mater. Interfaces 16, (2024), [6] J.J.B. Levinsky, **B. Beckmann** *et al.*, Nat. Commun. 15 (2024), [7] T. Niehoff, **B. Beckmann** *et al.*, Adv. Funct. Mater. 2505704 (2025)

Invited Talk MA 10.4 Mon 16:20 POT/0112

Nonlinear magnon dynamics: From the discovery of Floquet magnons to CMOS-compatible magnon computing — •Christopher Heins — Helmholtz-Zentrum Dresden-Rossendorf, Institute for Ion Beam Physics and Materials Research, Dresden, Germany

Magnetic vortices are prominent examples for topology in magnetism with a rich set of dynamic properties. They exhibit an intricate magnon spectrum and show a special eigen-resonance of the vortex texture itself, the gyroscopic motion of the vortex core. While there has been studies about magnon assisted reversal of the vortex core polarity, the impact of the vortex core motion on the magnon spectrum wasn't addressed so far. Both excitation types are clearly separated by one order of magnitude in their resonance frequencies, where magnons are in the lower GHz range and the vortex typically gyrates at a few hundred MHz. This clear separation allows for experiments studying the temporal evolution of the magnon spectrum when the motion of the vortex core is driven by an external stimulus. We present experimental and numerical studies on how the magnon eigenstates are transformed into Floquet bands, when the vortex ground state is periodically modulated in time by the gyroscopic motion of the vortex core [1]. The existence of the Floquet bands is evidenced by the appearance of magnon frequency combs, where the comb spacing is determined by the frequency of the gyroscopic motion. References: [1] C. Heins, et al., arXiv:2409.02583, accepted with Science

Invited Talk MA 10.5 Mon 16:45 POT/0112

The geometric memory of quantum wave functions — •Niclas Heinsdorf — Max Planck Institut für Festkörperforschung

Altermagnets are a newly identified type of collinear antiferromagnetism with vanishing net magnetic moment, characterized by lifted Kramers degeneracy in parts of the Brillouin zone. Their time-reversal symmetry-broken band structure has been observed experimentally and is theoretically well understood. On the contrary, altermagnetic fluctuations and the formation of the corresponding instabilities remain largely unexplored. We establish a correspondence between the quantum metric of normal and the altermagnetic spin-splitting of ordered phases. We analytically derive a criterion for the formation of instabilities and show that the quantum metric favors altermagnetism. We recover the expression for conventional q=0 instabilities where the spin-splitting terms of the normal-state model are locally absent. As an example, we construct an effective model of MnTe and illustrate the relationship between quantum geometry and altermagnetic fluctuations by explicitly computing the quantum metric and the generalized magnetic susceptibility.

Invited Talk MA 10.6 Mon 17:10 POT/0112

Altermagnets and Odd-parity-wave Magnets — •Anna Birk Hellenes — Institute of Physics of the Czech Academy of Sciences

The discovery of altermagnets was enabled by an unorthodox symmetry framework, spin groups, allowing to classify all collinear magnetic orders [1]. This raises the questions of whether (i) altermagnetism can be verified experimentally, (ii) new magnets with unknown symmetries can be realized, and (iii) whether they can be useful for spintronics.

In my thesis, I have contributed to answering these questions affirmatively. In this talk, I will review altermagnetic symmetries [1], present our theory-experiment verification of altermagnetism [2-4], and show that it enables spintronics phenomena such as giant magnetoresistance effects [5]. I will then discuss our theoretical prediction that odd-parity-wave magnetism arises in noncentrosymmetric, noncollinear magnets with a combined translation and time-reversal symmetry [6]. Contrary to common assumptions, they host non-relativistic spin-split electronic bands while preserving time-reversal symmetry:

unlike ferromagnets and altermagnets, which break it. Our work opens broad opportunities for exploring altermagnets and odd-parity-wave magnets with potential applications including giant magnetoresistance [5], transport anisotropy [6], and Edelstein [7] effects.

[1] Šmejkal et al. PRX 12, 031042 (2022), [2] Nature 626, 517-522 (2024), [3] Nat. Comm. 15, 2116 (2024), [4] arXiv:2511.01690, [5] Šmejkal, ABH & Jungwirth et al. PRX 12, 011028 (2022), [6] ABH & Šmejkal et al. arXiv:2309.01607, [7] Chakraborty, ABH & Sinova et al. arXiv:2411.16378.

30 min. discussion break and bestowal of INNOMAG e.V. Diplom-/Master Prize and Ph.D. Thesis Prize

MA 11: Electron Theory of Magnetism and Correlations (joint session MA/TT)

Time: Monday 15:00–18:00 Location: POT/0151

MA 11.1 Mon 15:00 POT/0151

Origin of pressure-induced anomalies in the nodal-line ferrimagnet $Mn_3Si_2Te_6$ — Varun Venkatasubramanian[1], Makoto Shimizu[2], •Daniel Guterding[3], and Harald O. Jeschke[1] — [1]Research Institute for Interdisciplinary Science, Okayama University, Okayama, Japan — [2]Department of Physics, Graduate School of Science, Kyoto University, Kyoto, Japan — [3]Technische Hochschule Brandenburg, Brandenburg an der Havel, Germany

The nodal-line ferrimagnet $Mn_3Si_2Te_6$ exhibits a pressure-induced insulator-to-metal transition (IMT), which coincides with pronounced anomalies in its magnetic ordering temperature and anomalous Hall conductivity. We employ density functional theory (DFT) in combination with classical Monte Carlo simulations to elucidate the origin of these effects. Pressure-dependent Heisenberg Hamiltonians extracted from DFT reveal a strong evolution of exchange couplings across the structural transition from the trigonal to the monoclinic phase, producing a dome-shaped variation of the ferrimagnetic ordering temperature in quantitative agreement with experiment. While our simulations capture the pressure-driven IMT and magnetic evolution, the anomalous Hall response cannot be fully explained by intrinsic Berry curvature effects, indicating additional extrinsic contributions.

[1] V. Venkatasubramanian, M. Shimizu, D. Guterding, and H. O. Jeschke, *Origin of pressure-induced anomalies in the nodal-line ferrimagnet $Mn_3Si_2Te_6$*, arXiv:2509.18238

MA 11.2 Mon 15:15 POT/0151

Near Room-Temperature Ferromagnetism and Insulator-Metal Transition in van der Waals Material $CrGeTe_3$ — Daniel Guterding[1], Jihaan Ebad-Allah[2], Gili Scharf[3], Han-Xiang Xu[4], Makoto Shimizu[5], Junya Otsuki[6], Alon Ron[3], Christine Kuntscher[2], and •Harald O. Jeschke[6] — [1]Technische Hochschule Brandenburg, Brandenburg an der Havel, Germany — [2]Augsburg University, Augsburg, Germany — [3]Tel Aviv University, Tel Aviv, Israel — [4]Chinese Academy of Sciences, Beijing, China — [5]Kyoto University, Kyoto, Japan — [6]Research Institute for Interdisciplinary Science, Okayama University, Okayama, Japan

We investigate how pressure tunes the electronic and magnetic properties of the van der Waals ferromagnet $CrGeTe_3$, a promising material for near room-temperature applications. Using DFT+DMFT, we trace the transition from semiconducting to metallic ferromagnet [1]. Optical conductivity reveals a mid-infrared feature, signalling orbital-selective correlations, while a double-exchange mechanism stabilizes high-temperature ferromagnetism [2]. The anomalous Hall effect shows extrinsic behaviour beyond pure Berry curvature effects [3]. These results highlight the interplay of magnetism and electronic correlations in achieving tunable ferromagnetism in $CrGeTe_3$, suggesting that pressure and charge carrier doping offer promising routes to control magnetism and transport in layered materials.

[1] H.-X. Xu *et al.*, Phys. Rev. B **108**, 125142 (2023)
[2] J. Ebad-Allah *et al.*, Phys. Rev. B **111**, L140402 (2025)
[3] G. Scharf *et al.*, Phys. Rev. Res. **7**, 013127 (2025)

MA 11.3 Mon 15:30 POT/0151

Ground State of the Topological Insulator Candidate Eu_2AuGe_3 — •Vinicius Estevo Silva Frehse[1], Aleksandr Sukhanov[1], Artem Korshunov[2], Eugen Weschke[3], Aly Abdeldaim[4], Priscila Rosa[5], and Marein Rahn[1] — [1]Universität Augsburg, Augsburg, Germany — [2]Donostia International Physics Center, San Sebastián, Spain — [3]Helmholz Zentrum Berlin, Berlin, Germany — [4]Diamond Light Source, Didcot, UK — [5]Los Alamos National Laboratory, Los Alamos, USA

Eu_2AuGe_3 is an unusual rare earth germanide in which quasi-trigonal europium sheets are interleaved with Au-Ge honeycomb layers, where high-throughput calculations indicate potential for topological band inversions. Bulk and transport data have revealed a series of (re-)ordering transitions upon cooling, as well as metamagnetic transitions at low temperature. Recently, we identified a broad transition around T_{CDW} = 130 K as the continuous freezing-out of a buckling mode of the honeycomb layers.

Here, we present preliminary evidence from neutron and resonant elastic X-ray scattering, which hints at helical magnetic order below T_N = 11 K. Unexpectedly for the nominally spin-only divalent europium, the magnetic order also appears to be accompanied by a modulated orbital order parameter. This phase is preceded by a transition at 23 K, where we observe a subtle doubling of the *ab*-plane, possibly related to the charge density wave formed during T_{CDW}.

MA 11.4 Mon 15:45 POT/0151

Electronic structure, magnetic and optical properties of antiferromagnetic 3*d*-oxides from a Wannier-localized optimally-tuned screened range-separated hybrid functional — •Alexander Shick[1,2], Guy Ohad[2], Jeffrey Neaton[3,4], and Leeor Kronik[2] — [1]FZU-Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [2]Weizmann Institute of Science, Rehovoth, Israel — [3]University of California, Berkeley, USA — [4]Lawrence Berkeley National Laboratory, Berkeley, USA

We apply the recently developed Wannier-localized, optimally tuned, screened range-separated hybrid (WOT-SRSH) functional to prototypical bulk antiferromagnetic insulators — MnO, NiO, and hematite (Fe_2O_3). Comparison to calculations based on well-established functionals, namely PBE0, and HSE06, as well as to self-consistent quasiparticle GW and dynamic mean field theory calculations, and to experiment, shows that the WOT-SRSH functional provides a good quantitative description of band gaps, spin magnetic moments, photoemission, and optical absorption spectra. This establishes WOT-SRSH as a uniform, non-empirical framework for band theory of electronic, magnetic, and optical properties of magnetic insulators.

MA 11.5 Mon 16:00 POT/0151

Spectroscopic evidence of Kondo resonance in 3*d* van der Waals ferromagnets — •Deepali Sharma[1,2], Neeraj Bhatt[1], Asif Ali[1], Rajeswari Roy Chowdhury[1], Chandan Patra[1], Ravi Prakash Singh[1], and Ravi Shankar Singh[1] — [1]IISER Bhopal, Bhopal, India — [2]TU Dortmund, Dortmund, Germany

Two-dimensional van der Waals (vdW) ferromagnets drive the advancement in spintronic applications and enable the exploration of exotic magnetism in low-dimensional systems. The entanglement of the dual–localized and itinerant–nature of electrons lies at the heart of the correlated electron systems giving rise to exotic ground state properties such as complex magnetism, heavy fermionic behavior, Kondo lattice formation, etc. Through temperature-dependent electronic structure of vdW ferromagnets, Co substituted Fe_3GeTe_2, probed using high-resolution photoemission spectroscopy and density functional theory combined with dynamical mean field theory (DFT + DMFT), we provide direct evidence of the emergence of Kondo resonance peak driven by complex interplay between localized and itinerant electrons. Further, in overall agreement with the experimental electronic structure and magnetic properties, DFT + DMFT also reveals non-Stoner magnetism. The findings provide a way forward to the understanding of complex interplay between electronic structure, exotic magnetism, and heavy fermionic behavior leading to the Kondo scenario in 3*d* vdW ferromagnets.

MA 11.6 Mon 16:15 POT/0151

T-linear and quadratic transport across the Cuprate and Nickelate phase diagram : pseudogap, strange-metal and Fermi-liquid — •Dongwook Kim[1], Motoharu Kitatani[2], Juraj Krsnik[3], and Karsten Held[4] — [1]Wiedner Hauptstraße 8-10, 1040 Wien — [2]3-2-1 Koto, Kamigori-cho, Ako-gun, Hyogo 678-1297, Japan — [3]Trg Republike Hrvatske 14. HR-10000 Zagreb Croatia — [4]Wiedner Hauptstraße 8-10, 1040 Wien

We investigate DC resistivity and nodal quasiparticle (QP) scattering in hole-doped cuprates-nickelate type superconductors by ladder dynamical vertex approximation (LDΓA). In the pseudogap regime of doping δ = 0.1-0.175, we observe a crossover from T-linear to T^2 resistivity at low T. For dopings δ = 0.2-0.25, the resistivity remains fully T-linear down to the lowest temperatures, indicating strange-metal behavior associated with a nearby quantum critical point (QCP). At higher doping of δ = 0.3 the T^2 recovery reappears, signaling exit from the quantum-critical regime. The nodal QP scattering rate and the first-Matsubara-frequency rule analysis independently confirm the same FL*NFL crossover, providing consistent support for the T-dependent transport obtained within LDΓA

15 min break

MA 11.7 Mon 16:45 POT/0151

Toward ab-initio simulation for resonant inelastic X-ray scattering in strongly correlated materials — •Yun Yen[1,2], Matthias Krack[2], and Michael Schüler[2,3] — [1]Institute for Theoretical Physics, Bremen Center for Computational Materials Science, University of Bremen, Bremen, Germany — [2]PSI Center for Scientific Computing, Theory and Data, Villigen PSI, Switzerland — [3]Department of Physics, University of Fribourg, Fribourg, Switzerland

X-ray absorption spectroscopy (XAS) and resonant inelastic X-ray scattering (RIXS) can be used to study low-energy excitations in complex materials, which are challenging to interpret due to strong correlations during the photoexcitation processes. We aim to develop ab-initio methods for XAS and RIXS, by constructing Anderson impurity models using Wannier-based tight-binding parameters and constrained random phase approximation. The spectrums are then computed via exact diagonalization and Krylov subspace methods. We will show a benchmark on spin spiral materials, where the d-d excitation intensity dependence can be related to the onset of magnetic order with the support of our methods.

MA 11.8 Mon 17:00 POT/0151

Magnetic Persistence in PrAlGe via RIXS and XAS modeling — •Juan Felipe Pulgarin Mosquera[1,2], Yun Yen[3], Tianlun Yu[4], Yeong-Ah Soh[4], Thorsten Schmitt[4], and Michael Schueler[1,2] — [1]PSI Center for Scientific Computing, Theory and Data, Villigen PSI, Switzerland — [2]University of Fribourg, Department of Physics, University of Fribourg, Fribourg , Switzerland — [3]Institute for Theoretical Physics and Bremen Center for Computational Materials Science, University of Bremen, Bremen, Germany — [4]PSI Center for Photon Sciences, Villigen-PSI, Switzerland

The interplay between topological electronic states and magnetism is in the spotlight of condensed matter for potential applications. PrAlGe is a prime candidate in this context, with several works reporting it as a magnetic Weyl semimetal. However, the microscopic relationship between the magnetic ordering, anomalous Hall effect and local spectroscopic signatures remains an open question. We study this phenomenon based on a combination of X-ray spectroscopy and first-principle calculations. We present our ab-initio approach to computing X-ray absorption spectroscopy and resonant inelastic X-ray scattering based on accurate Anderson Impurity model derived from density-functional theory with Hubbard corrections. This comparison is crucial for understanding the experimental finding that the ferromagnetic transition occurs at $T_c \sim 16$ K, significantly lower than the temperature scale at which the AHE and circular dichroism vanish $T_{AHE} \sim 35$ K). The survival of circular dichroism above T_c serves as a local probe for the persistence of local magnetic moments.

MA 11.9 Mon 17:15 POT/0151

Ab initio spin Hamiltonians and magnetism of Ce and Yb triangular-lattice compounds — Leonid V. Pourovskii[1,2], •Rafael D. Soares[3], and Alexander Wietek[3] — [1]CPHT, CNRS, École polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France — [2]Collège de France, Université PSL, 11 place Marcelin Berthelot, 75005 Paris, France — [3]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany

We calculate the crystal-field splitting, ground-state Kramers doublet and intersite exchange interactions within the ground-state doublet manifold for a representative set of Ce and Yb triangular-lattice compounds. These include the putative quantum spin liquids (QSL) $RbCeO_2$ and $YbZn_2GaO_5$ and the antiferromagnets $KCeO_2$ and $KCeS_2$. The calculated nearest-neighbor (NN) couplings are antiferromagnetic and exhibit noticeable anisotropy. The next-nearest-neighbor (NNN) couplings are ferromagnetic in the Ce systems and dominated by classical dipole–dipole interactions in the Yb case. Solving the resulting effective spin-1/2 models by exact diagonalization up to $N = 36$ sites, we predict ordered magnetic ground states for all systems, including the two QSL candidates. We explore the phase space of an anisotropic NN + isotropic NNN triangular-lattice model finding that a significant antiferromagnetic NNN coupling is required to stabilize QSL phases, while the NN exchange anisotropy is detrimental to them. Our findings highlight a possibly important role of deviations from the perfect triangular model in real materials.

MA 11.10 Mon 17:30 POT/0151

Transition metal dihalides: from band structure to magnetic properties — •Alexander Yaresko[1], Sebastien Hadjadj[2], and Maxim Ilyn[2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Centro de Física de Materiales, Donostia-San Sebastián, Spain

Transition metal dihalides TX_2 (T=Fe, Ni, X=Cl, Br) have recently attracted attention because of successful growth of monolayer-thick TX_2 films on various substrates, such as Au or $NbSe_2$, allowing to study 2D magnetism. We compare results of band structure calculations for bulk and monolayer FeX_2 and NiX_2. By mapping the total energies calculated for helical spin structures with various q to the Heisenberg model we show that the change of magnetic order within a layer from ferro- in $NiCl_2$ to helimagnetic in $NiBr_2$ can be explained by the increased strength of antiferromagnetic (AF) 3-rd neighbor exchange interaction J_3 which competes with FM nearest neighbor J_1. We found that inter-layer coupling J_{2c} stabilizes FM order within a layer. Thus, one can expect stronger tendency to a helimagnetic state in a NiX_2 monolayer.

In contrast to NiX_2, J_1 estimated from LDA+U spin-spiral calculations for FeX_2 is weak but shows substantial dependence on the strength of the Coulomb repulsion U. In agreement with experimental findings, calculations including spin-orbit coupling result in appreciable easy axis anisotropy with Fe magnetic moments normal to layers.

We also discuss various microscopic contributions to intra- and inter-layer exchange interactions.

MA 11.11 Mon 17:45 POT/0151

Coexistence of charge order and antiferromagnetism in three-dimensional Hubbard-Holstein model: A study (exploring phases) at and away from half-filling — •Sandip Halder and Moshe Schechter — Ben-Gurion University of the Negev, Beer-Sheva, Israel

The physics of correlated electron systems has long been explored through the Hubbard model and its extensions, including models with long-range hopping. Likewise, phenomena arising from electron-phonon coupling- such as charge order and superconductivity- have been extensively studied within the Holstein model, though largely in lower dimensions. In transition-metal oxides, however, both electron correlations (U) and electron-phonon coupling (V) coexist intrinsically, motivating a comprehensive study of the Hubbard-Holstein model in three dimensions.

Using an exact diagonalization-based semi-classical Monte Carlo (s-MC) method, we investigate the intriguing properties of this model. At half-filling, the system undergoes a first-order transition between a charge-ordered (CO) phase and an antiferromagnetic (AF) phase as U and V are varied. In the AF regime, near the phase boundary, hole doping drives the system from the AF state (n=1) to a CO state (n=0.5), and eventually to a disordered phase at low densities. Notably, a robust coexistence of AF and CO emerges around x=0.35 (n=0.65), with T_{CO} exceeding T_N, consistent with experiments on $La_{2-x}Sr_xNiO_4$. The study provides new insight into correlated materials and guiding future experimental explorations.

MA 12: Terahertz Spintronics

Time: Monday 15:00–16:30 Location: POT/0351

MA 12.1 Mon 15:00 POT/0351

Interface Modification of Spintronic THz emitters — •David Stein[1], Krishna Rani Sahoo[2], Alexander Heise[1], Stephan Glamsch[1], Jannis Bensmann[2], Robert Schmidt[2], Steffen Michaelis de Vasconcellos[2], Rudolf Bratschitsch[2], and Manfred Albrecht[1] — [1]Universität Augsburg, Augsburg, Germany — [2]Universität Münster, Münster, Germany

The spintronic Terahertz (THz) emission of thin magnetic/heavy metal bilayers with fs laser excitation is an excellent alternative to the well-known bulk nonlinear crystals. Many works have been published about different material combinations of spintronic emitters, but the properties of the bilayer interface and its influence on the THz emission is not well understood. We study Fe/Pt interfaces, which were modified by implantation with foreign atoms to investigate the influence of the interface on the THz emission. THz-Time Domain Spectroscopy and SQUID-VSM Magnetometry, as well as high-resolution Scanning Transmission Electron Microscopy (STEM) with Energy Dispersive X-Ray Spectroscopy (EDS) were performed to understand the effects of the modifications.

MA 12.2 Mon 15:15 POT/0351

Lightwave-driven spintronics by coherent breaking of time-reversal symmetry — •Philipp Weissenberger[1], Josef Riepl[1], Adrian Seith[1], Michael Aschenbrenner[1], Josef Freudenstein[1], Omer Kneller[1], Daniel Riese[1], Manuel Meierhofer[1], Konstantin Kokh[2], Oleg Tereshchenko[2], Jörg Wunderlich[1], Ulrich Höfer[1], Ferdinand Evers[1], Jan Wilhelm[1], and Rupert Huber[1] — [1]University of Regensburg, Germany — [2]Novosibirsk, Russia

Lightwave electronics has the potential to revolutionize high-speed information technology by using the carrier field of light to steer electrons at optical clock rates. Yet, expanding this subcycle control scheme to the spin, one of the most important quantum attributes, has remained a challenge. Additionally, time-reversal symmetry (TRS) prohibits a net spin polarization in non-magnetic solids, limiting ultrafast spintronics to magnetic systems with intrinsically broken TRS. Here, we transcend these boundaries by leveraging intense, phase-stable terahertz (THz) pulses to accelerate Dirac fermions in the topological state of Bi2Te3. Due to spin-momentum locking, the THz field drives ballistic, spin-

polarized currents. The nonequilibrium occupation coherently breaks TRS and leads to a net surface magnetization. Our all-optical measurements show that these dynamics follow the driving vector potential, proving their dissipationless nature and our magnetic switching abilities. Astonishingly, the data reveals an anisotropic coupling to higher-lying topological states. Our scheme could be transferred to a host of non-magnetic systems and boost ultrafast magnetic metrology.

MA 12.3 Mon 15:30 POT/0351

Spin Inertia as a Source of Topological Magnons — •Subhadip Ghosh[1], Mikhail Cherkasskii[2], Ritwik Mondal[1], Alexander Mook[3], and Levente Rozsa[4] — [1]IIT (ISM) Dhanbad, India. — [2]RWTH Aachen University, Germany. — [3]University of Munster, Germany — [4]BME, Budapest, Hungary

Ferromagnets exhibit not only the familiar precessional magnon bands, but also high-frequency nutational modes originating from spin inertia [1]. In this work, we show that the hybridization between these nutational and precessional branches opens a magnonic gap whose topology can become nontrivial. In a honeycomb ferromagnet, this topological phase is caused by the pseudodipolar coupling, which not only gaps out the well-known precessional Dirac cones [2,3] but also causes precessional and nutational modes to anticross. By computing the Chern numbers of the full magnon spectrum, we demonstrate that the nutational-precessional gap can host chiral, topologically protected edge states. We highlight the role of spin inertia as a source of topological magnonic phenomena.

[1] R. Mondal *et al.*, Phys. Rev. B 106, 134422 (2022). [2] A. Mook *et al.*, Phys. Rev. B. 90, 024412 (2014). [3] X. S. Wang *et al.*, Phys. Rev. Appl. 9, 024029 (2018).

MA 12.4 Mon 15:45 POT/0351

THz light field driven unidirectional spin Hall magnetoresistance in magnetic heterostructures — •Sergey Kovalev[1], Ruslan Salikhov[2], Igor Ilyakov[2], Anneke Reinold[1], Jan Deinert[2], Thales Oliveira[2], Alexey Ponomaryov[2], Gulloo Prajapati[2], Patrick Pilch[1], Ahmed Ghalgaoui[1], Steffen Kober[1], Jürgen Fassbender[2], Jürgen Lindner[2], and Zhe Wang[1] — [1]Technische Universität Dortmund, Dortmund, Germany — [2]Helmholtz Zentrum Dresden Rossendorf, Dresden, Germany

We demonstrate unidirectional spin Hall magnetoresistance (USMR) in magnetic heterostructures driven by terahertz (THz) light electric fields [1]. To isolate USMR from other spin transport phenomena, we performed anisotropy characterization of spintronic THz second-harmonic generation as a function of sample magnetization and THz pump polarization states. By investigating the temperature dependence of THz-driven USMR, we reveal distinct contributions to USMR dynamics on picosecond time scales. Our approach enables the characterization of ultrafast, field-driven spin-related magnetoresistance in free-standing heterostructures without the need for lithographic processing.

[1] R. Salikhov et al., "Ultrafast unidirectional spin Hall magnetoresistance driven by terahertz light field." Nat Commun 16, 2249 (2025)

MA 12.5 Mon 16:00 POT/0351

Orbital-torque driven excitation of Terahertz perpendicular standing spin wave (PSSW) modes — •Harshita Devda[1], Peter M. Oppeneer[2], and Ulrich Nowak[1] — [1]Fachbereich Physik, Universität Konstanz, Konstanz, Germany — [2]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

Layered ferromagnets support interface-sensitive THz spin dynamics, making the controlled excitation of such THz magnon modes relevant for spintronics applications. Recent experiments show that asymmetric NM/FM/NM trilayers couple efficiently to THz fields via interfacial spin-orbit torques (SOTs)[1], emphasizing the importance of interface effects in THz spin dynamics.

Here, we employ atomistic spin-dynamics simulations using ab-initio exchange parameters in thin NM/Co/NM trilayers to investigate ultrafast magnon excitation in presence of asymmetric and symmetric SOT interfaces. SOTs are implemented using the induced spin and orbital moments from first principles calculations. Our simulations show that nanometer thick Co-layers host exchange-dominated PSSWs in 1-3 THz range. Crucially, the efficient excitation of these THz modes is governed by interfacial field-like orbital torques, which follow directly from our recent study on layer-resolved SOTs[2]. This work establishes orbital torques as a robust route to ultrafast magnon generation.

[1]Salikhov et al., Nat. Phys. 19, 529-535 (2023)
[2]Devda et al.,Phys. Rev. B 112, 144438 (2025)

MA 12.6 Mon 16:15 POT/0351

Tuning terahertz emission from spintronic devices via interface engineering — Rahul Gupta[1,2], •Francesco Foggetti[3], Francesco Cosco[3], Venkatesh Mottamchetty[4], Martin Pavelka[3], Kasturie Jatkar[5], Anders Rydberg[3], Rimantas Brucas[3], Peter M. Oppeneer[3], and Peter Svedlindh[3] — [1]University of South Florida, Tampa, Florida, USA — [2]University of Gothenburg, Gothenburg, Sweden — [3]Uppsala University, Uppsala, Sweden — [4]Aarhus University, Aarhus, Denmark — [5]Stockholm University, Stockholm, Sweden

Spintronic terahertz (THz) emitters are emerging as compact and broadband sources. While common optimization approaches consist in the exploration of different materials and stacking geometries, the effects of the external interfaces have been poorly understood. Here we show that THz radiation amplitude from Pt/Fe grown on MgO and MgAl2O4 depends significantly on the interface reflection of spin currents, which is controlled by lattice mismatch and strain of the Fe/substrate interface, providing a powerful lever to tune THz emission. We use the superdiffusive transport theory to simulate the Pt/Fe bilayer, modeling the different interfaces via tunable interface reflection or via simulated substrate layer, resulting in very good agreement with the experimental data. Our results establish interface reflection governed by strain and lattice mismatch as a general design knob for optimizing spintronic THz emitters, opening new routes to engineer material platforms for next-generation THz technologies.

MA 13: Magnetic Heuslers and Semiconductors

Time: Monday 15:00–17:15 Location: POT/0361

MA 13.1 Mon 15:00 POT/0361

Investigation on the interplay of antisite disorder and magnetic ordering in $Co_2FeAl_{1-x}Si_x$ Heusler system — •Ahmad Omar[1], Matthias Frontzek[2], Robin Kramer[1], Bernd Büchner[1], and Sabine Wurmehl[1] — [1]Leibniz Institute for Solid State and Materials Research Dresden, Germany — [2]PSI Villigen, Switzerland

Quaternary Co-based Heusler compounds such as $Co_2FeAl_{1-x}Si_x$ system are predicted to demonstrate half-metallic ferromagnetism for the $L2_1$ ordered structure. However, the observed physical properties, are often in contrast to theory due to antisite disorder commonly present in practical samples. The $L2_1$-B_2 order-disorder transition is further convoluted with the ferromagnetic transition and is not well understood. Therefore, it is pertinent to understand the ordering phenomenon and develop routes to improve the order for practical realization of the desired properties. Herein, we present a systematic study of the impact of synthesis route and annealing parameters on the obtained order fraction in the samples, through detailed structural and magnetic characterization. In-situ neutron diffraction is performed during annealing to directly investigate the order-disorder transition. The interplay of disorder and the magnetic ordering is further studied through magnetic field annealing experiments. We aim to elucidate the structure-property relationships in the quaternary $Co_2FeAl_{1-x}Si_x$ system, developing methodology for tuning of the disorder through synthesis or post-processing routes, thus enabling a practical realization of half metallic ferromagnetism in the Heusler system.

MA 13.2 Mon 15:15 POT/0361

Impact of disorder on magnetic and vibrational properties of Ni-Mn-Sn Heusler alloys — •Olga Miroshkina[1], Benedikt Eggert[1], Benedikt Beckmann[2], Franziska Scheibel[2], Katharina Ollefs[1], Oliver Gutfleisch[2], Heiko Wende[1], and Markus E. Gruner[1] — [1]University of Duisburg-Essen, Duisburg, Germany — [2]Technical University of Darmstadt, Darmstadt, Germany

Ni-Mn-Sn Heusler alloys are attractive candidates for multi-stimuli caloric cooling. They undergo a magneto-structural phase transition at temperature that can be tuned via chemical disorder. In this work, we investigate the austenitic and martensitic phases near the composition $Ni_{50}Mn_{35}Sn_{15}$ by means of density functional theory complemented by magnetometry and nuclear resonant inelastic x-ray scattering (NRIXS). Bain-path calculations reveal strong competition between ferro-(FM) and ferrimagnetic (FiM) states in austenite and a clear FiM configuration in the $L1_0$ martensite. The FiM contribution in the cubic phase is confirmed by comparing the calculated Sn vibrational DOS with that extracted from NRIXS. In martensite, frustrated exchange introduced by Mn excess can prevail in the tetragonal FiM $L1_0$ phases and make nano-twinns competitive. We find that twins constructed according to the continuum theory of martensite are energetically even more favorable than $L1_0$. A striking outcome is that all Mn/Sn-disordered configurations are energetically more favorable than the ordered ones, with the FiM 4O and 10M phases remaining the most competitive structures. Financial support within the DFG Projects MI 3273/1 and CRC/TRR 270 is gratefully acknowledged.

MA 13.3 Mon 15:30 POT/0361

Finite Size-Effects in Martensite Microstructure of Magnetic Shape Memory Films — Satyakam Kar[1,2], Aman Singh[1], Kornelius Nielsch[1], Heiko Reith[1], and •Sebastian Fähler[3] — [1]Leibniz IFW Dresden, 01069 Dresden, Germany — [2]TU Dresden, Institute of Materials Science, 01062 Dresden, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Magnetic shape memory alloys, owing to their multifunctional properties, are a promising material system for integration into microsystems. Their multifunctionality arises from the coexistence of ferroelasticity and ferromagnetism. While size-effects in ferromagnetic microstructure are well understood, corresponding experiments on the influence of finite size on the ferroelastic martensite microstructure are sparse. In this study, we use epitaxially grown Ni-Mn-Ga-based films as a model system to investigate the influence of a finite size in the martensite microstructure under constrained and freestanding conditions. Our results show that the microfabricated patterns, in both conditions, retain the characteristics of their continuous film microstructures. Film thickness has a strong influence, as this is the smallest extension investigated in our study. We analyze similarities and differences between ferromagnetic and ferroelastic microstructure, as understanding finite size effects is decisive for using these multifunctional materials in microsystems with reduced size.

MA 13.4 Mon 15:45 POT/0361

Microstructure Design via Additive Manufacturing of Heusler Alloys for Multicaloric Applications — •Nene Narh Teinor[1,2], Adrian Guder[3], Johannes Puy[1], Christian Lauhoff[3], Thomas Niendorf[3], Oliver Gutfleisch[1], and Franziska Scheibel[1,2] — [1]Institute of Materials Science, Technical University of Darmstadt, Germany — [2]Additive Manufacturing Center, Technical University of Darmstadt, Darmstadt, Germany — [3]Institute of Materials Engineering, University of Kassel, Germany

Heusler alloys like NiMnSn and NiCoMnTi show strong potential for solid-state cooling due to their first-order magnetostructural transitions (FOMST). However, their functional performance is highly sensitive to processing conditions. In this work, bulk samples are produced via Laser Powder Bed Fusion (PBF-LB/M) using gas-atomized powders to explore the influence of additive manufacturing parameters on microstructure and caloric properties. By varying laser power, scan speed, and strategy, we achieve controlled tuning of martensitic, austenitic, and Curie temperatures, as well as reduced thermal hysteresis. Structural, compositional, and magnetic analyses reveal how rapid solidification enhances the sharpness and reversibility of FOMST. We demonstrate that additive manufacturing not only preserves the functional properties of these alloys but also enables active enhancement of their tunability of transition behavior compared to conventionally processed samples. We acknowledge Deutsche Forschungsgemeinschaft (DFG) support through the CRC/TRR 270 (Project ID 405553726)

MA 13.5 Mon 16:00 POT/0361

Modelling the martensitic transformation in Ni-Mn-based Heusler compounds with machine-learning force-fields — •Markus E. Gruner, Mike J. Bruckhoff, and Olga Miroshkina — Faculty of Physics and CENIDE, University of Duisburg-Essen, D-47048 Duisburg

Functional properties of Ni-Mn-based Heusler alloys, such as Ni_2MnGa, depend on the presence of hierarchically twinned, modulated structures in the martensite phase. These can be interpreted as an adaptive, self-organized arrangement of [101]-aligned nanotwins consisting of non-modulated tetragonal building blocks. Density functional theory (DFT) suggests that these martensites are connected to cubic austenite via a downhill transformation path. This is owed to a Fermi surface reconstruction, softening the corresponding acoustic phonons of austenite. Modeling free energy surfaces at finite temperatures or the dynamics of the martensitic transition as probed in recent ultrafast laser heating experiments [1] is too expensive for conventional DFT. Machine-learning force fields (ML-FF) trained on DFT data offer a possibility to account for electronic instabilities and allow to explore the impact of adaptive nanotwining on the martensitic transition using ML-FF in classical molecular dynamics simulations. Funding by the DFG via TRR270 (B06), SFB1242 (C02) and MI3273/1 is gratefully acknowledged.

[1] Y. Ge, F. Ganss, D. Schmidt, D. Hensel, M. J. Bruckhoff, S. Sadashivaiah, B. Neumann, M. Brede, M. E. Gruner, P. Gaal, K. Lünser, S. Fähler, arXiv:2509.06513.

MA 13.6 Mon 16:15 POT/0361

Enhanced anomalous Hall response via nodal line tuning in Co2VSn(1-x)Alx topological semimetal — •Sunil Wilfred DSouza[1], Shivani Rastogi[2], Gaurav Shukla[3], Nidhi Shukla[2], Jan Minár[1], and Sanjay Singh[2] — [1]New Technologies Research Centre, University of West Bohemia, 30100 Pilsen, Czech Republic — [2]School of Materials Science and Technology, Indian Institute of Technology (Banaras Hindu University), Varanasi 221005, India — [3]National Institute for Materials Science (NIMS), Tsukuba 305-0047, Japan

Topological semimetals (TSMs) with nodal-line states exhibit strong Berry-curvature driven transport. We Investigate Co2VSn(1-x)Alx (x = 0-0.75) to understand how hole doping tunes the nodal line relative to the Fermi level. Al substitution shifts the nodal-line states upward, leading to a maximum intrinsic anomalous Hall conductivity (AHC) of 203 S/cm at x = 0.5, representing a significant enhancement over the undoped compound. First-principles calculations corroborate the nodal line in Co2VSn, its gapping under SOC, and its progressive alignment with the Fermi level upon Al doping. The correlation between nodal-line tuning and enhanced AHC highlights an effective strategy for controlling Berry-curvature driven transport in magnetic TSMs.

MA 13.7 Mon 16:30 POT/0361

Manipulating the first-order magnetostructural phase transition in Ni-Mn-Sn Heusler alloy through nano-functionalization — •Johannes Puy[1], Nadine Stratmann[2], Hamed Shokri[3], Bilal Gökce[3], Stephan Barcikowski[2], Oliver Gutfleisch[1], Anna Ziefuss[2], and Franziska Scheibel[1] — [1]TU Darmstadt, Darmstadt, Germany — [2]Universität Duisburg-Essen, Essen, Germany — [3]BU Wuppertal, Wuppertal, Germany

Ni-Mn-based Heusler alloys are considered as a promising candidate for magnetocaloric or multicaloric cooling applications, as they exhibit an inverse magnetocaloric and conventional elastocaloric effect, which arise from a first-order magnetostructural phase transition (FOMST). However, the practical use of these alloys is limited by the thermal hysteresis associated with the FOMST and their intrinsic brittleness. This work demonstrates a novel approach to tailor the FOMST characteritics and the mechanical stability of spark-plasma-sintered (SPS) Ni-Mn-Sn by nano-functionalization. Silver and zirconium diboride nanoparticles (NP) are synthesized by pulsed laser fragmentation of microparticles (MP-LFL) and subsequently used to functionalize Ni-Mn-Sn powder (150 - 75 μm) at varying mass loadings. This enables targeted modification of the sintered particle interfaces, which act as martensite nucleation sites, but also as origin of fracture under compressive stress. We systematically characterize the influence of NP-functionalization on the microstructure, the temperature-induced FOMST and the mechanical stability. This work was supported by the DFG within the CRC/TRR 270 (Project ID No. 405553726).

MA 13.8 Mon 16:45 POT/0361

Fe^{3+}-Centers as Structural Probes in Fe-Doped $Cs_2AgBiBr_6$ Semiconducting Perovskite — •Volodymyr Vasylkovskyi[1], Timur Biktagirov[2], Anastasiia Kultaeva[1], Carlos Canhassi[3], Mykola Slipchenko[4], Yakov Kopelevich[3], and Vladimir Dyakonov[1] — [1]Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany — [2]Physics Department, Paderborn University, D-33098 Paderborn, Germany — [3]Gleb Wataghin Institute of Physics, University of Campinas, 13083-859 Campinas, Brazil — [4]Institute for Scintillation Materials, Kharkiv, Ukraine

Fe-doping introduces new functionality into halide double perovskites alongside modifying optical properties. We report controlled growth of Fe-doped $Cs_2AgBiBr_6$ single crystals and correlate their structural, optical, and magnetic parameters. ICP analysis confirms Fe incorporation below 0.1% relative to Bi, which induce defect-related sub-gap absorption and photoluminescence shift. EPR measurements reveal an S = 5/2 Fe^{3+} spin center whose anisotropy follows the phase transition below 120 K. DFT calculations, guided by angular-dependent EPR, identify these centers as impurity-vacancy complexes, likely Fe_{Bi}-V_{Br}. SQUID magnetometry shows ferromagnetic-type hysteresis at room temperature, with rising spontaneous magnetization below 20-30 K and magnetization irreversibility under zero-field and field-cooling, confirming ferromagnetism from Fe-related defect complexes. Even small Fe amounts significantly alter optical and magnetic behavior of $Cs_2AgBiBr_6$, emphasizing the role of controlled doping and defect engineering in lead-free double perovskites.

MA 13.9 Mon 17:00 POT/0361

Pressure-dependence of the thermoelectric properties of $MnIn_2Te_4$ — •Shubham Rakesh Singh, Mohammed Ghadiyali, and Udo Schwingenschlögl — Physical Science and Engineering Division (PSE), King Abdullah University of Science and Technology (KAUST), Thuwal 23955-6900, Saudi Arabia

We investigate the thermoelectric properties of $MnIn_2Te_4$ in its two experimentally characterized phases. The tetragonal phase ($I\bar{4}2m$) undergoes a pressure-induced transition to an orthorhombic phase ($Pnma$) at 1.3 GPa. First-principles calculations reveal for both phases a small energy difference between antiferromagnetic and ferromagnetic states. The band gap is 1.04 (0.70) eV in the tetragonal phase and 1.25 (1.10) eV in the orthorhombic phase for the antiferromagnetic (ferromagnetic) state. A higher power factor is achieved by n-type than by p-type carriers. At 700 K, for example, the more densely packed orthorhombic phase exhibits a 56% reduction in the lattice thermal conductivity as compared with the tetragonal phase, yielding high thermoelectric figures of merit of 1.23 for n-type carriers and 0.96 for p-type carriers at optimal carrier concentration.

MA 14: PhD Focus Session: What about the lattice? Lessons from (ultrafast) magnetism

This focus session brings together experimental, theoretical and numerical perspectives to highlight recent discoveries and unresolved questions on ultrafast magnetization effects facilitated by spin-lattice interactions. In recent years, the transfer of magnetic angular momentum during ultrafast demagnetization processes has been observed experimentally. Studies have revealed both the microscopic mechanism through circularly polarized phonons and the macroscopic mechanical response in the form of the ultrafast Einstein-de Haas effect. Further, the complementary ultrafast Barnett effect has been demonstrated, where angular momentum is transferred into the spin system from non-equilibrium angular momentum sources (e.g. lattice vibrations or optical fields) Furthermore, inertial effects in spin dynamics were measured by observing additional nutation frequencies on top of the precessional motion Theoretical work suggests that these frequencies arise due to the spin-lattice coupling, however, the underlying mechanisms are not yet fully understood. In order to predict and explain these different types of phenomena, spin-lattice dynamics simulations have been developed in recent years. These allow energy and angular momentum to be exchanged between the magnetic spin system and the lattice.

Organizers: Felix Hartmann, hartmann3@uni-potsdam.de; Fried-Conrad Weber, fried-conrad.weber@uni-potsdam.de; Finja Tietjen, finja.tietjen@chalmers.se; Daniel Schick, daniel.schick@uni-konstanz.de; Jasmin Jarecki, jasmin.jarecki@mbi-berlin.de

Time: Tuesday 9:30–12:40 Location: HSZ/0002

Introduction and Welcome

Invited Talk MA 14.1 Tue 9:35 HSZ/0002

Femtophonomagnetism — •Sangeeta Sharma[1] and John Dewhurst[1,2] — [1]Max Born Institute, Berlin, Germany — [2]Max Planck Inst. Halle, Germany

From the outset of research into femtomagnetism, the field in which spins are manipulated by light on femtosecond or faster time scales, several questions have arisen and remain highly debated: How does the light interact with spin moments? How is the angular momentum conserved between the nuclei, spin, and angular momentum during this interaction? What causes the ultrafast optical switching of magnetic structures? What is the ultimate time limit on the speed of spin manipulation? What is the impact of nuclear dynamics on the light-spin interaction?

In my talk I will advocate a parameter free ab-initio approach to treating ultrafast light-matter interactions, and discuss how this approach has led both to new answers to these old questions but also to the uncovering of novel and hitherto unsuspected early time spin dynamics phenomena [1, 2]. In particular I will show that phonons strongly influence the spin dynamics[3], demonstrating nuclear system can play a profound role in controlling femtosecond magnetization of materials.

[1] Dewhust et al., Nano Lett. 18, 1842 (2018).
[2] Siegrist et al. Nature 571, 240 (2019)
[3] Sharma et al. Sci. Advs. 8, eabq2021 (2022)

Invited Talk MA 14.2 Tue 10:20 HSZ/0002

THz-driven dynamical ferroicity in paraelectric and diamagnetic perovskites — •Martina Basini — ETH Zürich, Department of Phyisics, August-Piccard-Hoff,1, 8049, Zürich, Switzerland

The emergence of collective order in matter is among the most fundamental and intriguing phenomena in physics. In recent years, the dynamical control and creation of novel ordered states of matter not accessible in thermodynamic equilibrium have received much attention. The theoretical concept of dynamical multiferroicity has been introduced to describe the emergence of magnetization due to time-dependent electric polarization in non-ferromagnetic materials. Here, we provide experimental evidence of magnetization in the archetypal paraelectric and diamagnetic perovskites SrTiO3 and KTaO3 due to this mechanism. To induce such a magnetic response, we resonantly drive the infrared-active soft phonon mode with an intense circularly polarized terahertz electric field and detect the time-resolved magneto-optical Kerr effect. Our findings show a new path for the control of magnetism, for example, for ultrafast magnetic switches, by coherently controlling the lattice vibrations with light.

Invited Talk MA 14.3 Tue 10:50 HSZ/0002

Angular momentum transfer and chiral phonons from first principles — •Markus Weissenhofer[1], Philipp Rieger[1], MS Mrudul[1], Luca Mikadze[1], Sergiy Mankovsky[2], Svitlana Polesya[2], Hubert Ebert[2], Ulrich Nowak[3], and Peter M. Oppeneer[1] — [1]Uppsala University, Uppsala, Sweden — [2]Ludwig Maximilian Universität, München, Germany — [3]Universität Konstanz, Konstanz, Germany

Transfer and manipulation of angular momentum is a key aspect in spintronics. Recently, it has been shown that angular momentum transfer between spins and lattice is possible on ultrashort timescales [1].

To contribute to the understanding of this transfer, we have developed a theoretical multiscale framework for spin-lattice coupling, which is linked to ab-initio calculations on the one hand and magnetoelastic continuum theory on the other [2], allowing for the study of a wide range of magnetomechanical phenomena.

Here I will demonstrate how this framework can be used to calculate magnon-phonon coupling parameters, emphasizing the importance of a Dzyaloshiskii-Moriya type interaction for angular momentum transfer [2] and revealing the existence of chiral phonons in iron arising from a chirality-selective coupling [3].

[1] Tauchert al., Nature 602, 73 (2022); Luo et al., Science 382, 698 (2023).
[2] Mankovsky et al., PRL 129, 067202 (2022); Weißenhofer et al., PRB 108, L060404 (2023).
[3] Weißenhofer et al., PRL 135, 216701(2025).

15 min break

Invited Talk MA 14.4 Tue 11:35 HSZ/0002

Inertial Spin Dynamics: A Signature of Non-Markovian Interactions in Ferromagnets — •Vivek Unikandanunni[1,5], Felix Hartmann[2], Matias Bargheer[2], Eric Fullerton[3], Stefano Bonetti[4,5], and Janet Anders[2] — [1]Institute of Applied Physics, University of Bern,Switzerland — [2]Institute of Physics and Astronomy, University of Potsdam, Germany — [3]Center for Memory and Recording Research, University of California San Diego, USA — [4]Department of Molecular Sciences and Nanosystems, Ca Foscari University of Venice, Italy — [5]Department of Physics, Stockholm University, Stockholm, Sweden

We report direct experimental observation of intrinsic inertial spin dynamics in ferromagnetic thin films, manifested as a damped THz frequency oscillation of the magnetization. Using a broadband tabletop THz source, we resonantly drive epitaxial cobalt and directly measure the frequency and relaxation time of the inertial response, which is well described by the inertial Landau-Lifshitz-Gilbert (LLG) equation. We find that the frequency and relaxation time of the inertial dynamics are dependent on the structural symmetry of the sample.

Broadband measurements further reveal a multi-peaked magnetic spectrum that cannot be captured by the inertial LLG alone. An open-quantum-system approach incorporating spin-phonon coupling through a memory kernel yields a non-Markovian LLG equation that reproduces the full experimental spectra demonstrating the fundamental role of non-Markovian memory effects in ultrafast spin dynamics.

Invited Talk MA 14.5 Tue 12:05 HSZ/0002

Atomistic simulations of ultrafast spin-lattice dynamics — •Richard Evans[1] and Mara Strungaru[2] — [1]University of York, York, United Kingdom — [2]University of Manchester, Manchester, United Kingdom

Atomistic spin dynamics (ASD) has become a standard method for studying finite temperature processes in magnetic materials and devices. In some systems, such as magnetic insulators, coupled spin-lattice dynamics can play a dominant role in the thermal and dynamic properties that have so far been neglected in spin-only models. Recent exciting results in ultrafast dynamics have shown that the spin-lattice interaction is a critically important component to the physical properties of a magnetic material. Spin-Lattice Dynamics (SLD) is a relatively recent theoretical development aiming to directly couple an atomistic spin model with a molecular dynamics solver to incorporate the fascinating and complicated dynamics of these coupled systems into a practical numerical framework. In this talk I will introduce the theoretical background and numerical methods for SLD as recently implemented in the VAMPIRE software package, including its parallelisation and scalability on the UK National Supercomputer

ARCHER2. I will present recent results on coherent ultrafast THz switching where we found that it is possible to induce magnetic switching through a coherent phonon excitation. I will conclude with a brief perspective on open problems in spin-lattice dynamics, including numerical challenges, quantum thermostats and correlated noise, and how to model electron processes in metallic magnetic systems.

Closing Remarks

MA 15: Focus Session: Quantum Sensing with Solid State Spin defects I (joint session TT/MA)

The electron spins of defects in solid state materials show remarkable quantum coherence, making them excellent sensors. Recent advances in material engineering and measurement techniques lead to continuous improvements in the sensitivity and resolution of established single spin sensors such as the Nitrogen-Vacancy center in diamond, and the development of new defect sensors in materials such as Silicon Carbide and hexagonal Boron Nitride. In condensed matter physics, such sensors are often being used for exploring the structure of magnets, superconductors, topological phases, etc. This focus session will highlight most of the recent experimental and theoretical advances, current challenges, and emerging directions, focusing both on the improvements of the defects themselves, and their use for exploring novel phenomena in condensed matter physics.

Coordinators: Aparajita Singha (TU Dresden), Uri Vool (Max Planck Institute for Chemical Physics of Solids)

Time: Tuesday 9:30–12:45 Location: HSZ/0003

See TT 24 for details of this session.

MA 16: Skyrmions I

Time: Tuesday 9:30–12:45 Location: HSZ/0004

MA 16.1 Tue 9:30 HSZ/0004

Charge Order, Spin textures, and Electronic Structure of Eu(Ga,Al)4 — Steven Gebel[1], Aleksandr Sukhanov[2], Artem Korshunov[3], Jaime Moya[4], Kevin Allen[5], Emilia Morosan[5], and •Marein Rahn[2] — [1]TU Dresden, Germany — [2]Universität Augsburg, Germany — [3]ESRF, Grenoble, France — [4]Princeton University, USA — [5]Rice University, USA

The tetragonal intermetallic series $Eu(Ga,Al)_4$, is known for a range of interesting phenomena, ranging from the nodal line semimetal EuGa4 to centrosymmetric skyrmion phases in $EuAl_4$. It would be of great interest to design the band topology of these materials and, in particular, to understand how it may couple to electronic correlations. To this end, one must clarify by what mechanisms the multifaceted spin- and charge-ordering instabilities of this series arise from the underlying electronic band structure. For instance, structural modifications and charge density waves exist throughout the series, but show a variable response to hydrostatic pressure – hinting at competing mechanisms. We provide an overview of the ordered phases in $Eu(Ga,Al)_4$ and then show how X-ray crystallography using diamond anvil pressure cells draws a clear line between different structural instabilities. Complementary measurements using inelastic X-ray scattering also provide evidence on the underlying electron-phonon coupling mechanisms. Our results provide a tentative x-P-T phase diagram of $Eu(Ga_{1-x}Al_x)_4$ and highlight interesting questions, e.g. regarding the origin of anomalous Hall effects in $EuGa_4$ and the nature of a new pressure-induced structural phase of $EuAl_4$.

MA 16.2 Tue 9:45 HSZ/0004

Topological pumping of skyrmionic textures in spiral multiferroics — •Luca Maranzana[1,2], Maxim Mostovoy[3], Naoto Nagaosa[4,5], and Sergey Artyukhin[1] — [1]Quantum Materials Theory, Italian Institute of Technology, Via Morego 30, Genoa, Italy — [2]Department of Physics, University of Genoa, Via Dodecaneso 33, Genoa, Italy — [3]Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 3, 9747 AG Groningen, Netherlands — [4]RIKEN Center for Emergent Matter Science (CEMS), Wako, Saitama 351-0198, Japan — [5]Fundamental Quantum Science Program, TRIP Headquarters, RIKEN, Wako 351-0198, Japan

Precise positioning of topological defects is crucial for racetrack memories, where their positions along a magnetic nanotrack encode information. Conventional approaches rely on engineered pinning landscapes, which increase power consumption. Here, we show that spiral multiferroics serve as a natural ruler for electric-field-driven positioning of skyrmionic textures, extending the concepts introduced in [1]. An oscillating electric field, assisted by anisotropy or a static magnetic field, displaces the topological defect by exactly one spiral period per full oscillation of the field. Such adiabatic pumping, reminiscent of Thouless pumping, is topologically protected and remains robust against small perturbations. Our work proposes a route to electrically driven, topologically protected transport of spin textures and positions spiral multiferroics as a natural platform for skyrmion racetracks.

[1] L. Maranzana, M. Mostovoy, N. Nagaosa, and S. Artyukhin, arXiv:2502.13083 (2025).

MA 16.3 Tue 10:00 HSZ/0004

Statistical Signature of Chirality as a Probe of Skyrmion Topology and Collapse Dynamics — Shiyu Zhou[1], •Kai Litzius[2], Felix Büttner[2,3], and Lucas Caretta[1,4] — [1]Department of Physics, Brown University, Providence, Rhode Island 02912, USA — [2]Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, 14109 Berlin, Germany — [4]School of Engineering, Brown University, Providence, Rhode Island 02912, USA

Magnetic skyrmions are topological spin textures whose robustness has driven intense interest for spintronic applications, yet direct experimental evidence linking topology to stability has been limited. We introduce an accessible, material-agnostic method to probe skyrmion topology statistically by measuring annihilation field distributions using Kerr microscopy. By tuning in-plane magnetic fields, we drive transitions from topologically nontrivial to trivial skyrmion states and observe a clear shift in annihilation behavior: skyrmions show broad, thermally activated distributions, while trivial bubbles collapse deterministically with narrow distributions. Micromagnetic simulations corroborate this correlation between topology and collapse statistics. Our approach enables straightforward chirality detection and skyrmion state control without specialized imaging or transport probes. The ability to toggle between deterministic and stochastic collapse suggests new device concepts, including synchronized deletion for memory and topology-tunable randomness for probabilistic applications.

MA 16.4 Tue 10:15 HSZ/0004

observation of a distorted tilted conical spiral at the surface of Cu_2OSeO_3 — •Sina Mehboodi[1], Victor Ukleev[2], Chen Luo[2], Radu Abrudan[2], Florin Radu[2], Christian Back[1], and Aisha Aqeel[3] — [1]School of Natural Sciences, Technical University of Munich, Garching, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [3]Institute of Physics, University of Augsburg, Augsburg, Germany

Chiral magnets such as Cu_2OSeO_3 host a rich variety of noncollinear spin textures [1]. Using resonant elastic X-ray scattering (REXS), where the magnetic satellites are captured as scattered intensity on a CCD detector, we observed a well-ordered surface texture referred to as a distorted tilted conical (dTC) spiral phase. This phase displays strong anharmonicity, evidenced by pronounced higher-order magnetic satellites. Tilting the applied magnetic field causes a continuous reorientation of the dTC propagation vector and increases its modulation wavevector, revealing a high sensitivity of the surface spiral to field direction. Importantly, by combining REXS with rocking-curve analysis, we determine the full scattering vector of dTC, about 0.0718 nm^{-1}. This value is significantly smaller than the reported bulk TC wavevector (≈ 0.095 nm^{-1}) [2], providing direct evidence that the surface spiral is intrinsically distorted and cannot be explained by a simple bulk-like conical modulation [3].

[1] A. Aqeel, et al., Phys. Rev. Lett. 126, 017202 (2021). [2] E. Marchiori et al., Commun. Mater. 5, 202 (2024). [3] S. Mehboodi et al. Sci. Technol. Adv. Mater. 26, 2532366 (2025).

MA 16.5 Tue 10:30 HSZ/0004

Optical manipulation of magnetic skyrmions and antiskyrmions — •Dola Chakrabartty[1], Andreas Wendeln[2,3], Manuel Zahn[1,4], Sascha Schäfer[2,3], and István Kézsmárki[1] — [1]Experimentalphysik V, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, Augsburg, D-86135, Germany — [2]Regensburg Center for Ultrafast Nanoscopy, University of Regensburg, Regensburg, 93040, Germany. — [3]Department of Physics, University of Regensburg, Regensburg, 93040, Germany. — [4]NTNU Trondheim, Trondheim, 7034, Norway

Topological magnetic textures like skyrmions and antiskyrmions, have potential applications in next-generation spintronic devices. Notably, skyrmions and antiskyrmions can be viewed as particle- and antiparticle-like entities, respectively, with opposite topological charges and the potential to annihilate each other or be created in pairs. The controlled and fast manipulation of these spin textures are crucial for their practical applications.

In this work, we utilized in-situ femtosecond optical pulses in Lorentz microscopy and investigated the possibility of manipulating skyrmions and antiskyrmions. Our preliminary results show that ultrafast laser excitation can induce a helicity switching of elliptical skyrmions as well as the transformation between different spin textures, such as skyrmions, antiskyrmions, non-topological bubbles and stripes. A statistical analysis of our observations provides insights into the energy landscape of these magnetic patterns. Our findings suggest that laser pulses can control topological magnetic states.

MA 16.6 Tue 10:45 HSZ/0004

Emergent reactance induced by the deformation of a current-drive skyrmion lattice — •Matthew Littlehales[1,2], Max Birch[3], Akiko Kikkawa[3], Yasujiro Taguchi[3], Diego Alba Venero[2], Peter Hatton[1], Naoto Nagaosa[3,4], Yoshinori Tokura[3,5,6], and Tomoyuki Yokouchi[3] — [1]Department of Physics, Durham University, South Road, Durham, DH1 3LE, UK — [2]ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, Didcot, OX11 0QX, UK — [3]RIKEN Center for Emergent Matter Science (CEMS), Wako, Japan — [4]Fundamental Quantum Science Program (FQSP), TRIP Headquarters, RIKEN, Wako, Japan — [5]Department of Applied Physics, University of Tokyo, Tokyo, Japan — [6]Tokyo College, University of Tokyo, Tokyo, Japan

Emergent electromagnetism offers an opportunity to develop novel applications by exploiting quantum mechanics. In condensed matter systems, the Berry phase acquired by conduction electrons acts as an emergent electromagnetic field, facilitating phenomena akin to classical electromagnetism. Magnetic skyrmions, spin vortices with non-trivial topology, offer a unique opportunity to investigate emergent electromagnetism. For example, non-trivial transport responses from magnetic skyrmions arise from the emergent Lorentz force and electromagnetic induction. Here, we present two new examples of emergent electric fields arising simultaneously from skyrmion lattice dynamics in MnSi. We find out-of-phase components in the electrical transport, reminiscent of a reactance, and attribute their existence to inertial, and deformative, current-driven skyrmion lattice dynamics.

15 min break

MA 16.7 Tue 11:15 HSZ/0004

***Ab inito* quantum transport for sub-10 nm skyrmions in 2D magnets** — •Moritz A. Goerzen, Salomé Trillot, and Dongzhe Li — CEMES, Université de Toulouse, CNRS, France

Topological spin textures, such as magnetic skyrmions, play a central role in modern magnetism and have attracted significant interest in both fundamental studies and spintronics applications. *Ab initio* theory can provide a direct connection to experiments, giving access to the material-dependent physics behind the observed effects. However, the high computational cost makes it difficult to model chiral skyrmions, which typically span several nanometers and arise from competing magnetic interactions. Here, we present a novel workflow capable of treating the electronic structure and transport properties of sub-10 nm skyrmions at the full *ab initio* level. We then apply this technique to investigate the electrical detection and chirality-induced orbitronics effects in 2D magnets. In particular, we demonstrate how non-collinear magnetoresistance, chirality-induced orbital moments, and orbital Hall effects evolve with skyrmion size, helicity, and spin-orbit coupling.

MA 16.8 Tue 11:30 HSZ/0004

Magnetic anisotropies resolved in the skyrmion-host GaV_4S_8 by high-field electron spin resonance spectroscopy — •Ignác Fejes[1], Titusz Fehér[1], Norbert Marcell Nemes[1], András Jánossy[2], Dávid Szaller[1,2,3], Sándor Bordács[3,5], Vladimir Tsurkan[3], and István Kézsmárki[4] — [1]Department of Physics, Institute of Physics, Budapest University of Technology and Economics, Muegyetem rkp. 3., H-1111 Budapest, Hungary — [2]HUN-REN-BME Condensed Matter Physics Research Group, Budapest University of Technology and Economics, Muegyetem rkp. 3., H-1111 Budapest, Hungary — [3]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, D-86135 Augsburg, Germany — [4]GFMC, Departamento de Fisica de Materiales Universidad Complutense de Madrid, 28040 — [5]Institute of Applied Physics, MD 2028, Chisinau, R. Moldova

Appearance of exotic types of magnetic ordering, such as skyrmions, strongly depends on the magnetic anisotropies present in a material, particularly in axially symmetric systems where second-order anisotropy in spin-orbit coupling is allowed. Here, we used high-field electron spin resonance spectroscopy (ESR) to study the field and orientation dependence of the spin excitation in the field-polarized state of GaV_4S_8. Below T_S = 44 K, the material transforms from a cubic phase to a polar rhombohedral phase, giving rise to multiple structural domains at low temperatures. We assigned the observed resonance modes to the corresponding polar domains and identified the relevant anisotropies - magnetocrystalline and g-factor - of GaV_4S_8.

MA 16.9 Tue 11:45 HSZ/0004

Isolated Magnetic Hopfions — Xiaowen Chen[1], •Nikolai S. Kiselev[2], Filipp N. Rybakov[3], Donghai Yang[1], and Fengshan Zheng[1] — [1]South China University of Technology, Guangzhou, China — [2]Forschungszentrum Jülich, Germany — [3]Uppsala University, Sweden

Hopfions are three-dimensional topological solitons formed by closed loops of vortex strings. In magnetic crystals, hopfions have so far been observed only in unusual configurations in which they are linked to skyrmion strings [1]. Although theory predicts the existence of stable, isolated hopfions in frustrated magnets [2] and chiral magnets [3], their experimental realization has remained elusive. Here we report laser-induced nucleation and direct TEM observation of isolated magnetic hopfions in the B20-type FeGe crystal [4]. We map out the nucleation conditions as a function of laser fluence and external magnetic field. Good agreement between experimental data and micromagnetic simulations unambiguously confirms the emergence of isolated hopfions and reveals their detailed structure. We derive the relevant topological invariant for hopfions embedded in helical or conical backgrounds and calculate its integer values for the observed objects. We demonstrate that these hopfions are stable without geometrical confinement and can coexist and interact with other topological spin textures. [1] F. Zheng, et al., Nature **623**, 718 (2023). [2] F. N. Rybakov et al., APL Mater. **10**, 111113 (2022). [3] J.-S. B. Tai & I. I. Smalyukh, Phys. Rev. Lett. **121**, 187201 (2018). [4] X. Chen, et al., preprint on Research Square https://doi.org/10.21203/rs.3.rs-7435743/v1

MA 16.10 Tue 12:00 HSZ/0004

Strain-controlled topological magnetic textures in antiskyrmion hosting materials — •Somasree Bhattacharjee[1], István Kézsmárki[2], and Jan Masell[1] — [1]Institute of Theoretical Solid State Physics (TFP), Karlsruhe Institute of Technology (KIT), 76049 Karlsruhe, Germany — [2]Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86159 Augsburg, Germany

In non-centrosymmetric crystal structures with D_{2d} or S_4 symmetry, anisotropic Dzyaloshinskii-Moriya interaction (DMI) stabilizes antiskyrmions which was recently confirmed experimentally [1,2]. In these materials, easy-axis anisotropy additionally stabilizes skyrmions and non-topological bubbles in certain ranges of external magnetic fields and lamella thicknesses. The competition between magnetic dipolar interaction and DMI renders skyrmions elliptical depending on their handedness. Also, dipolar interaction stabilizes skyrmion caps on top of antiskyrmions which renders them rectangular [3]. In this work, we investigate how external mechanical strain can be used as an additional tuning parameter for the stability of these topological magnetic textures. We show that strain breaks the degeneracy of distinct types of elongated skyrmions and antiskyrmions, which can be used to controllably switch the helicity of the textures. [1] A. Nayak et al. Nature 548, 561 (2017), [2] K. Karube et al. Nat. Mater. 20, 335 (2021), [3] F. S. Yasin, J. Masell, et al., Adv. Mater. 36 (16), 2311737 (2024)

MA 16.11 Tue 12:15 HSZ/0004

Multistable skyrmions in thin nanodots — •Mateusz Zelent[1,2] and Maciej Krawczyk[2] — [1]Fachbereich Physik and Landesforschungszentrum Optimas, Rheinland-pfälzische Technische Universität Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]Faculty of Physics and Astronomy, Adam Mickiewicz University, Poznan, ul. Uniwersytetu Poznańskiego 2, Poznan, Poland

We present a new method for controlling and manipulating magnetic skyrmions in ultrathin multilayer structures by employing spatially tailored magnetostatic

fields produced by ferromagnetic rings. Through a combination of analytical calculations and micromagnetic simulations, we demonstrate that the stray field generated by a Co/Pd ferromagnetic ring with perpendicular magnetic anisotropy can markedly increase the stability of skyrmions in an Ir/Co/Pt nanodot even when the Dzyaloshinskii Moriya interaction is entirely absent. Our analysis reveals a multistable behaviour, in which skyrmions can exist with two or even three distinct diameters, depending on the magnetization direction of the ring. The associated energy barriers separating these states are substantial, indicating possible applications in binary or multilevel magnetic data storage. We further show that transitions between these states can be triggered in a controlled and robust manner using short magnetic-field pulses. Overall, our approach offers a versatile strategy for engineering the magnetostatic energy landscape and designing skyrmion-based devices with customizable stability characteristics.

MA 16.12 Tue 12:30 HSZ/0004

First-Principles calculation of skyrmion collapse via the geodesic nudged elastic band approach — •Nihad Abuawwad[1], Daniel Wortmann[1], Gregor Michalicek[1], and Stefan Blügel[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich & JARA, 52425 Jülich, Germany — [2]Institute for Theoretical Physics, RWTH Aachen University, 52074 Aachen, Germany

Magnetic skyrmions are often investigated using spin models parameterized from first-principles calculations and achieving a fully *ab initio* description of skyrmion energetics and collapse mechanisms remains a significant challenge. In this work, we present a high-performance computing density functional theory (DFT) framework to compute both the skyrmion structure and its minimum-energy collapse pathway. Using the all-electron FLEUR code [1] within the AiiDA-FLEUR workflow environment [2], we construct an automated geodesic nudged elastic band (GNEB) workflow designed to determine the skyrmion collapse mechanism entirely from first principles. The method generates a sequence of intermediate magnetic states via geodesic interpolation between an initial skyrmion configuration and the final ferromagnetic state, and each image is evaluated under constrained magnetic moments to obtain accurate total energies and true magnetic forces. The resulting energy profile reveals the minimum energy path (MEP) and the associated barrier governing the topological skyrmion collapse. We compared these with the spin-model approach.

[1] D. Wortmann, et al. FLEUR, Zenodo (2023). [2] J. Broeder, et al., Proc. Extreme Data Workshop 40, 43*48 (2019).

MA 17: Multiferroics and Magnetoelectric Coupling (joint session MA/FM)

Time: Tuesday 9:30–12:30 Location: POT/0112

MA 17.1 Tue 9:30 POT/0112

Electric polarization driven by non-collinear spin alignment: first principles calculations — •Sergiy Mankovsky[1,3], Svitlana Polesya[1], Jan Minar[2], Hongbin Zhang[3], and Hubert Ebert[1] — [1]Ludwig Maximilian University of Munich, Munich, DE — [2]University of West Bohemia, Pilsen, CZ — [3]TU Darmstadt, Darmstadt, DE

We present an approach for first principles investigations of the spin driven electric polarization in type II multiferroics. We propose a parametrization of the polarization with the parameters calculated using the multiple scattering Green function (KKR-GF) formalism. On this basis, the induced electric polarization of a unit cell can be represented in terms of three-site parameters. Those antisymmetric with respect to a spin permutation can be seen as an ab-initio based counter-part to the phenomenological parameters used in the inverse-DMI model. Beyond to this, our new approach gives direct access to the element- and site-resolved electric polarization. To demonstrate the capability of the approach, we consider several examples, for which the magneto-electric effect is observed either as a consequence of an applied magnetic field (Cr_2O_3), or as a result of a phase transition to a spin-spiral magnetic state (MnI_2 and $AgCrO_2$).

MA 17.2 Tue 9:45 POT/0112

Competition Between Multiferroic and Magnetic Soliton Lattice States in DyFeO3 — •Nikita Andriushin[1], Stanislav Nikitin[2], Oystein Fjellvag[1,3], Ekaterina Pomjakushina[2], Alexandra Turrini[2], Sergey Artyukhin[4], Christof Schneider[2], and Maxim Mostovoy[5] — [1]TU Dresden, Germany — [2]PSI, Switzerland — [3]IFE, Norway — [4]IIT, Italy — [5]University of Groningen, The Netherlands

Simultaneous breaking of time-reversal and inversion symmetries in multiferroics couples ferroelectricity to magnetism and produces unusual phenomena relevant for next-generation electronics. A notable case is $DyFeO_3$, which under magnetic fields shows a giant linear magnetoelectric response and a large spontaneous polarization arising from coexisting Fe and Dy orders. Using high-resolution neutron diffraction, we demonstrate that at zero field $DyFeO_3$ hosts an incommensurate magnetic soliton lattice formed by spatially ordered Dy domain walls with an average size of 231(8) Å. Long-range interactions between these walls are mediated by magnons in the Fe subsystem, analogous to a Yukawa force. An applied magnetic field destroys the incommensurate order, restores the linear magnetoelectric response, and stabilizes the ferroelectric state. The magnetic domain walls carry electric charge, and the soliton array dimerizes when both electric and magnetic fields are applied. Simulations using experimental parameters indicate that competition between ferroelectric and incommensurate states can be effectively tuned by an electric field.

MA 17.3 Tue 10:00 POT/0112

Magnetoelectric coupling in antiferromagnetic $BiCoO_3$ — •Veronica Goian[1], Fedir Borodavka[1], Petr Proschek[2], Maxim Savinov[1], Christelle Kadlec[1], Hong Dong Nguyen[1], Andrei A. Belik[3], and Stanislav Kamba[1] — [1]Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic — [2]Department of Condensed Matter Physics, Charles University, Prague Czech Republic — [3]National Institute for Materials Science: Tsukuba, Ibaraki, Japan

$BiCoO_3$ is a potential multiferroic material with a C-type antiferromagnetic phase transition at T_N=470 K and a hypothetical ferroelectric phase transition around 1000 K (the sample decomposes at around 470 °C).[1] First-principles calculations predict an unusually strong antimagnetoelectric coupling in $BiCoO_3$.[2] However, no experimental measurements have been reported in the literature to determine the magnetoelectric coupling or related structural properties. This is mainly because $BiCoO_3$ requires high-pressure and high-temperature sintering. We have measured the dielectric permittivity, ferroelectric hysteresis loops, and Raman, THz, and IR spectra to probe the ferroelectric behavior. In addition, we found that $BiCoO_3$ exhibits well-measurable nonlinear magnetoelectric coupling.

[1] Oka et al., J. Am. Chem. Soc., 132, 9438-9443 (2010)
[2] Braun et al., Phys. Rev. B, 110, 144442(2024)

MA 17.4 Tue 10:15 POT/0112

Investigation of the piezomagnetic effect in $CaBaCo_4O_7$ — •Jyotiranjan Rout[1], Yusuke Tokunaga[2], Yasujiro Taguchi[2], Yoshinori Tokura[2], Bernd Büchner[1,3], and Vilmos Kocsis[1] — [1]IFW-Dresden — [2]RIKEN, CEMS, Japan — [3]TU-Dresden

In a magnetoelectric material the electric and magnetic responses are intertwined and cross control via the application of external magnetic and electric field are enabled. Ferroelectric polarization implies a special distortion of the lattice where dipolar moment related to the separation of the positive and negative ions are not compensated within the unit cell. Therefore we immediately can imagine the intricate and complicated connection between the magnetoelectric and magnetoelastic properties of a multiferroic.

The Swedenborgite $CaBaCo_4O_7$ exhibits a polar structure, which is accompanied by a ferrimagnetic order at T_C=62 K and a record large change in the ferroelectric polarization. Correspondingly, former magnetoelastic measurements have indeed confirmed the presence of a giant magnetoelastic distortion close to T_C; However, less is known about the magnetoelastic anisotropies.

Here, we report a detailed study of the magnetoelastic anisotropy, completing the connection between magnetoelasticity and magnetoelectricity in this material family. We also report on an unusual feature of the piezomagnetic effect, which suggests the importance of the orbitals in the piezomagnetoelectric effects.

MA 17.5 Tue 10:30 POT/0112

Multiferroic altermagnetism and magneto-orbital excitations in monolayer VCl3 — •Luigi Camerano[1,2], Adolfo Otero Fumega[3], Alessandro Stroppa[2], Jose Lado[3], and Gianni Profeta[1,2] — [1]University of L'aquila, 67100 L'Aquila, Italy — [2]CNR-SPIN L'Aquila, 67100 L'Aquila, Italy — [3]Aalto University, 02150 Espoo, Finland

Van der Waals monolayers featuring magnetic states provide fundamental building blocks for artificial quantum matter. In this contribution I will present the emergence of a symmetry broken multiferroic ground state featuring magneto-orbital excitations and nematic d-wave altermagnetism in monolayer VCl3 [1-4]. All these physics arises from a pure electronic symmetry breaking ultimately stabilizing an antiferro-orbital order ground state showing the emergence of an electronic polarization. Recent experimental evidence report signatures of symmetry breakings and ferroelectricity combined with 2D magnetism, establishing monolayer VCl3 as a novel 2D multiferroic driven by orbital ordering.

1. Mastrippolito D., Camerano L. et al. Phys. Rev. B 108,045126 (2023)
2. Camerano, L. et al. 2D Mater. 11, 025027 (2024)
3. Camerano, L. et al. Nano Lett. 25, 4825,4831 (2025)
4. Camerano, L. et al. npj 2D Mater Appl 9, 75 (2025)

MA 17.6 Tue 10:45 POT/0112

Electric control of antiferromagnetic states in an insulator — •Somnath Ghara[1], Maximilian Winkler[1], Sebastian Schmid[1,2], Lilian Prodan[1], Korbinian Geirhos[1], Vladimir Tsurkan[1,3], Wenbo Ge[4], Weida Wu[4], András Halbritter[2], Stephan Krohns[1], and István Kézsmárki[1] — [1]EP5, Institute of Physics, University of Augsburg, Germany — [2]Department of Physics, Budapest University of Technology and Economics, Hungary — [3]Institute of Applied Physics, Moldova State University, Republic of Moldova — [4]Department of Physics and Astronomy, Rutgers University, USA

Electric control of antiferromagnetic (AFM) order is highly desirable for the development of ultrafast and energy-efficient spintronic devices. In this talk, I will show that the strong linear magnetoelectric coupling in the collinear AFM insulator Co_3O_4 enables full isothermal control of AFM order by electric fields deep within its AFM phase, i.e. the Néel vector can be either reversed instantaneously or rotated smoothly. Importantly, we found that even in macroscopic volumes of Co_3O_4, the non-volatile switching between time-reversed AFM states occurs on timescales as short as a few tens of nanoseconds. These observations suggest that the quasi-cubic AFM insulators, such as Co_3O_4, provide an ideal platform for ultrafast manipulation of microscopic AFM domains and may lead to the realization of antiferromagnet-based spintronic devices.

Ref: S. Ghara et al., Phys. Rev. Lett. 135, 126704 (2025).

15 min break

MA 17.7 Tue 11:15 POT/0112

Optical detection of magnetic order in SmFe3(BO3)4 — •Bálint Beke[1], Bence Szász[1], I. A. Gudim[2], L. N. Bezmaternykh[2], Dávid Szaller[1], and Sándor Bordács[1] — [1]Budapest University of Technology and Economics, Budapest, Hungary — [2]Krasnoyarsk, Russia

The chiral crystal structure of $SmFe_3(BO_3)_4$ hosts an easy-plane antiferromagnetic phase below 32 K. Due to the broken inversion, the magnetic order induces electric polarization in this compound, but this polarization averages out to zero when domains are randomly oriented in the ab plane. We studied the 4f-4f excitations of Sm^{3+} ions using polarization resolved magneto-optical spectroscopy. Low magnetic fields, <2 T give rise to linear dichroism that we associate with the rearrangement of antiferromagnetic domains. In finite fields, we could determine the polarization selection rules in a state where the orientation of the antiferromagnetic domains is well defined. Moreover, we detected non-reciprocal absorption of light, which is a finite frequency fingerprint of the optical magnetoelectric effect.

MA 17.8 Tue 11:30 POT/0112

A high-temperature multiferroic $Tb_2(MoO_4)_3$ — •Shimon Tajima, Hidetoshi Masuda, Yoichi Nii, Shojiro Kimura, and Yoshinori Onose — Institute for Materials Research, Tohoku University, Sendai, Japan

We demonstrated magnetic control of ferroelectric polarization at 432 K in ferroelectric and ferroelastic $Tb_2(MoO_4)_3$, in which the polarity of ferroelectric polarization is coupled to the orthorhombic strain below the transition temperature 432 K.

The paramagnetic but strongly magnetoelastic Tb^{3+} magnetic moments enable the magnetic control of ferroelectric and ferroelastic domains; the ferroelectric polarization is controlled depending on whether the magnetic field is applied along [110] or [1$\bar{1}$0].

MA 17.9 Tue 11:45 POT/0112

Towards topological switching in multiferroics — •Alessandro Granero and Sergey Artyukhin — Italian Institute of Technology (IIT), Genova, Italy

Magnetoelectric switching in GdMn2O5 [1] is the first known example of topological ferroic switching, where magnetic field sweeps across the spin-reorientation transition induce incremental 90° spin rotations described by a topological winding number. While the behavior has been rationalized with a microscopic model, symmetry conditions and minimal model ingredients that enable this behavior are poorly understood. Here we use a symmetry-based Landau theory approach and demonstrate that a toy model with two frustrated antiferromagnetic subsystems and a low-symmetry anisotropy captures the topological switching behavior. The model reveals how sweeps of the driving field move the free-energy minimum continuously in spin-orientation space, in contrast to conventional ferroelectric switching that relies on fixed *P minima and domain-wall nucleation. Multiple switching pathways enabled by the simultaneous presence of E and H fields are summarized by a "switching diagram" [2], linking regions of the H and E field amplitudes to distinct sequences of magnetoelectric transitions. Small parameter variations near diagram boundaries redirect the system along different routes. The results establish a minimal model for topological switching in GdMn2O5 and guide the search for topological switching phenomena in other materials. [1] L. Ponet, et al.: Nature 607, 81-85 (2022) [2] M. Ryzhkov, A. Granero et al.: Communication Materials, in press

MA 17.10 Tue 12:00 POT/0112

Observation of antiferromagnetic domains by low-temperature photoluminescence microscopy — •Bence Szász — Physics Department, Budapest University of Technology and Economics, Budapest, Hungary

The optical oscillator strengths of crystal-field transitions in magnetoelectric antiferromagnets can serve as specific signatures of the underlying magnetic order. In this work, I investigate the feasibility of identifying magnetic domains using a low-temperature optical photoluminescence microscopy system.

MA 17.11 Tue 12:15 POT/0112

Spectroscopy of coupled magnetic and electric resonances — •Dávid Szaller[1,2], Artem M Kuzmenko[3], Alexander A Mukhin[3], Alexey Shuvaev[2], and Andrei Pimenov[2] — [1]HUN-REN-BME Condensed Matter Physics Research Group, and Department of Physics, Institute of Physics, Budapest University of Technology and Economics, Muegyetem rkp. 3., H-1111 Budapest, Hungary — [2]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [3]Moscow, Russia

Controllable non-reciprocal propagation of light is an intensively investigated field of optics, with studies motivated both by fundamental questions and possible telecommunication applications. So far, polarization-independent, switchable one-way transparency has been demonstrated at certain resonances of multiferroic crystals at cryogenic temperatures and in high magnetic fields, limiting the practical implementation. As an alternative approach, we present one-way transparency of an artificial layered structure consisting of split-ring metamaterial and magnetic substrate layers interacting in the dynamic regime [1]. Our quasi-optical experiments in the GHz frequency range show that this unique combination breaks time and space inversion symmetries in external magnetic field. The ease of tuning the dynamic response and the controllable one-way transparency make this approach promising for real-world applications.

[1] A. M. Kuzmenko et al., Phys. Rev. B 112, 134434 (2025).

MA 18: Caloric Effects in Ferromagnetic Materials (joint session MA/TT)

Time: Tuesday 9:30–11:30 Location: POT/0151

Invited Talk MA 18.1 Tue 9:30 POT/0151

Magnetic Cooling: From applications at room temperature to hydrogen liquefaction — •T. Gottschall[1], E. Bykov[1], M. Strassheim[1], T. Platte[2], C. Fujta[2], D. Benke[2], M. Fries[2], W. Liu[3], A. Döring[3], K. Skokov[3], O. Gutfleisch[3], and J. Wosnitza[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]MAGNOTHERM Solutions GmbH, Darmstadt, Germany — [3]Technical University of Darmstadt, Darmstadt, Germany

Magnetic cooling can be utilized to construct environmentally friendly cooling devices, air conditioners, and heat pumps. Recently, low temperatures became the focus of attention as an area of application for magnetocaloric cooling, namely for hydrogen liquefaction. The conventional liquefaction process uses up to 40 % of the lower heating value of the gas we are compressing, just to liquefy it! Magnetocaloric materials enable an alternative and more efficient approach. A large number of compounds are already known that show magnetocaloric effects in the desired temperature range and new candidates are constantly being added. In this work, we would like to discuss our current progress for the creation of a materials library for cryogenic applications. The basis for this is our characterization infrastructure for materials research at TU Darmstadt and the Dresden High Magnetic Field Laboratory in static and pulsed magnetic fields. Furthermore, we also provide an overview of the recent results in the demonstrator development of a magnetic hydrogen liquefier within the framework of the European project HyLICAL.

MA 18.2 Tue 10:00 POT/0151

Hydrogen tunned transition temperature of GdFeSi for magnetocaloric hydrogen liquefaction application — •Allan Döring[1], Wei Liu[1], Marc Strassheim[2], Tino Gottschall[2], Konstantin Skokov[1], and Oliver Gutfleisch[1] — [1]Institute of Materials Science, Functional Materials, Technical University of Darmstadt, Darmstadt, Germany — [2]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany

Hydrogen can play an important role in the future carbon-neutral society. Among several alternatives to store this energy carrier, the liquid H2 (LH2) stands out for its higher volume-to-energy ratio. However, the actual method of H2 liquefaction sums up to 34% of the costs of LH2. The magnetocaloric cooling could be one alternative to improve the efficiency of the process. Thus, it is essential to conduct research on materials exhibiting a strong magnetocaloric effect (MCE) within the temperature range of 20 K to 77 K. The peak of the MCE is at transition temperatures, such as the Curie temperature (TC). The mag-

netocaloric effect peak of GdFeSi is at 125 K. In this study, the TC of GdFeSi was shifted to lower temperatures by hydrogenation process, achieving a shift of over 90 K. By the anisotropic crystal expansion, GdFeSiH exhibited and higher magnetocaloric effect than the pristine alloy, not only by the isothermal entropy change, but also directly measured adiabatic temperature change. We acknowledge the HyLICAL project for the funding of this research through grant 101101461, and Deutsche Forschungsgemeinschaft (DFG) within the CRC/TRR 270 (Project-ID 405553726).

MA 18.3 Tue 10:15 POT/0151

First-principles investigation of chemical substitution and interstitial doping in La(Fe,Si)$_{13}$ — •Anita Yadav and Markus E. Gruner — University of Duisburg-Essen, 47057 Duisburg, Germany

$La(Fe_xSi_{1-x})_{13}$ is a prominent magnetocaloric material, characterized by a sharp first-order phase transition and a large associated entropy change. Its behavior arises from an intricate coupling among the magnetic, electronic, and lattice degrees of freedom, which makes the material highly responsive to external factors and enables targeted tuning of its magnetocaloric response [1,2]. The operating range can be modified through substitution and interstitial loading, which can alter the local atomic environment and reshape the coupling between structural and magnetic subsystems. In this work, we employ first-principles calculations in the framework of density functional theory (DFT) to systematically screen the impact of chemical substitution and loading of light elements on interstitial sites with respect to structural stability, lattice expansion, magnetic interactions, and thermodynamic behavior. Furthermore, we explore the benefits of machine-learning force-fields based on our DFT results for an efficient modeling of the thermodynamic properties of $La(Fe_xSi_{1-x})_{13}$-based compounds. Funding by the DFG via TRR270 (B06) is gratefully acknowledged.

[1] M. E. Gruner *et al.*, Phys. Rev. Lett. **114**, 057202 (2015)
[2] K. P. Skokov *et al.*, Appl. Phys. Rev. **10**, 031408 (2023)

MA 18.4 Tue 10:30 POT/0151

Magnetocaloric Laves phases based on light rare earths: Addressing Criticality — •M. Strassheim[1,2], L. Beyer[3,4], J. Wosnitza[1,2], and T. Gottschall[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Leibniz Institute for Solid State and Materials Research Dresden, Germany — [4]TU Bergakademie Freiberg, Germany

Laves-phase intermetallic compounds based on heavy rare-earth elements have long been recognized for their excellent magnetocaloric performance at low temperatures, making them promising candidates for cryogenic cooling applications. However, the reliance on heavy rare earths poses challenges in terms of cost, availability, and sustainability. In this work, we explore the magnetocaloric properties of the light rare-earth-based Laves phase $CeFe_2$. By the substitution of Al, its unstable ferromagnetism can be disturbed enough to establish an antiferromagnetic phase below 80 K. Using a combination of structural, magnetic, and direct adiabatic temperature change measurements at the Dresden High Field Laboratory, we investigate the potential of this antiferromagnetic state for its potential in magnetocaloric hydrogen liquefaction.

MA 18.5 Tue 10:45 POT/0151

Pressure effect on the magnetocaloric response of RCo_2 Laves Phases — •Catalina Salazar-Mejia[1], E. Bykov[1], W. Liu[2], K. Skokov[2], O. Gutfleisch[2], J. Wosnitza[1,3], and T. Gottschall[1] — [1]High Magnetic Field Laboratory (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Institut für Materialwissenschaft, TU Darmstadt, Germany — [3]Institut für Festkörper- und Materialphysik, TU Dresden, Germany

Rare-earth Laves phases are potential candidates for magnetic refrigeration at cryogenic temperatures. They exhibit large magnetocaloric effects and their transition temperatures can be tuned through elemental substitutions. In this work, we investigate the effect of hydrostatic pressure on the magnetism and magnetocaloric effect of RCo_2 Laves phases with rare-earth elements R = Tb, Dy, Ho, and Er. In general, we observe that the Curie temperature, T_C, decreases with applied pressure in all alloys. T_C is most sensitive to pressure in $TbCo_2$, with $dT_C/dp \approx -22$ K/GPa, and this value decreases systematically along the series, reaching $dT_C/dp \approx -7.7$ K/GPa in $ErCo_2$. More interestingly, hydrostatic pressure has an almost negligible effect on the magnetocaloric response - specifically on the isothermal entropy change, ΔS_T, with the exception of $HoCo_2$, where ΔS_T increases by about 26% under an applied pressure of approximately 1 GPa and for a magnetic field change of 5 T.

MA 18.6 Tue 11:00 POT/0151

Manipulating Magnetocaloric Properties Through Magnetic Exchange at $Mn_{3-x}GaC$/Fe Interfaces — •Ivan Tarasov and Ulf Wiedwald — Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany

Magnetocaloric materials enable solid-state cooling by exploiting temperature changes under magnetic-field variation. Manganese-based antiperovskites (APVs, Mn_3AX) are promising materials due to their sharp, tunable first-order magnetostructural transition (FOMST). A key challenge is to control the working temperature window and enhance the magnetocaloric response within a given material system. Tailoring magnetic exchange interactions offers a new strategy.

Here, we investigate APV/Fe bilayers, focusing on interface-driven exchange effects. Uncoupled $Mn_2GaC_{1.1}$ films show a sharp FOMST at 189 K with a strong $\partial M/\partial T$ peak. A 5 nm Fe cap lowers the transition to 175 K, broadens hysteresis, and suppresses the $\partial M/\partial T$ peak above 1 T. The bare APV exhibits $\Delta S_m \approx 10$ J kg^{-1} K^{-1} at $B = 6$ T, whereas coupling reduces this to ~ 1 J kg^{-1} K^{-1} at $B = 5$ T. In multi-domain bilayers, $\partial M/\partial T$ increases by 15% (AFM–FM) and 46% (FM–PM) for a Fe film thickness of $t = 2.6$ nm, but disappears for $t = 21$ nm, accompanied by an anomaly near 50 K linked to interfacial AFM ordering.

Funding by the Deutsche Forschungsgemeinschaft (DFG) within CRC/TRR 270, project B02 (Project-ID 405553726) is gratefully acknowledged.

MA 18.7 Tue 11:15 POT/0151

Frustration and Antiferromagnetic Ordering in Low-Temperature Materials for Adiabatic Demagnetization — •Anton Jesche, Tim Treu, Marvin Klinger, Jorginho Villar Guerrero, and Philipp Gegenwart — EP VI, Institute of Physics, University of Augsburg, Germany

The development of improved materials for adiabatic demagnetization refrigeration (ADR) has been driven increasingly by research on magnetically frustrated systems, where competing interactions can suppress magnetic ordering to very low temperatures [1]. Such behavior is particularly attractive for low-temperature cooling and has led to several promising rare-earth-based compounds. Notable examples include $KBaYb(BO_3)_2$, which reaches temperatures near 20 mK [2], and $NaGdP_2O_7$, which demonstrates extended hold times below 2 K in standard cryogenic environments [3].

This contribution will highlight selected Yb- and Gd-based materials and discuss the influence of frustration and antiferromagnetic (AFM) ordering on their cooling performance. Using $NaGdP_2O_7$ as a representative case, we examine how magnetic entropy near AFM transitions affects ADR behavior under varying magnetic fields and temperatures. We further show that high-resolution thermodynamic information, such as heat capacity, can be extracted directly from ADR curves.

[1] M. E. Zhitomirsky, Phys. Rev. B, 2003, 67, 104421
[2] Y. Tokiwa, Commun. Mater. 2021, 2, 42
[3] P. Telang, Phys. Rev. B, 2025, 111, 064434

MA 19: Frustrated Magnets I (joint session MA/TT)

Time: Tuesday 9:30–12:30 Location: POT/0361

MA 19.1 Tue 9:30 POT/0361

Spontaneous symmetry breaking in the Heisenberg antiferromagnet on a triangular lattice — •Bastian Pradenas[1,2], Grigor Adamyan[1,3], and Oleg Tchernyshyov[1] — [1]William H. Miller III Department of Physics and Astronomy, Johns Hopkins University, Baltimore, USA — [2]Leibniz Institute for Solid State and Materials Research, IFW, Dresden, Germany — [3]Department of Physics, Massachusetts Institute of Technology, Cambridge, USA

We present a detailed investigation of an overlooked symmetry structure in non-collinear antiferromagnets that gives rise to an emergent quantum number for magnons. Focusing on the triangular-lattice Heisenberg antiferromagnet, we show that its spin order parameter transforms under an enlarged symmetry group, $SO(3)_L \times SO(2)_R$, rather than the conventional spin-rotation group SO(3). Although this larger symmetry is spontaneously broken by the ground state, a residual subgroup survives, leading to conserved Noether charges that, upon quantization, endow magnons with an additional quantum number—*isospin*—beyond their energy and momentum. Our results provide a comprehensive framework for understanding symmetry, degeneracy, and quantum numbers in non-collinear magnetic systems, and bridge an unexpected connection between the paradigms of symmetry breaking in non-collinear antiferromagnets and chiral symmetry breaking in particle physics.

MA 19.2 Tue 9:45 POT/0361

Antiferro octupolar order in the 5d^1 double perovskite Sr_2MgReO_6 and its spectroscopic signatures — •Dario Fiore Mosca[1] and Leonid Pourovskii[2,3] — [1]University of Vienna, Faculty of Physics and Center for Computational Materials Science, Vienna, Austria — [2]CPHT, CNRS, Ecole polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France — [3]College de France, Université PSL, 11 place Marcelin Berthelot, 75005 Paris, France

Hidden-order phases governed by high-rank multipolar order parameters have recently been identified in several cubic 5d double perovskites. Because experimental probes often couple weakly to high-rank moments, multipolar orders can remain elusive or be misinterpreted as lower-rank phases. A notable example is the $5d^1$ double perovskite Sr_2MgReO_6, originally proposed as a spin glass and later reclassified as a conventional dipolar antiferromagnet.

In this work, we show instead that Sr_2MgReO_6 hosts a hidden antiferroic order of magnetic octupoles. The dominant tetragonal crystal field isolates a doublet carrying octupolar degrees of freedom, while weak dipolar moments arise only through admixture of the excited j = 1/2 spin-orbit multiplet. This octupolar order produces characteristic quasigapless magnetic excitations and superstructural neutron-diffraction intensities that peak at large scattering momenta.

This results highlights the tunability of multipolar interactions in spin-orbit entangled materials and places Sr_2MgReO_6 with unconventional octupolar phases.

MA 19.3 Tue 10:00 POT/0361

Field-dependent CEF excitations in Ce_2Bi — •Nikolai Pavlovskii[1], Alexander Sukhanov[2], Anton Kulbakov[1], Michael Smidman[3], Federico Mazza[4], Darren Peets[1], Kaushick Parui[1], Ross Stewart[5], Ross Piltz[6], and Dmytro Inosov[1] — [1]TU Dresden, Germany — [2]University of Augsburg, Germany — [3]Zhejiang University, China — [4]TU Vienna, Austria — [5]ISIS, UK — [6]ANSTO, Australia

Ce_2Bi is a cerium-based intermetallic compound where crystal-field (CEF) splitting and anisotropic magnetic interactions occur on comparable energy scales. To identify the relevant low-energy degrees of freedom, we investigate the field dependence of CEF-related excitations in single-crystalline Ce_2Bi using neutron-scattering techniques. Single-crystal diffraction establishes the crystallographic symmetry at the Ce site, providing the structural framework required for interpreting the magnetic excitations. The excitation spectrum shows a clear magnetic mode within the $J = 5/2$ manifold whose energy and intensity vary strongly with applied field. Crucially, the mode displays clear dispersion, demonstrating the presence of exchange interactions; as a result, what was previously interpreted as a localized CEF level is revealed to be a dispersive magnetic exciton. The field-induced evolution of this exciton constrains the mixing within the CEF manifold and the anisotropy of the ground-state Kramers doublet.

MA 19.4 Tue 10:15 POT/0361

High-field magnetic excitations in a kagome antiferromagnet — •Yoshihiko Ihara[1], Dmytro Inosov[2], Darren Peets[2], Moyu Kato[1], and Hiroyuki Yoshida[1] — [1]Hokkaido University, Sapporo, Japan — [2]TU Dresden, Dresden, Germany

Magnetic ground states in kagome antiferromagnets have been intensively studied to reveal the quantum mechanically disordered magnetic states. By applying high magnetic fields, further intriguing phenomena have been introduced such as the plateau in magnetization curve at the 1/9 of the full saturation value in $YCu_3(OH)_{6.5}Br_{2.5}$. [S. Jeon et al., Nat. Phys. **20**, 435 (2024), S. Suetsugu et al., PRL **132**, 226701 (2024), G. Zheng et al., PNAS **122**, e2421390112 (2025)]. Although higher magnetic fields induce another magnetization plateau at the 1/3 of the full saturation, the field strength required to access the 1/3 plateau is more than 50 T and is too large to perform most of the microscopic experiments. Thus, we focus on another Cu-based mineral $InCu_3(OH)_6Cl_3$, which shows the 1/3 plateau around 10 T due to smaller energy scale of exchange interactions [M. Kato et al., Commun. Phys. **7**, 424 (2024)]. This allows us to perform NMR experiments in the entire field range reaching the full saturation. The measured nuclear spin-lattice relaxation rate demonstrates that the magnetic excitations are gapped in the 1/3 plateau state and the gap size increases with fields [M. Kato et al., JPSJ **94**, 083704 (2025)]. We will also discuss the magnetic excitations above the 1/3 plateau based on the results obtained in the high-field magnet in Tohoku Univ.

MA 19.5 Tue 10:30 POT/0361

Evidence for a Near-Ideal Jeff = 1/2 Ground State in Triangular-Lattice Na2BaCo(PO4)2 — •Miguel M. F. Carvalho[1,2], Sheng H. Chen[1], Yu C. Ku[3,4], Anagha Jose[5], Ryan Morrow[5], Chang Y. Kuo[3,4], Chun F. Chang[1], Zhiwei Hu[1], Maurits W. Haverkort[6], and Liu H. Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids,Dresden — [2]Institute of Physics II, University of Cologne — [3]Department of Electrophysics, National Yang Ming Chiao Tung University, Hsinchu, Taiwan — [4]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [5]Institut fuer Festkoerperphysik, Leibniz IFW, Dresden — [6]Institute for theoretical physics, Heidelberg University

We investigated the local Co 3d electronic structure of Na2BaCo(PO4)2 using polarization-dependent X-ray absorption spectroscopy (XAS) together with full multiplet cluster calculations. To obtain reliable spectra from this strongly insulating material, we employed the line-fitting inverse partial fluorescence yield (IPFY) method. Our combined experimental and theoretical analysis shows that the CoO6 octahedra exhibit only a very small effective trigonal distortion of about 11 meV, placing the system close to the ideal conditions for a Jeff = 1/2 ground state. Using our cluster model, we are also able to simulate the magnetic susceptibility along different crystallographic directions, . Overall, these results establish Na2BaCo(PO4)2 as a promising platform for investigating exotic magnetic behavior linked to Jeff = 1/2 states on triangular lattices.

MA 19.6 Tue 10:45 POT/0361

Dimensional reduction and fractionalized magnetization plateaus in the scalene-distorted triangular-lattice magnet kobyashevite — •Kaushick Parui[1], Anton Kulbakov[1], Roman Gumeniuk[2], Maria Teresa Fernandez-Diaz[3], Sergey Granovsky[1], Sergei Zvyagin[4], Dmytro Inosov[1], and Darren Peets[1,5] — [1]TU Dresden, Germany — [2]TU Bergakademie Freiberg, Germany — [3]ILL, France — [4]HZDR, Germany — [5]ct.qmat, TU Dresden, Germany

Quantum magnetism intertwined with lattice distortion can give rise to exotic ground states, yet studies on scalene-distorted triangular-lattice antiferromagnets remain scarce. Here, we report the crystal and magnetic structures, as well as magnetic and thermodynamic properties, of kobyashevite, $Cu_5(SO_4)_2(OH)_6{\cdot}4H_2O$. This compound hosts a scalene-distorted triangular lattice and exhibits antiferromagnetic order at 4 K, with a possible second transition at 0.64 K. High-field magnetization and specific-heat measurements reveal a cascade of field-induced states, manifested as magnetization plateaus, suggestive of a rich magnetic phase diagram. Neutron diffraction uncovers a dimensionally-reduced commensurate magnetic structure with propagation vector $\mathbf{k} = (0\,0\,\frac{1}{2})$, consisting of coupled alternating ferromagnetic and antiferromagnetic spin chains, while the Cu4 spins remain idle at 1.5 K. Collectively, these results establish kobyashevite as a promising platform for exploring the interplay of frustration, distortion, and dimensional reduction in quantum magnets.

15 min break

MA 19.7 Tue 11:15 POT/0361

Atomically sharp magnetic solitons for racetrack memory at the spatial limit — K Allen[1], K Du[2], J Bouaziz[3], S Mishra[1], G Bihlmayer[3], Y Zhang[1], Y Hao[4], V Ukleev[5], C Luo[5], F Radu[5], Y Gao[1], Ch Lane[6], J-X Zhu[6], M Yi[1], H Cao[4], S-W Cheong[2], •Stefan Blügel[3], and Emilia Morosan[1] — [1]Dept. of Physics and Astronomy & Rice Center for Quantum Materials, Rice University, Houston, 77005, TX, USA — [2]Dept. of Physics and Astronomy, Rutgers University, Piscataway, 08854, NJ, USA — [3]Peter-Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany — [4]Neutron Scattering Division, Oak Ridge Natl Lab, Oak Ridge, 37831, TN, USA — [5]Helmholtz-Zentrum Berlin, 14109 Berlin, Germany — [6]Theoretical Division, Los Alamos Nat. Lab., Los Alamos, 87545, NM, USA

We discuss the physics of a metallic square-net lattice rare-earth compound that exhibits RKKY interactions leading to magnetic frustration whose effective exchange interactions competes with the uniaxial anisotropy resulting in a rare ferrimagnetic up-up-down phase. Applying magnetic fields, atomically sharp solitons can be precipitated that have all the foundational credentials for a racetrack memory at the spatial limit. We present DFT calculations relating the RKKY interaction and the magnetic anisotropy to the electronic structure. We performed atomistic spin-dynamics calculations relating the interaction parameters to the soliton formation. A combination of experiments will be presented that provide evidence of the 1D magnetic solitons.

MA 19.8 Tue 11:30 POT/0361

Guest*Controlled Quantum Magnetism in a Flexible Metal-Organic Framework — •Fang Liu[1], Armin Schulz[2], Axel Lubk[4], Alexej Pashkin[3], Sergej Granovski[1], Shuhan Wang[1], Weinel Kristina[4], Herzog Max[4], and Stefan Kaiser[1] — [1]Institute of Solid State and Materials Physic, Dresden University of Technology — [2]Max Planck Institute for Solid State Research, Stuttgart — [3]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [4]Leibniz Institute for Solid State and Materials Research, Dresden

Metal-organic frameworks provide an unusual setting where magnetic frustration and structural flexibility coexist. In our system, two distinct states emerge: a guest-stabilized regime with signatures of a potential quantum spin liquid, and a guest-free state exhibiting weak magnetic ordering. Raman and infrared spectroscopy reveal pronounced differences in lattice modes between these phases. Complementary Raman and THz measurements further uncover contrasting magnetic backgrounds. These findings establish a guest-controlled route to tuning magnetic quantum states in MOFs.

MA 19.9 Tue 11:45 POT/0361

Investigation of spin-correlated phases in quasi two-dimensional layered honeycomb oxide — •Aprajita Joshi[1], Anjali Kumari[2,3], Shalini Badola[1], Anup Kumar Bera[2,3], and Surajit Saha[1] — [1]Indian Institute of Science Education and Research Bhopal, 462066, India — [2]Bhabha Atomic Research Centre, Mumbai 400085, India — [3]Homi Bhabha National Institute, Mumbai 400094, India

Honeycomb oxides are an intriguing class of materials characterised by low dimensionality and strong magnetic frustration, which leads to exotic quantum spin correlations. Here, we investigated a quasi-two-dimensional magnetic ox-

ide Na2Co2TeO6, which exhibits several intriguing magnetic phases, including the zigzag antiferromagnetic interaction and Kitaev paramagnetic spin interactions. We explored the intricate relationship between these phases and phonons using temperature-dependent Raman measurements. Our findings reveal the signature of magnetoelastic coupling across the long-range and short-range magnetic ordering temperatures. Furthermore, Na2Co2TeO6, which has a noncentrosymmetric crystal structure, showcases ferroelectric order below 80 K. The evolution of Raman spectra reveals the presence of a ferroelectric order coupled phonon mode in Na2Co2TeO6 below this temperature.

MA 19.10 Tue 12:00 POT/0361

Characterizing entanglement at finite temperature: how does a paramagnet become a quantum spin liquid? — Snigdh Sabharwal[1,2], •Matthias Gohlke[1], Paul Skrzypczyk[2], and Nic Shannon[1] — [1]Okinawa Institute of Science and Technology, Onna, Japan — [2]H. H. Wills Physics Lab., University of Bristol, Bristol, UK

Quantum spin liquids (QSL) are generically many body entangled states of matter that form when quantum fluctuations meet the extensive ground state degeneracy of a classical spin liquid. Entanglement properties have enabled to characterise gapped QSL at zero temperature, however, much less is known about how quantum many body entanglement evolves at finite temperature.

Here, we use entanglement depth and genuine multipartite entanglement (GME) to study how entanglement and its local structure emerge when cooling a frustrated magnet from the high-temperature paramagnet down to the low-temperature QSL state. Within a case study on the Kitaev Honeycomb model, we obtain two characteristic bounds: (1) a lower bound on the upper temperature below which separability breaks and quantum entanglement must be present, while (2) a lower temperature scale is obtained when GME on plaquettes becomes finite signifying the coherent, structured entanglement that is characteristic for QSL ground states [1], i.e. the flux free state of the Kitaev spin liquid. We provide a framework to discuss the relevant temperature scales for QSL in frustrated magnets [2].

[1] L. Lyu, D. Chandorkar, et al., arXiv:2505.18124
[2] S. Sabharwal, M. Gohlke, et al., arXiv:2511.15144

MA 19.11 Tue 12:15 POT/0361

Fate of the Triangular Dirac spin liquid under an external magnetic field — •Sasank Budaraju[1,2], Josef Willsher[3], Federico Becca[4], Johannes Knolle[1,2], and Frank Pollmann[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany — [3]Max-Planck-Institut fur Physik komplexer Systeme, 01187 Dresden, Germany — [4]Dipartimento di Fisica, Universita di Trieste, Strada Costiera 11, I-34151 Trieste, Italy

We investigate the J1-J2 Heisenberg model under an external Zeeman field using the Variational Monte Carlo approach. Simple variational ansatzes are proposed for several candidate ordered states, and their energetics are compared on large clusters to obtain the phase diagram for small/moderate fields. For small J2, we capture a continuous transition from the Y to the "Up-Up-Down" (UUD) states as predicted by spin-wave theory. Additionally, around the highly frustrated region, we demonstrate that the ground state in the presence of a small field is a condensate of monopoles, which are gapless gauge excitations of the U (1) spin liquid. The monopole condensate is shown to be the ground state for a significant region of phase diagram, which we estimate using finite size numerics. Our results imply that the Dirac spin liquid is unstable to a condensation of monopoles in the presence of external fields.

MA 20: Altermagnets III

Time: Tuesday 14:00–15:30 Location: HSZ/0002

MA 20.1 Tue 14:00 HSZ/0002

Curvature-induced magnetization of altermagnetic films — •Kostiantyn Yershov[1,2], Volodymyr Kravchuk[1,2], and Jeroen van den Brink[1] — [1]Leibniz Institute for Solid State and Materials Research, 01069 Dresden, German — [2]Bogolyubov Institute for Theoretical Physics, 03143 Kyiv, Ukraine

Here we generalize the previously developed phenomenology of the d-wave altermagnetic films for the case of a curvilinear film bent in a stretching-free manner. We show that a stretching-free bending of a thin altermangnetic film with nonzero curvature gradients induces local magnetization that is approximately tangential to the film. The origin of curvature-induced magnetization is nonuniformity of the Neel vector distribution generated by the non-zero curvature gradients. The magnitude of the curvature-induced magnetization is determined by the curvature gradient and the direction of bending relative to the crystallographic axes. The maximal effect is achieved when bending is in the direction of maximum altermagnetic splitting in the magnon spectrum. For a periodically bent film of sinusoidal shape possesses a total magnetic moment per period $\propto A^2 q^4$ where A and q are the bending amplitude and wave vector, respectively. The total magnetic moment is perpendicular to the plane of the unbent film and its direction (up or down) is determined by the bending direction.

MA 20.2 Tue 14:15 HSZ/0002

Strain controlled g -to d-wave transition in altermagnetic CrSb — Bennet Karetta[1], •Xanthe Verbeek[1], Rodrigo Jaeschke-Ubiergo[1], Libor Šmejkal[2,3,4], and Jairo Sinova[1,5] — [1]Insitut für Physik, Johannes Gutenberg-Universität Mainz, D-55099 Mainz, Germany — [2]Max-Planck-Institut für Physik Komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany — [3]Max-Planck-Institut für Chemische Physik Fester Stoffe, Nöthnitzer Str. 40, 01187 Dresden, Germany — [4]Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnická 10, Prague 6, Czech Republic — [5]Department of Physics, Texas A&M University, College Station, Texas 77843-4242, USA

We demonstrate a strain-induced transition in the g-wave altermagnet CrSb, revealing how shear strain can tune spin symmetries and enable new responses. Focusing on the spin-splitter effect, which allows for pure spin currents but is forbidden in unstrained CrSb, we identify four shear-strain directions that lower the symmetry and enable spin conductivity. These strains induce three d-wave altermagnetic states and one uncompensated magnetic phase, each with distinct spin symmetries. Using both a minimal model and first-principles calculations, we confirm the emergence of these phases and show that their key features remain robust in the presence of spin-orbit coupling. We predict a spin-splitter effect of up to 5% under just 1% strain, showing that even small deformations can generate sizable spin-splitter currents. Our findings highlight strain as a precise and effective tool for controlling symmetry-driven spin phenomena in altermagnets.

MA 20.3 Tue 14:30 HSZ/0002

Designing non-relativistic spin-splitting in transition metal oxide bulk and heterostructures — •Subhadeep Bandyopadhyay and Rossitza Pentcheva — Department of Physics, University of Duisburg-Essen, Duisburg, Germany

Non-relativistic spin splitting (NRSS) of bands in collinear antiferromagnets is an exotic phenomenon, that has currently shifted in the focus, owing to the great potential for various spintronic applications. Studies showed that the inhomogeneous distribution of the real space magnetization density, originating from the ferroically ordered magnetic octupole moments[1] is the key to this exotic phenomenon, which stems from the global time reversal symmetry (TRS) breaking in antiferromagnets. In perovskite ABO_3 materials, we find an intriguing correlation between the antiferroic distortion patterns and the antiferromagnetic order, that breaks TRS to induce NRSS[2].

Here we explore how structural distortions and antiferromagnetism combine to induce NRSS in perovskites. Building on that insight, we demonstrate the recipe to design and control the NRSS. Beyond the bulk compounds, the discussion is extended to the perovskite heterostructures, where interface-driven structural distortions and modifications of the electronic properties are crucial.

1. S Bhowal and N A Spaldin, Phys. Rev. X 14, 011019 (2024)
2. S. Bandyopadhyay, S Picozzi, S Bhowal, Phys. Rev. B 112, 064405, (2025)

MA 20.4 Tue 14:45 HSZ/0002

hall viscosity of altermagnet — •iksu jang[1], rui aquino[2], rafael fernandes[3,4], and jörg schmalian[1,5] — [1]Institute for Theory of Condensed Matter, Karlsruhe Institute of Technology, Karlsruhe 76131, Germany — [2]ICTP, South American Institute for Fundamental Research Instituto de Física Teórica da UNESP, Universidade Estadual Paulista, Rua Doutor Bento Teobaldo Ferraz 271, 01140-070 São Paulo, Brasil — [3]Department of Physics, The Grainger College of Engineering, University of Illinois Urbana-Champaign, Urbana, Illinois 61801, USA — [4]Anthony J. Leggett Institute for Condensed Matter Theory, The Grainger College of Engineering, University of Illinois Urbana-Champaign, Urbana, Illinois 61801, USA — [5]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, Karlsruhe 76131, Germany

Altermagnets have garnered significant interest due to their ability to exhibit spin splitting without spin orbit coupling and their symmetry-driven phenomena, such as elastic quantum criticality and elasto-Hall responses. In this work, we investigate the Hall viscosity of altermagnets subject to strain. Using group-theoretical analysis and tight-binding calculations, we show that altermagnetic systems with various form factors can host a finite Hall viscosity. We additionally propose that the acoustic Faraday effect offers a viable route for its experimental detection.

MA 20.5 Tue 15:00 HSZ/0002

Dynamical orbital pumping in altermagnets — •Guidobeth Sáez-Toro[1], Mirco Sastges[2], Myunil Choi[3], Dongwook Go[3], and Yuriy Mokrousov[2] — [1]Departamento de Física, Facultad de Ciencias, Universidad de Chile, Santiago 7800024, Chile — [2]Peter Grünberg Institute (PGI-6), Forschungszentrum Jülich, 52425 Jülich, Germany — [3]Department of Physics, Korea University, Seoul 02841, Republic of Korea

Altermagnets constitute a recently recognized class of magnetic materials in which symmetry breaking between sublattices and orbital degrees of freedom gives rise to unconventional magnetic responses. A direct consequence of this symmetry structure is that time-dependent magnetization generates a purely orbital pumping mechanism, $\partial_t \langle \mathbf{L} \rangle_\alpha = \chi^L_{\alpha\beta} (\hat{\mathbf{m}} \times \partial_t \hat{\mathbf{m}})_\beta$, mediated by spin-orbit coupling. We investigate this effect by driving the Néel order in a minimal tight-binding model on a square altermagnetic lattice, based on an antiferromagnetic array of spins with an orbital crystal field breaking both C_4 rotational and sublattice exchange symmetries. Our results reveal a pronounced sublattice dependence of the orbital response, providing a clear microscopic distinction between antiferromagnetic and ferromagnetic configurations. Using the Bastin-Smrcka-Streda Kubo formula, we compute the full response tensor and show that orbital pumping naturally decomposes into two robust contributions, analogous to field-like and damping-like components. These findings establish orbital pumping as a distinctive dynamical signature of altermagnets and highlight its potential for next-generation orbitronic functionalities.

MA 20.6 Tue 15:15 HSZ/0002

Unique responses in odd-parity nodal p-wave magnets — •Atasi Chakraborty[1], Anna Birk Hellenes[1], Rodrigo Jaeschke Ubiergo[1], Tomas Jungwirth[2,3], Libor Šmejkal[2,4], and Jairo Sinova[1,5] — [1]Institut für Physik, Johannes Gutenberg Universität Mainz — [2]Institute of Physics, Academy of Sciences of the Czech Republic — [3]School of Physics and Astronomy, University of Nottingham — [4]Max Planck Institute for the Physics of Complex Systems,Dresden — [5]Department of Physics, Texas A & M University

The recent discovery of Altermagnetism – spin-split even-parity compensated magnets – highlights how spin symmetries can reveal exchange-driven phenomena that has previously been overlooked. Building on this insight, we explore spin symmetry criteria [1,3] to identify the odd-parity magnetic states in non-collinear systems, focusing on effects driven purely by exchange interactions, independent of spin-orbit coupling. In this talk, I will focus on the lowest-order (pwave) nodal odd-parity magnets, and discuss their characteristic responses [1, 2]. We show that these p-wave magnetic phases spontaneously break crystal symmetries, leading to pronounced exchange-mediated resistive anisotropy [1] and exhibit a large, purely non-relativistic, anisotropic out-of-plane charge-to-spin conversion [2], fundamentally distinct from the conventional Rashba-Edelstein effect.

1. Hellenes, Jungwirth, Ubiergo, Chakraborty, Sinova, Šmejkal, arXiv:2309.01607v3 (2020). 2. Chakraborty, Hellenes, Ubiergo, Jungwirth, Šmejkal, Sinova, Nature Communications 16, 7270 (2025). 3. Jungwirth, Fernandes, Sinova, Šmejkal, arXiv:2409.10034v1 (2024)

MA 21: Skyrmions II

Time: Tuesday 14:00–15:30 Location: HSZ/0004

MA 21.1 Tue 14:00 HSZ/0004

Real-Time Modeling of Skyrmion Dynamics in Arbitrary 2D Spatially Dependent Pinning Potential Landscapes — •Simon M. Fröhlich, Tobias Sparmann, Maarten A. Brems, Jan Rothörl, Fabian Kammerbauer, Klaus Raab, Sachin Krishnia, Mathias Kläui, and Peter Virnau — Institute of Physics, Johannes Gutenberg University Mainz

We investigate how non-flat pinning landscapes influence skyrmion dynamics and develop a quantitative framework that links experimental measurements to predictive simulations. Using real-time magneto-optical Kerr microscopy, we track skyrmion hopping and dynamics in a magnetic thin-film system and extract dwell times and transition statistics across pinning sites. This data is used to construct parameters for a coarse-grained Thiele model, for which we introduce a two-stage parameter identification procedure that directly maps experimental observables onto simulation units. This calibration resolves a key barrier to quantitative quasiparticle-level modeling by enabling reconstruction of pinning energies not directly accessible on experimental timescales. We validate the resulting simulation framework by predicting the density dependence of skyrmion diffusion and confirming it through long-time measurements. The approach provides a robust, simulation-ready description of the pinning landscape and establishes a pathway for predictive in-silico exploration of skyrmion dynamics and device concepts on experimentally relevant time and length scales.

MA 21.2 Tue 14:15 HSZ/0004

Theoretical study on excitation in anti-Skyrmion lattice — •László Udvardi, Mátyás Török, and László Szunyogh — Department of Theoretical Physics, Budapest University of Technology and Economic

Magnetic Skyrmions exhibit intriguing and novel phenomena due to their topologically non-trivial spin textures. Their exceptional stability makes them possible candidates for information carriers for future spintronic devices.

We have determined the parameters appearing in a classical spin model from first principle for $Pt_{95}Ir_{05}$/Pd(111) overlayer. Optimizing the energy of the spin model several local minima have been identified as a Skyrmion with various topological charges. We demonstrate that the frustration of the isotropic exchange interactions is responsible for the creation of these various types of skyrmionic structures. Our study is focused on objects with topological charge of Q=1 anti-Skyrmion. Anti-skyrmions exhibit attractive inter-particle interaction and they have tendency to form clusters or skyrmionic lattice. The excitation spectrum of an anti-skyrmon lattice with various external magnetic field has been calculated. The low energy excitation responsible for the low temperature behavior of the system shows similarities to nematic liquid crystals.

MA 21.3 Tue 14:30 HSZ/0004

Skyrmion topological Hall effect in Ta/CoFeB/MgO at room temperature detected with Kerr microscopy — •Hauke Lars Heyen[1], Michael Vogel[2], Florian Gossing[2], Jakob Walowski[1], Jeffrey McCord[2], and Markus Münzenberg[1] — [1]Institute of Physics, University Greifswald, Germany — [2]Institute of Materials Science, Nanoscale Magnetic Materials and Magnetic Domains, CAU Kiel, Germany

The topological Hall effect is interesting for characterizing materials and their non-trivial spin structures. It arises from spin textures with a finite topological charge, such as skyrmions. In this work, we measured the topological Hall effect originating from topologically protected skyrmions in Ta/CoFeB/MgO single-layer films. Since the small topological Hall contribution appears on top of the dominating anomalous Hall effect, its direct detection in this material system is challenging. Electrical Hall effect measurements contain both effects and to separate these, Kerr-microscopy (MOKE) measurements are carried out simultaneously to Hall effect measurements. We further verify the results with thermal and electrical transport measurements to calculate a topological quantity that contains the topological Nernst and Hall effect respectively. Those measurements are conducted using the experimental scheme introduced in [1].

[1] R. Schlitz et al. All Electrical Access to Topological Transport Features in Mn1.8PtSn Films. Nano Letters, 19(4):2366-2370, March 2019.

MA 21.4 Tue 14:45 HSZ/0004

Optimization of magnetic skyrmion diffusion in thin films — •Alen John[1,2], Maria Andromachi Syskaki[1], Jürgen Langer[1], Gerhard Jakob[2], and Mathias Kläui[2] — [1]Singulus Technologies AG, 63796 Kahl am Main, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, 55128 Mainz, Germany

Topological magnetic solitons, particularly skyrmions, have garnered significant interest for their potential in unconventional computing and sensing applications. In this work, we outline an optimized fabrication strategy for generating and stabilizing low-pinning magnetic skyrmions in magnetic thin films using magnetron sputtering. We focus on Ta/CoFeB/MgO heterostructures with perpendicular magnetic anisotropy and systematically vary key deposition parameters including sputter power and Ar pressure to optimize skyrmion formation. Furthermore, we incorporate an ultrathin Ta dusting layer at the CoFeB/MgO interface to precisely tune the interfacial anisotropy. This combined approach enables the realization of ultralow-pinning thin-film systems that reliably host room-temperature, thermally diffusing skyrmions. Such samples represent a promising platform for emerging applications in unconventional computing paradigms, including reservoir computing[1].

[1] J. Zázvorka et al., Nat. Nanotechnol. 14, 658 (2019)

MA 21.5 Tue 15:00 HSZ/0004

Impact of higher-order exchange on the lifetime of skyrmions and anti-skyrmions — Hendrik Schrautzer[1], Moritz Goerzen[2,3], •Bjarne Beyer[3], Pavel Bessarab[1,4], Soumyajyoti Haldar[3], and Stefan Heinze[3,5] — [1]Science Institute and Faculty of Physical Sciences, University of Iceland, Reykjavik, Iceland — [2]CEMES, Université de Toulouse, CNRS, Toulouse, France — [3]Institute of Theoretical Physics and Astrophysics, University of Kiel, Germany — [4]Department of Physics and Electrical Engineering, Linnaeus University, Kalmar, Sweden — [5]Kiel Nano, Surface, and Interface Science (KiNSIS), University of Kiel, Germany

Reliable control of skyrmion lifetime is essential for realizing spintronic devices, yet the role of higher-order interactions (HOI) – which can lead to skyrmion

stabilization – remains largely unexplored. Here we calculate lifetimes of isolated skyrmions and antiskyrmions at transition-metal interfaces based on an atomistic spin model that includes fourth-order exchange [1]. Within harmonic transition-state theory, we evaluate both energetic and entropic contributions and find substantially enhanced lifetimes when HOI are included. The four-spin four-site interaction raises the energy barrier and lowers the curvature of the energy landscape in the vicinity of the collapse saddle point, increasing the pre-exponential factor of the arrhenius Law. Further HOI allow thermally stable skyrmions and antiskyrmions even in absence of Dzyaloshinskii-Moriya interaction, interesting in the context of 2D van der Waals magnets lacking inversion symmetry.

[1] H. Schrautzer *et al.*, arxiv:2511.05278 (2025).

MA 21.6 Tue 15:15 HSZ/0004

Real-time observation of topological defect dynamics mediating two-dimensional skyrmion lattice melting — Raphael Gruber[1], •Edoardo Mangini[1], Maria-Andromachi Syskaki[1], Elizabeth Jefremovas[1], Sachin Krishnia[1], Asle Sudbø[2], Peter Virnau[2], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg University, Staudingerweg 7, Mainz, Germany — [2]Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, Trondheim, Norway

Magnetic skyrmions, topologically non-trivial chiral magnetic quasi-particles, can be stabilized in magnetic thin-film stacks [1]. By precisely controlling the externally applied in-plane and out-of-plane magnetic fields, two-dimensional dense arrays of skyrmions—so-called skyrmion lattices—can be formed [2]. Through suitable geometrical confinement, both orientational and translational order can be induced in these lattices. Such systems provide experimental insight into the dynamics of phase transitions in two-dimensional particle systems.

In this work, we show a two-step topological lattice-melting experiment, in which phase transitions are triggered in a skyrmion lattice by tuning the skyrmion size. The Kerr microscopy setup, in conjunction with machine learning approaches, enables real-time tracking of skyrmions, allowing us to investigate the emergence and dynamics of topological lattice defects throughout the phase transitions [3].

[1] K. Everschor-Sitte et al., J. Appl. Phys. 124, 24, 2018
[2] J. Zázvorka et al., Adv. Funct. Mater. 30, 46, 2020
[3] R. Gruber et al., Nat. Nanotechnol. 20, 10, 2025

MA 22: Focus Session: Materials Discovery II – High throughput searches for functional magnetic materials (joint session FM/MA)

chairs: Jan Schultheiß (Norwegian University of Science and Technology, NO), Hiroki Taniguchi (Nagoya University, JP)

Discovering new functional materials is crucial to advance today's technologies, ranging from caloric cooling via catalysis to next-generation energy conversion and storage, such as thermoelectric, ferroelectric, and ionic conductor materials. New materials also form the basis for potential applications in quantum information technologies. This session provides a platform to highlight functional materials discoveries and how they come about. Notably, systematic searches with high-throughput synthesis approaches, as well as predictions from materials informatics, have helped to go beyond serendipitous discoveries in recent years. However, intuition guided by general principles remains an important factor. In this session, we particularly welcome contributions that showcase the discovery of new functional materials with original approaches. Diverse material systems - from well-established to emerging and niche classes across condensed-matter and materials physics - will be featured. Bringing together diverse discoveries in a single session will help delineate general principles and inspire future work.

Time: Tuesday 14:00–15:30 Location: BEY/0138

See FM 9 for details of this session.

MA 23: Cooperative Phenomena: Spin Structures and Magnetic Phase Transitions (joint session MA/TT)

Time: Tuesday 14:00–15:30 Location: POT/0151

MA 23.1 Tue 14:00 POT/0151

Stochastic Simulation of Phase Transitions in the Dissipative 2D XYZ-Model — •Franz Pöschl[1,2,3], Przemyslaw Zielinski[1,2,3], Xin Zhang[1,2,3], and Peter Rabl[1,2,3] — [1]Technical University of Munich, TUM School of Nat- ural Sciences, Physics Department, 85748 Garching, Germany — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany

The simulation of large, open quantum spin systems is a hard problem and for most cases it is not possible to get exact solutions. Therefore, we use methods in the class of the Truncated Wigner Approximations to tackle this problem. In our work we investigated the hybrid discrete-continuous truncated Wigner approximation and used it to determine the phase diagram of the dissipative 2D XYZ-model. We were able to simulate systems with several thousands of spins due to the linear scaling of the method and numerical optimization of our code. Hence we were able to simulate the phase transitions of the model and also characterize the different phases in the open quantum system.

MA 23.2 Tue 14:15 POT/0151

Large magnetoreflectance and optical anisotropy due to 4f flat bands in the frustrated kagome magnet HoAgGe — •Felix Schilberth[1,2], Luke DeFreitas[3], Khan Zhao[4,5], Florian Le Mardelé[6], Ivan Mohelsky[6], Milan Orlita[6], Philipp Gegenwart[5], Hua Chen[3], István Kézsmárki[1], and Sándor Bordács[2] — [1]Experimentalphysik V, Unversity of Augsburg — [2]Department of Physics, BME Budapest — [3]Department of Physics, Colorado State University — [4]School of Physics, Beihang University — [5]Experimentalphysik VI, Unversity of Augsburg — [6]LNCMI, Université Grenoble Alpes

We report peculiar optical properties of the frustrated itinerant magnet HoAgGe, which exhibits multiple magnetically ordered states obeying the kagome spin-ice rule. The optical conductivity is higher for light polarization perpendicular to the kagome plane both for the free carrier response and the interband transitions. The latter have strong contributions from Ho 4f flat bands located near the Fermi level, as revealed by our *ab initio* calculations, explaining the unusual anisotropy of the optical properties and the pronounced temperature dependence of the interband transitions for out-of-plane light polarization. The key role of Ho 4f states is further supported by the large variation of the magneto-reflectivity, following the field dependence of the magnetization in contrast to that of the magnetotransport data. Such heavy-electron bands near the Fermi level offer an efficient way to control transport and optical properties and we show that their ultrafast magneto-optical response is susceptible to the magnetic order.

MA 23.3 Tue 14:30 POT/0151

Transition between critical antiferromagnetic phases in the J1-J2 spin chain — Adam McRoberts[1], •Chris Hooley[2], and Andrew Green[3] — [1]International Centre for Theoretical Physics, Trieste, Italy — [2]Coventry University, Coventry, United Kingdom — [3]University College London, London, United Kingdom

The J1-J2 spin chain is one of the canonical models of quantum magnetism, and has long been known to host a critical antiferromagnetic phase with power-law

decay of spin correlations. We show that there are, in fact, two distinct critical antiferromagnetic phases, where the roles of the local dimer field and its dual field are interchanged: the 'Affleck-Haldane' phase near the Heisenberg point J2 = 0, where the dimer field that parametrises local singlet order is gapless and part of a joint O(4) Neel-singlet order parameter; and the 'Zirnbauer' phase which appears at sufficiently large ferromagnetic J2, where the dimer field is gapped out and its dual field - the instanton density of the O(3) Neel field - is critical instead. The phases are so-named because each realises one of the competing pictures for how the O(3) non-linear sigma model with a topological theta term renormalises to the su(2) level 1 Wess-Zumino-Witten model. We support these predictions with density matrix renormalisation group calculations.

MA 23.4 Tue 14:45 POT/0151

Field-induced transitions in the charge-ordered Kagome metal FeGe — •Lilian Prodan[1], Jeremy Sourd[2], Pavlo Khanenko[2], Yurii Skourski[2], Sergei Zherlitsyn[2], and István Kézsmárki[1] — [1]EPV, Institute of Physics, University of Augsburg - Augsburg, Germany — [2]HLD-EMFL, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Kagome metals with strong electronic correlations have recently attracted significant interest as fertile platforms for emergent phenomena such as unconventional magnetism, topological transport, and symmetry-breaking instabilities. Among them, FeGe stands out due to its intriguing combination of noncollinear magnetism and charge ordering, making it a prime candidate for studying the coupling between spin, charge, and lattice degrees of freedom [1]. This compound orders antiferromagnetically below $\sim$ 410 K, develops a charge-density-wave state near $\sim$ 110 K, and forms a noncollinear spin structure below $\sim$ 60 K. To explore how these orders interact, we performed magnetization, sound-velocity, and magnetostriction measurements in static and pulsed magnetic fields up to 60 T. Our results reveal previously unreported transitions at high magnetic fields and allow us to construct an extended H-T phase diagram for FeGe. [1] X. Teng, et al., Nature **609**, 490-495 (2022).

MA 23.5 Tue 15:00 POT/0151

Successive field-induced phase transitions in the kagome magnet $ErMn_6Sn_6$ — •A. Kurtanidze[1,2], Sh. Yamamoto[1], K. Uhlirova[3], Y. Skourski[1], S. Zherlitsyn[1], J. Sourd[1], T. Herrmannsdörfer[1], E. Weschke[4], O. Prokhnenko[4], H. Nojiri[5], B. Eggert[6], A. Aubert[7], K. Kummer[8], K. Skokov[7], H. Wende[6], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Materials Growth and Measurement Laboratory (MGML), Charles University, Prague, Czech Republic — [4]Helmholtz-Zentrum Berlin für Materialien und Energie, BESSY II, Berlin, Germany — [5]Institute for Materials Research, Tohoku University, Sendai, Japan — [6]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Germany — [7]Functional Materials, Material Science, TU Darmstadt, Germany — [8]ESRF, The European Synchrotron, Grenoble, France

The ternary stannides RMn_6Sn_6 (R = Sc, Y, Gd-Lu) with hexagonal $HfFe_6Ge_6$-type structure ($P6/mmm$) are a key platform for exploring coupled topological electronic and magnetic properties. We focused on single crystals of $ErMn_6Sn_6$ and observed successive field-induced phase transitions. Using element-specific x-ray magnetic circular and linear dichroism (XMCD/XMLD) measurements in pulsed magnetic fields up to 30 T, we revealed the microscopic nature of these transitions, supported by thermodynamic data. We discuss Er and Mn moment reorientations and their link to macroscopic results.

MA 23.6 Tue 15:15 POT/0151

Depinning by shaking of skyrmions by oscillating magnetic fields — •Rajendra Loke[1], Alla Bezvershenko[2], Petra Becker Bohaty[3], Achim Rosch[2], and Joachim Hemberger[1] — [1]II. Physikalisches Institut, University of Cologne, Zülpicher Str. 77, 50937 Cologne, Germany — [2]Institut for Theoretical Physics, University of Cologne , Zülpicher Str. 77, 50937 Cologne, Germany — [3]Institut for Geology und Mineralogy, University of Cologne , Zülpicher St. 49b, 50674 Cologne, Germanyy

Here we present our recent result on shaking the skyrmion lattice by oscillating transvers magnetic field. When a transvers field is applied in addition to the longitudinal external field, skyrmion strings try to align themselves parallel to the effective field. To do so, the tips of the skyrmion strings have to move large distances and thus have to overcome pinning forces before being able to follow the field lines. We employ linear and non-linear AC susceptometry as experimental probe. The signature of this pinning-depinning transition is observable as contribution to the magnetic susceptibility, to the magnetic loss, and as well in the higher harmonic susceptibility. According to theoretical predictions, due to the chiral nature of the material the depinning is connected to translational motion of the skyrmions.

[1] Jan Müller et al. PhysRevLett.119.137201 (2017) [2] Felix Rucker et al. arXiv: 2504.01133v1 [3] Nina del Ser et al. SciPost Phys. 15, 065 (2023).

MA 24: Weyl Semimetals (joint session MA/TT)

Time: Tuesday 14:00–15:30 Location: POT/0361

MA 24.1 Tue 14:00 POT/0361

Ferrimagnetism and the causes of discontinuous magnetic behavior in Kagome Weyl-semimetal Co3Sn2S2 — •Abdul-Vakhab Tcakaev[1], Benjamin Katter[1], Stefan Enzner[2], Eugen Weschke[3], Sebastian Wintz[3], Gohil S. Thakur[4], Michael Ruck[4], Giorgio Sangiovanni[2], and Vladimir Hinkov[1] — [1]Experimentelle Physik IV, Fakultät für Physik und Astronomie, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Computational Quantum Materials, Fakultät für Physik und Astronomie, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [3]Helmholtz-Zentrum Berlin for Materials and Energy, Albert-Einstein-Straße 15, 12489 Berlin, Germany — [4]Technical University of Dresden, Helmholtzstr. 10 01069 Dresden

The Kagome Weyl semimetal Co3Sn2S2 shows puzzling magnetic anomalies that have been interpreted as hidden phase transitions. Combining element-specific XMCD, SQUID magnetometry, STXM, DFT, and inelastic neutron scattering, we establish a ferrimagnetic ground state in which Co moments are partially compensated by antiparallel Sn moments and stabilized by strong uniaxial magnetocrystalline anisotropy. Temperature-dependent XMCD and STXM show that the discontinuous drop of remanent magnetization on zero-field warming arises from abrupt domain nucleation controlled by demagnetization effects, rather than from an intrinsic change of the spin structure. This yields a consistent microscopic picture of the magnetism in Co3Sn2S2 relevant for its Weyl and anomalous Hall properties.

MA 24.2 Tue 14:15 POT/0361

High-field THz Probing of the Crossover between Weyl and Weyl-Kondo Physics in $Mn_{3+x}Sn_{1-x}$ — •Erik W. de Vos[1], Zekai Chen[1], Debankit Priyadarshi[1], Anusree V. Puleri[2], Uri Vool[2], Claudia Felser[2], Edouard Lesne[2], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zurich, Zurich, Switzerland — [2]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany

We present temperature-dependent high-field THz spectroscopy measurements on a substitution series of the noncollinear antiferromagnet $Mn_{3+x}Sn_{1-x}$. When the Mn substitution is increased from x=0 to x=0.5, $Mn_{3+x}Sn_{1-x}$ has been found to transition from a pure Weyl semimetal to a Weyl-Kondo insulator. This is accompanied by the emergence of a hybridization gap of 10.2 meV [1]. Our study uses high-field THz radiation to probe and drive the non-linear response of $Mn_{3+x}Sn_{1-x}$ through the onset of Kondo-driven correlations. Via this high-field resonant excitation, we directly probe the dynamic response across the transition from a Weyl semimetal to a Weyl-Kondo insulating state.

[1] Sci. Adv. 6, eabc1977 (2020)

MA 24.3 Tue 14:30 POT/0361

Peierls-induced topological Weyl semimetal in $PtBi_2$ — •Anders C. Mathisen[1], Stefanie S. Brinkman[1], Xin L. Tan[1], Øyvind Finnseth[1], Fabian Göhler[1], Chul-Hee Min[1], Jens Buck[2], Kai Rossnagel[2], Grisha Shipunov[3], Anna Isaeva[3], Jorge I. Facio[4], and Hendrik Bentmann[1] — [1]Center for Quantum Spintronics, Department of Physics, NTNU, Norway — [2]Kiel University & DESY, Germany — [3]Institute of Physics, University of Amsterdam, The Netherlands — [4]Instituto Balseiro, National University of Cuyo, Argentina

$PtBi_2$ is attracting interest because of its exotic electronic properties, including bulk Weyl nodes, Fermi-arc surface states, and unconventional surface superconductivity. The emergence of Weyl nodes in materials is commonly attributed to accidental crossings between non-degenerate valence and conduction bands, while little emphasis has been placed on the physical mechanisms that induce Weyl physics. Recent theory indicates that reduced translational symmetry in the Peierls-distorted crystal structure of $PtBi_2$ constitutes a mechanism for the formation of Weyl nodes [1]. In this talk, we will present an investigation of the bulk electronic structure of $PtBi_2$ using soft X-ray angle-resolved photoelectron spectroscopy. Based on an analysis of the spectral weight across wide regions in momentum space, we show how the Peierls-distortion in $PtBi_2$ promotes the formation of Weyl nodes.

[1] S. Palumbo *et al.*, Interplay between inversion and translation symmetries in trigonal $PtBi_2$. Phys. Rev. B **112**, 205125 (2025)

MA 24.4 Tue 14:45 POT/0361

Phonon-driven axial fields enable terahertz Kerr rotation in WTe2 — •Soma Dutta, Vishal Shokeen, Ruslan Chulkov, David Muradas Belinchón, M. Venkata Kamalakar, Oscar Gråsäs, and Hermann Dürr — Department of Physics and Astronomy, Uppsala University, Box 516, 75120 Uppsala, Sweden

Weyl semimetals provide a platform for studying the coupling between lattice dynamics and topological electronic structure through the motion of Weyl nodes and their associated Berry curvature (see Sie et al., Nature 565, 61, 2019). Here we report the observation of terahertz-frequency Kerr rotation in the noncentrosymmetric Weyl semimetal WTe_2, generated in the absence of an external magnetic field. Using ultrafast pump-probe polarimetry, we identify coherent oscillations at 0.24 THz and 2.4 THz that originate from interlayer shear vibrations and optical phonon modes, respectively. The 0.24 THz shear mode exhibits maximum amplitude along the a-axis and is strongly suppressed along b, indicating an odd mirror-symmetry character. By modeling the strain-induced modification of the Weyl-node separation, we show that this shear phonon produces an axial vector potential whose sign depends on the direction of atomic displacement. Spatial gradients of this axial potential generate a pseudo-magnetic field with a sign structure that naturally accounts for the observed phase inversion. Our results provide direct evidence for phonon-driven axial electromagnetic fields in a Weyl semimetal and demonstrate a route for ultrafast control of topological optical responses through coherent lattice motion. *Ab initio* calculations will further clarify the Kerr response mechanism.

MA 24.5 Tue 15:00 POT/0361

Magnetoconductance in Chiral Topological Semimetals — •Ricardo Manuel Sousa Barbosa and Annika Johansson — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle (Saale), Germany

Chiral topological semimetals [1] are a class of quantum materials whose crystal symmetries enforce multifold band crossings with nonzero topological charge, hosting symmetry-protected chiral fermionic quasiparticles, long surface Fermi arcs, and enhanced optical and transport responses. These Weyl semimetals [2] are three-dimensional materials that exhibit multiple Weyl nodes that act as point-like sources and sinks of Berry curvature in momentum space, and provide a condensed-matter realization of the chiral anomaly [3], a field-induced non-conservation of electrons associated with a given Weyl node, which manifests as a positive longitudinal magnetoconductance.

We investigate the magnetotransport properties of compounds in space group 198 [4], which host four- and six-fold degenerate Weyl nodes at the Γ and *R* points, respectively, with Chern numbers up to ±4. Using a semiclassical approach, we compute the resulting magnetoconductance, enabling a detailed analysis of the unconventional electronic responses characteristic of these materials.

[1] N.B.M. Schröter *et al.*, Nature Physics **15**, 759-765 (2019); [2] M. Z. Hasan *et al.*, Annu. Rev. Condens. Matter Phys. **8**, 289-309 (2017); [3] F. Bladuini *et al.*, Nat. Commun. **15**, 6526 (2024) [4] D.A. Pshenay-Severin *et al.*, J. Phys.: Condens. Matter **30**, 135501 (2018)

MA 24.6 Tue 15:15 POT/0361

Giant Anomalous Hall Effect Tuned by Atomic Order in Fe3Pt — •Yibo Wang and Enke Liu — Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

The Berry curvature induced anomalous Hall effect (AHE) has attracted considerable interest in recent years [1,2]. In Fe3Pt, a nodal line situated near the Fermi level generates a pronounced Berry curvature hotspot [3], giving rise to an intrinsic anomalous Hall conductivity (AHC) of 1250 S/cm according to our measurement. Building on this large intrinsic contribution, we sought to enhance the total AHE by deliberately increasing the extrinsic AHC through control of atomic ordering. By annealing Fe3Pt samples at various temperatures and for different durations, we were able to tune the extrinsic AHC continuously from nearly 0 S/cm up to 550 S/cm. The most striking result was obtained for a specimen that was annealed for ten days; at 2 K this sample exhibited a total AHC of 1892 S/cm. This value is a significant value among magnetic topological materials and represents a 50 % increase over the intrinsic contribution alone. These findings confirm the success of the proposed strategy: leveraging a substantial intrinsic Berry curvature AHC and subsequently amplifying the total AHC through extrinsic AHC through mechanisms such as atomic engineering. The approach provides a practical pathway for achieving exceptionally large anomalous Hall responses in magnetic topological systems. [1]Nat. Phys. 14, 1125-1131 (2018). [2] Nat. Phys. 14, 1119-1124 (2018). [3] Adv. Mater. 35, 2301339 (2023).

MA 25: Focus Session: Chiral phonons and crystals coupled to magnetic order I

Conventional magnetism arises from electron spin and orbital angular momentum, forming the basis of spintronics and orbitronics. Recent advances, however, have revealed that magnetism is also intimately linked to the chirality and angular momentum of the crystal lattice itself, often mediated by circular lattice vibrations known as chiral or axial phonons. These discoveries have uncovered novel mechanisms of spin and phonon transport and enabled direct access to phonon chirality and angular momentum as fundamental physical quantities. These developments prompt a re-examination of angular momentum coupling in solids, including well-established phenomena such as the Einstein-de Haas and Barnett effects, as well as the role of phonon angular momentum in the equilibrium state of magnetic materials. Chiral and axial phonons emerge as a powerful new platform for controlling magnetic order and dynamics, bridging lattice, spin, and angular momentum physics. This focus session aims to highlight recent breakthroughs in phonon angular momentum and magnetism and to connect the rapidly expanding field of chiral phononics with the broader magnetism community, spanning both experimental and theoretical perspectives.

As part of this focus session, we offer an excursion to the high-field THz user facilities at HZDR with an introduction to the planned Dresden Advanced Light Infrastructure (DALI). See MA 32 for details.

Organizers: Dominik Juraschek, d.m.juraschek@tue.nl; Michael Fechner, michael.fechner@mpsd.mpg.de; Sebastian Maehrlein, s.maehrlein@hzdr.de

Time: Wednesday 9:30–12:45 Location: HSZ/0002

Invited Talk MA 25.1 Wed 9:30 HSZ/0002

Coherent phononic control of chirality — •Michael Först — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Chirality is a pervasive property of matter that underpins many important phenomena across physics, chemistry and biology. Given its broad significance, the development of protocols for rational control of chirality in solid state systems is highly desirable, especially if this effect can be tuned continuously and in two directions.

I will show that coherent optical excitation of the crystal lattice at terahertz frequencies can induce chirality in the non-chiral solid BPO_4. By resonantly driving one of two orthogonal, doubly degenerate phonon modes and exploiting their nonlinear coupling to symmetry-lowering lattice distortions, chiral structures of either handedness can be selectively created. These findings offer new prospects for controlling of out-of-equilibrium phenomena in complex materials.

Invited Talk MA 25.2 Wed 10:00 HSZ/0002

Towards a modern theory of chiralization (and can chiral phonons help us get there?) — •Nicola Spaldin — Materials Theory, ETH Zürich, Switzerland

The goal of this talk is to answer the question: Given two chiral crystals, which one is the most chiral? In order to compare the amount of chirality, we propose the concept of "chiralization", representing the amount of chiral moment per unit volume, as a bulk macroscopic thermodynamic quantity, analogous to magnetization or polarization. Such a quantity will allow us to identify the conjugate field for chirality, classify achiral to ferrochiral phase transitions in terms of an appropriate order parameter, determine the multipole(s) associated with chirality, and predict phenomena in chiral materials. We begin by analyzing ferroaxial materials, which are protochiral, in the sense that they have a symmetry-lowering structural phase transition that breaks mirrors but preserves inversion, and are often characterized by rotations of sub-units around an axis yielding domains of opposite handedness. We show that the electric toroidal dipole, calculated as the

cross product of the spin and orbital angular momenta, is a suitable order parameter for ferroaxial phase transitions. We outline the difficulties in extending the physics of ferroaxial materials to ferrochiral materials, and indicate how our emerging understanding of chiral phonons might help.

MA 25.3 Wed 10:30 HSZ/0002

Coherent Transfer of Pseudo- and Real Angular Momentum via Lattice Anharmonicity — •Olga Minakova[1], Carolina Paiva[2], Maximilian Frenzel[1], Michael Spencer[1], Joanna Urban[1], Martin Wolf[1], Dominik Juraschek[2,3], and Sebastian Maehrlein[1,4,5] — [1]FHI Berlin — [2]Tel Aviv U. — [3]TU Eindhoven — [4]HZDR — [5]TU Dresden

Rotational symmetry in crystals enforces conservation of phonon pseudo-angular momentum. However, direct evidence for angular momentum transfer between phonon modes has been lacking. We demonstrate coherent angular momentum transfer between doubly degenerate phonons through a resonant three-phonon interaction [1]. Circularly polarized THz pulses drive an IR-active phonon in Bi2Se3, imprinting the helicity of the field and generating ionic loops possessing real angular momentum. Anharmonic coupling then upconverts two such IR phonons into a Raman-active phonon at twice the frequency, transferring energy, linear momentum, and angular momentum. The THz-driven Kerr effect directly resolves the Raman phonon trajectory, revealing a helicity reversal, which perfectly fulfills pseudo-angular momentum conservation in the discrete C3 rotational symmetry of the lattice. Group theory analysis and DFT confirm this helicity flip and simultaneously reveal transfer of real angular momentum as circular ionic motion. These results constitute the first direct experimental evidence of angular momentum conservation in phonon-phonon interactions.

[1] O. Minakova et. al., arXiv:2503.11626 (2025)

MA 25.4 Wed 10:45 HSZ/0002

Rotational Umklapp scattering in chiral nonlinear phononics — •Yu-Chi Huang[1], Carolina Paiva[2], and Dominik Juraschek[1] — [1]Eindhoven University of Technology, Eindhoven, Netherlands — [2]Tel Aviv University, Tel Aviv, Israel

Chiral phonons, circularly polarized lattice vibrations propagating perpendicular to their rotational plane, commonly arise in chiral materials and have attracted considerable attention in condensed matter physics lately. Due to *n*-fold rotational crystal symmetry, they enable rotational phonon-phonon Umklapp scattering through nonlinear phonon coupling. This process is the angular-momentum analog of the conventional Umklapp scattering conserving linear crystal momentum. Recent pump-probe experiments have measured the effect in Bi_2Se_3, and we here develop a general theory using α-quartz (α-SiO_2) as an example. Our results offer insight into the fundamentals of angular momentum conservation in solids.

15 min break

Invited Talk MA 25.5 Wed 11:15 HSZ/0002

Observation and control of chiral phonons in non-centrosymmetric materials — •Hiroki Ueda — Paul Scherrer Institute, Villigen, Switzerland

The field of chiral phonons has rapidly grown with the emergence of various intriguing phenomena, including magnetism, transport, and light-matter interactions. Chiral phonons are rotational phonon modes propagating out of the rotational plane, breaking improper rotational symmetry. I will present direct demonstrations of chiral phonons in chiral crystal α-SiO2 and polar crystals LiNbO3 and BaTiO3 using resonant inelastic X-ray scattering (RIXS) with circularly polarized X-rays. Angular momentum transfer between circularly polarized photons and chiral phonons imposes the selection rule in the RIXS process, enabling observation of chiral phonons through circular dichroism in phonon excitation peaks. Furthermore, in BaTiO3, we demonstrate in situ electrical switching of phonon chirality, opening pathways for dynamic control of chiral phononic properties.

MA 25.6 Wed 11:45 HSZ/0002

Associated magnetism of circular ionic motion probed with ultrafast x-ray pulses — •Clifford Allington[1], Matthew Lutz[2], E. Ho[2], F. Graf[3], M. Basini[3], H. Ueda[2], A. Elliot[2], M. Biggs[2], R. Finn[2], S-W Huang[1], M. Grimes[1], M. Henstridge[4], M. Hoffmann[4], R. Alonso-Mori[4], D. Zhu[4], Q. Nguyen[4], V. Esposito[4], T. Sato[4], E. Skoropota[1], E. Paris[1], A. Camps[1], E. Razzoli[1], R. Mankowsky[1], F. Capotondi[5], N. Jaouen[6], M. Radovic[1], M. Savoini[1,3], E. Abreu[3], S. Johnson[1,3], Jeremy Johnson[2], and Urs Staub[1] — [1]Paul Scherrer Institute — [2]Brigham Young University — [3]ETH Zurich — [4]SLAC National Accelerator Laboratory — [5]Elettra Sincrotrone Trieste — [6]Synchrotron SOLEIL

It has been proposed that the coherent circular motion of ions creates a magnetic field. This effect, termed dynamical multiferroicity (DM), has been evidenced experimentally in diamagnetic materials such as SrTiO3 using circular terahertz (THz)-pump optical-probe methodologies. However, the fields reported are much larger than predicted, raising questions on the exact nature of the transient state. Thus, we performed a suite of circular THz-pump experiments on the paramagnetic EuTiO3, a material directly analogous to SrTiO3 but with a S = 7/2 spin on the Eu2+ ion. We have measured the circular motion of ions by femtosecond x-ray diffraction as well as an optical-probe signal which changes sign upon changing the helicity of the THz-pump, consistent with DM. However, no induced Eu2+ moment was found within the resolution of time-resolved x-ray magnetic circular dichroism, providing a quantitative upper limit on the resulting field.

MA 25.7 Wed 12:00 HSZ/0002

Real-time laser-driven (chiral) phonon dynamics from atomistic simulations — •Mike Pols and Nicola A. Spaldin — Materials Theory, ETH Zürich, Zürich, CH-8093, Switzerland

I will present an approach to simulate the real-time dynamics of excited phonons in materials. Using machine-learning interatomic potentials (MLIPs) together with laser-driven molecular dynamics simulations, we can capture the response of materials to driven (chiral) phonon excitations and directly capture their nonlinear vibrational dynamics. Driving phonon modes into the nonlinear regime can induce a wide range of material properties, such as strain and magnetism [1]. While first-principles modeling has provided valuable insights into these dynamics, the commonly used coupled-oscillator method requires the computation of numerous higher-order coupling coefficients [2], limiting its scalability.

Our MLIP-based approach enables the direct simulation of the full anharmonic lattice response. It effectively models both IR- and Raman-active modes, with finite-temperature effects, and the nonlinear couplings to high orders. Using this method, we explore the vibrational dynamics of linear and chiral phonons in oxide perovskites, enabling predictive simulations of the behavior and coupling of phonons in functional materials.

[1] A. Disa et al., Nat. Phys. 17, 1087 (2021).
[2] A. Subedi et al., Phys. Rev. B 89, 220301 (2014).

MA 25.8 Wed 12:15 HSZ/0002

THz field-induced magnetic-like response in the quantum paraelectric diamagnet $KTaO_3$ — •Christelle Kadlec[1], Filip Kadlec[1], Dalibor Repček[1], Martina Basini[2], Petr Kužel[1], Jan-Christoph Deinert[3], Sergey Kovalev[3], Mattia Udina[4], Igor Ilyakov[3], Alexey Ponomaryov[3], and Stanislav Kamba[1] — [1]Institute of Physics, Prague, Czechia — [2]ETH Zurich, Switzerland — [3]HZDR, Dresden, Germany — [4]CESQ-ISIS, Strasbourg, France

The current efforts on developing new ways of data manipulation are aimed at ultrafast control of magnetization in magnetic materials, as well as at inducing magnetic moments in diamagnetics. We demonstrate that in the diamagnetic quantum paraelectric $KTaO_3$, the electric field of circularly polarized THz pulses with an amplitude of 300 kV/cm induces a transient magnetic-like response by resonantly pumping its degenerate soft phonon. The transient phonon-mediated magnetic-like response was measured via the rotation of the polarisation of a probe light. However, such response usually contains contributions from both the magneto-optic THz-field-induced Faraday effect and the electro-optic THz-field-induced Kerr effect (TKE). In order to distinguish between them, we separately measured the TKE by applying a linearly polarized THz pump beam. Moreover, we present a theoretical analysis of the TKE, showing that its contribution can be suppressed by subtracting the experimental data generated by opposite elliptically polarized THz radiation. Thus, we are able to unambiguously identify a magnetic-like behavior of the $KTaO_3$ crystal manifested by the extracted Faraday rotation.

MA 25.9 Wed 12:30 HSZ/0002

Phonon-induced chirality — •Dominik Juraschek — Eindhoven University of Technology, Eindhoven, Netherlands

Controlling and utilizing solid-state chirality is a central challenge in condensed matter physics, because it does not couple to applied magnetic or electric fields, in contrast to magnetism and ferroelectricity. In this talk I show that geometric chiral phonons, lattice vibrations whose instantaneous atomic displacements break inversion and mirror symmetries, can transiently drive an achiral crystal into a chiral state. Using group-theoretical analysis, we identified selection rules for phonon-induced geometric chirality across all 32 point groups and demonstrate that ultrashort mid-infrared and terahertz pulses can excite pairs of IR-active phonons whose nonlinear coupling rectifies a geometric chiral phonon. I further demonstrate that chiral order exhibits fundamental excitations which we term "chiralons," similar to the recently discovered ferrons in ferroelectric order. Our results highlight an emerging functionality of chiral phononics beyond phonon angular momentum.

MA 26: Focus Session: Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects I (joint session TT/DS/MA)

Nickel, a direct neighbor of copper in the periodic table, has been considered a promising candidate for high-temperature superconductivity since the early 1990s. After more than three decades of research, this prediction was confirmed with the discovery of superconductivity in nickelates, marking the beginning of the "nickel age" of superconductivity. Recent advances include Sm-based infinite-layer nickelates with transition temperatures approaching 40 K, as well as bilayer nickelates exhibiting superconductivity above 90 K under pressure and up to 60 K under compressive epitaxial strain. These results highlight the crucial roles of structural engineering, epitaxial strain, and precise synthesis control, and they open new frontiers for both fundamental understanding and materials design. This focus session aims to define key scientific challenges ahead, strengthen collaboration within Germany and Europe, and accelerate progress toward higher superconducting transition temperatures.

Coordinators: Marta Gibert (TU Wien), Mattias Hepting (MPI FKF Stuttgart), Ilya M. Eremin (Ruhr-University Bochum)

Time: Wednesday 9:30–12:45 Location: HSZ/0003

See TT 39 for details of this session.

MA 27: Ultrafast Magnetization Effects I

Time: Wednesday 9:30–12:45 Location: HSZ/0004

Invited Talk MA 27.1 Wed 9:30 HSZ/0004

Towards sub-10fs magnetization switching — Reza Rouzegar[1], Oliver Franke[1], Gal Lemut[1], Oliver Gueckstock[1], Junwei Tong[1], Dieter Engel[2], Xianmin Zhang[3], Georg Woltersdorf[4], Piet W. Brouwer[1], Tobias Kampfrath[1], and •Quentin Remy[1] — [1]Department of Physics, Freie Universität Berlin, 14195 Berlin, Germany — [2]Max-Born-Institut für nichtlineare Optik und Kurzzeitspektroskopie, 12489 Berlin, Germany — [3]Key Laboratory for Anisotropy and Texture of Materials (Ministry of Education), School of Material Science and Engineering, Northeastern University, Shenyang 110819, China — [4]Institut für Physik, Martin-Luther-Universität Halle, 06120 Halle, Germany

Femtosecond laser pulses can induce sub-picosecond demagnetization, enabling ultrafast magnetic writing, spin transport, and broadband THz generation. Yet the microscopic processes in the first ~ 10 fs remain poorly understood. Three-temperature models describe energy flow among electrons, spins, and the lattice but neglect angular-momentum transfer, essential for spin dissipation.

Using ultrabroadband THz emission spectroscopy with ~ 10 fs resolution, we find that electron-magnon (em) scattering drives the nonequilibrium spin dynamics, generating both spin flips and magnons in under 10 fs, well before ~ 100 fs demagnetization. Angular momentum is then dissipated primarily through magnon-lattice interactions. Having established em scattering as the dominant sub-10-fs mechanism, we show that THz pulses can harness this coupling to reverse magnetization, pointing to sub-10-fs spin control.

MA 27.2 Wed 10:00 HSZ/0004

Ultrafast Control of Spin Periodicity in a Helical Heisenberg Antiferromagnet — •Hyein Jung[1,2], Abeer Arora[2], Deeksha Gupta[3], Franziska Walther[4], Kristin Kliemt[4], Victoria C. A. Taylor[2], Túlio de Castro[2], Hanqian Lu[1,2], Christian Schüssler-Langeheine[3], Niko Pontius[3], Urs Staub[5], Cornelius Krellner[4], Laurenz Rettig[2], Ralph Ernstorfer[1,2], and Yoav W. Windsor[1,2] — [1]Technische Universität Berlin, Berlin, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [4]Goethe-Universität Frankfurt, Frankfurt, Germany — [5]Paul Scherrer Institut, Villigen, Switzerland

The ultrafast manipulation of spin structures is a promising route toward the next generation spintronic devices. In this work, we study the helical Heisenberg antiferromagnet $EuCo_2P_2$ using resonant soft X-ray diffraction (RXD). By probing the magnetic Bragg reflections, we are experimentally sensitive both to the antiferromagnetic (AF) order parameter and to the 4f spin periodicity. We measure their response under three distinct perturbations: (a) femtosecond laser excitation (ultrafast RXD), (b) external magnetic fields, and (c) temperature variation. Employing a Heisenberg model, we directly reveal how the observables respond to each of the perturbations we apply. We further probe the response of the crystal lattice under the same conditions as the spin order and draw a relation between the dynamics of the two. These results offer insight into different routes to control AF spin order and its couplings.

MA 27.3 Wed 10:15 HSZ/0004

Time-resolved coherent small-angle EUV scattering of magnetic thin film structures — •Konstanze Korell[1], Sergey Zayko[1], Hung-Tzu Chang[1], Timo Schmidt[2], Murat Sivis[1,3], Manfred Albrecht[2], and Claus Ropers[1,3] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]Experimental Physics IV, University of Augsburg, Germany — [3]4th Physical Institute - Solids and Nanostructures, University of Göttingen, Germany

Laser excitation yields control over magnetic structures on the femtosecond timescale, yet the corresponding nanoscale response remains difficult to access. Ultrafast coherent diffractive imaging has recently provided real-space insights [1], limited, however, to reversible dynamics. Here, by carrying out coherent speckle diffraction, we combine the strengths of diffraction with the coherence of a source capable of coherent imaging. Through this, we get insights to reversible and irreversible processes. Using a femtosecond high harmonic generation source, we measure pump-probe scattering from magnetic thin films in a laboratory-based setup. We discuss both the opportunities and limitations of this approach providing a basis for the interpretation of nanoscale magnetic dynamics in future ultrafast experiments.

[1] H.-T. Chang et. al, arXiv:2504.17917 (2025)

MA 27.4 Wed 10:30 HSZ/0004

Exploitation of Spin Wave Resonances in Miniaturized Magnetic Electron Optics for Ultrafast Electron Beam Manipulation — •Max Herzog[1], Johannes Schultz[1], and Axel Lubk[1,2] — [1]IFF, IFW Dresden, Helmholtzstraße 20, 01069 Dresden — [2]IFMP, TU Dresden, Haeckelstraße 3, 01069 Dresden

Magnetic electron optics that can be switched on sub-nanosecond time scales are useful for the setup of stroboscopic measurements in scanning and transmission electron microscopes. Scaling laws indicate that devices become permeable for alternating magnetic fields with GHz frequency by miniaturizing them to micrometer length scales, therefore decreasing their induction. On these length scales, spin waves can be excited in the magnetic pole pieces which can drastically increase the micro optics effectivity when their resonance condition is met. We fabricate such magnetic multipole optics using lithographic techniques with pole piece sizes in the tens of μm, a thickness of up to 800 nm, a pole piece distance of 25 μm as well as variable geometries in order to optimize the resonant behavior. Due to those resonances, the characterized micro optics show an especially strong deflection of the TEMs 300 keV electron beam of more than 100 μrad at 3 GHz excitation frequency. Conducted electron spin resonance measurements confirm the possibility to excite spin waves in the magnetic pole pieces in the same frequency range. This allows for the application of models of the dispersion relation to determine favorable values for parameters like thickness, exchange interaction, and saturation magnetization in order to achieve the desired resonance frequency.

MA 27.5 Wed 10:45 HSZ/0004

Terahertz Spectroscopy of non-collinear magnetic state in ferrimagnetic iron garnet — •Tushar Baruah[1], Andrzej Stupakiewicz[2], Paul H. M. van Loosdrecht[1], and Evgeny A. Mashkovich[1] — [1]II. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany. — [2]Faculty of Physics, University of Bialystok, Ciolkowskiego 1L, 15-245 Bialystok, Poland.

Data storage technologies and magnetic control research, in general, focuses primarily on magnets with anti-ferromagnetic exchange interactions for their ultra-

fast picosecond-scale dynamics. Among them, ferrimagnets are particularly appealing, as they combine high Terahertz (THz)-scale eigenfrequencies with the feasibility of ground state control. Non-collinear magnetic states in ferrimagnets exhibit complex spin dynamics, whose ultrafast behaviour remains partly understood. Using a table-top high-power broadband THz pump-optical probe setup integrated with a 10T superconducting magnet, we directly probe the field and temperature dependent spin dynamics in Bi-substituted Gadolinium iron garnet, which is a ferrimagnet with non-collinear magnetic state and a magnetic moment compensation point temperature. Our results show magnetisation dynamics in non-collinear state driven by overlap of exchange modes and THz cavity modes formed by multiple reflections inside the sample.

15 min break

MA 27.6 Wed 11:15 HSZ/0004

Spin-lattice coupling control of ultrafast order melting in antiferromagnetic insulators — Aleksandr Buzdakov[1], •Ravi Kaushik[1], Nikolai Khokhlov[2], Johan Mentink[2], Sergey Artyukhin[1], and Aleksei Kimel[2] — [1]Istituto Italiano di Tecnologia, Via Morego 30, 16163 Genova, Italy — [2]Radboud University Nijmegen, Institute for Molecules and Materials, 6525 AJ Nijmegen, The Netherlands

Ultrafast order melting in magnetic insulators is governed by two processes: intrinsic intra-spin relaxation and spin-lattice energy transfer. Antiferromagnets, which lack net magnetization, can in principle evade angular-momentum constraints and display markedly faster order-parameter dynamics than ferromagnets, but experimental rates vary widely across materials. Here we combine first-principles magnetostriction calculations, phonon and magnon spectral analysis, atomistic spin-dynamics simulations and time-resolved second-harmonic generation to disentangle these pathways and explain material-dependent disparities. Focusing on two structurally similar antiferromagnets, Cr_2O_3 and $FeBO_3$, we show that the strength of spin-phonon coupling - revealed by magnetostrictive response and phonon-magnon spectral overlap - dictates the dramatic difference in order-melting rates. We also achieved accelerated dynamics in Cr_2O_3 and show sub-2-ps order melting in both experiment and simulation. Our results identify spin-phonon coupling as the decisive control parameter for ultrafast antiferromagnetic dynamics and provide a practical framework to design faster switching in antiferromagnetic spintronic devices.

MA 27.7 Wed 11:30 HSZ/0004

Nonlinear optical probing of a strongly correlated phase transition in epitaxial $NdNiO_3$ thin films — •Christian Tzschaschel[1,2], Felix Utsch[1], Qi Song[2], Spencer Doyle[3], Grace A. Pan[3], Julia A. Mundy[3], and Stefan Eisebitt[2,4] — [1]Department of Physics, University of Zurich, Switzerland — [2]Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, Berlin, Germany — [3]Department of Physics, Harvard University, USA — [4]IOAP, TU Berlin, Germany

The family of rare-earth nickelates is a prime example of strongly correlated oxide materials displaying a wealth of physical phenomena from antiferromagnetism to superconductivity. $NdNiO_3$ specifically exhibits a metal-to-insulator phase transition upon cooling that is concomitant with the emergence of antiferromagnetic order.

Here, we use nonlinear optical second harmonic generation (SHG) in the near-infrared regime to gain insight into the symmetry and ultrafast dynamics of this correlated electronic and magnetic phase transition. In static measurements, we observe a symmetry reduction from orthorhombic in the paramagnetic phase to monoclinic in the antiferromagnetically ordered phase. Upon optical excitation, we observe a quench of the SHG signal and a restoration of the orthorhombic state within 125 fs. Our study highlights the capabilities of nonlinear optics and advances the understanding of strongly correlated quantum materials.

MA 27.8 Wed 11:45 HSZ/0004

Ultrafast angular momentum transfer in RKKY-coupled 4f antiferromagnets — S.-E. Lee[1], Y.W. Windsor[1,2], D. Zahn[1], A. Kraiker[3], K. Kummer[3], K. Kliemt[4], C. Krellner[4], C. Schüssler-Langeheine[5], N. Pontius[5], U. Staub[6], D.V. Vyalikh[7], A. Ernst[8], and •L. Rettig[1,9] — [1]Fritz-Haber-Institut der MPG, DE — [2]TU Berlin, DE — [3]ESRF, Grenoble, FR — [4]Goethe-Universität Frankfurt, DE — [5]Helmholtz-Zentrum Berlin, DE — [6]PSI, Villigen, CH — [7]DIPC, San Sebastian, ES — [8]Johannes Kepler University, Linz, AU — [9]RPTU Kaiserslautern-Landau, DE

Antiferromagnets allow for direct angular momentum (AM) transfer between opposing spins, thereby avoiding AM transfer to the lattice, which limits ultrafast magnetization dynamics in ferromagnets. Here, we study the ultrafast magnetization dynamics in 4f antiferromagnetic intermetallics of type $LnRh_2Si_2$ (Ln=Pr, Nd, Sm, Gd, Tb, Dy, Ho) where we modify the magnitude of the on-site RKKY coupling strength via substitution of Ln ions. By combining time-resolved soft X-ray diffraction with ab-initio calculations, we find that the rate of AM transfer between opposing moments is directly determined by this coupling [1]. Moreover, the influence of itinerant conduction electrons has been explored in the Series GdT_2Si_2 by varying the transition metal T (T=Co, Rh, Ir). Here, we find a more than twofold increase in ultrafast AM transfer rate between the materials, which we associate with modifications in the conduction electron susceptibility due to differences in their density of states [2].

[1] Nat. Mater. 21, 514 (2022) [2] PRR 6, 043019 (2024)

MA 27.9 Wed 12:00 HSZ/0004

Time-resolved wide-field SHG imaging of ferroic materials — •Andrin Caviezel, Jan Gerrit Horstmann, Thomas Lottermoser, and Manfred Fiebig — Department of Materials, ETH Zurich, Zurich, Switzerland

We investigate the ultrafast dynamics of van der Waals ferroics using time-resolved second harmonic generation (SHG) wide-field imaging. Controlling antiferromagnetic order on ultrafast timescales is of central relevance for spintronic applications, and van der Waals ferroics constitute highly promising material platforms. However, achieving such control requires an experimental technique that is simultaneously sensitive to ferroic order and combines micrometer spatial with femtosecond temporal resolution. Here, we present a setup for direct wide-field visualization of ferroic domain structures by exploiting SHG generated from high-energy pulses of an amplified laser system. The adjustable wavelength and polarization of pump and probe pulses, together with tailored pulse sequences for excitation, enable sensitive detection and selective manipulation of magnetic order. Our approach provides access to ultrafast processes in bulk ferroics with microscopic domain patterns as well as in micrometer-sized flakes of van der Waals ferroics under cryogenic conditions, opening new pathways for understanding and steering their nonequilibrium dynamics.

MA 27.10 Wed 12:15 HSZ/0004

Photoinduced demagnetization and carrier dynamics in $SrRuO_3$ thin films probed by time resolved THz spectroscopy — •Ankhijur Islam Sekh[1], Harun Mert Iyiisler[1], Phillip Leiprecht[2], Mathias Beck[2], Paul Leiderer[2], Gad Koren[3], Ionela Lindfors-Vrejoiu[4], Paul H.M. van Loosdrecht[4], and Jure Demsar[1] — [1]JGU Mainz — [2]University of Konstanz — [3]Technion, Haifa — [4]University of Cologne

$SrRuO_3$ is an itinerant ferromagnet (Tc ≈ 150 K) whose T^2 resistivity below 30K signals a ferromagnetic Fermi-liquid ground state. We present the temperature (T) and excitation fluence (F) dependent photoinduced conductivity dynamics of thin films grown by MBE and PLD, following excitation with fs near-infrared pulses. We show that photoinduced changes in THz conductivity are governed by the changes in the scattering rate of the intraband Drude response. The T- and F-dependent photoconductivity dynamics suggest that rapid carrier thermalization is accompanied by magnon generation, consistent with a high spin-flip scattering rate due to strong spin-orbit coupling. Accordingly, over a broad T and F-range, the photoconductivity transients track the evolution of the magnon population. At temperatures below 20K and at lowest F, we observe a delayed rise in photoconductivity, which reflects the reduced e-e thermalization rate with its characteristic Fermi-liquid T^2 dependence.

MA 27.11 Wed 12:30 HSZ/0004

Element-specific magnetization dynamics of epitaxial ultrathin Co/Pt heterostructures — •Puloma Singh[1], Corentin Aulagnet[2], Thomas Jauk[3], Sangeeta Sharma[1,4], Martin Schultze[3], Stéphane Mangin[2], Clemens von Korff Schmising[1], and Stefan Eisebitt[1,5] — [1]Max Born Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Berlin, Germany — [2]Université de Lorraine, CNRS, Institut Jean Lamour, Nancy, France — [3]Institut für Experimentalphysik, Technische Universität Graz, Graz, EU, Austria — [4]Institute for Theoretical Solid-state Physics, Freie Universität Berlin, Berlin, Germany — [5]Technische Universität Berlin, Institut für Optik und Atomare Physik, Berlin, Germany

Magnetic systems comprising 3d ferromagnetic transition metals and 4d/5d heavy metals are of interest because of their potential application in future energy storage technology. The microscopic process involved after femtosecond laser excitation is complex and is still controversially discussed in the existing literature. We present a systematic and element specific study of epitaxial, ultrathin Co films (0.8 and 1.0 nm) sandwiched by Pt layers. We compare the ultrafast response for the different Co thicknesses as well as for out-of-plane and in-plane magnetic anisotropy by a combination of pump-probe spectroscopy in the optical and extreme ultraviolet spectral range. Exploiting the Pt $O_{2,3}$ and N_7 and Co $M_{2,3}$ resonances, we accurately disentangle the intrinsic and proximity induced magnetic moments of Co and Pt. We find consistently larger demagnetization amplitudes of the Pt magnetization compared to Co and a very pronounced thickness dependence.

MA 28: Focus Session: Quantum Sensing with Solid State Spin defects II (joint session TT/HL/MA)

Time: Wednesday 9:30–10:30 Location: HSZ/0101

See TT 40 for details of this session.

MA 29: Spin Transport and Orbitronics, Spin-Hall Effects I (joint session MA/TT)

Time: Wednesday 9:30–12:45 Location: POT/0112

Invited Talk MA 29.1 Wed 9:30 POT/0112

Exploring the interplay between spin and chirality — •Angela Wittmann — Johannes Gutenberg University Mainz, Germany

Chirality is omnipresent in nature, bridging magnetic and molecular spin phenomena. At the core of this connection lies the chiral-induced spin selectivity (CISS) effect, describing the highly efficient generation of spin polarized currents in chiral molecules. Despite extensive experimental evidence, the underlying mechanisms of CISS remain debated. Here, we explore how chirality is directly linked to the intrinsic magnetic moments in molecules and how molecular design can be harnessed to control spin phenomena at hybrid chiral molecule magnetic interfaces [1]. Our findings pave a pathway towards functional "chiralitronic" devices - turning a fundamental puzzle into a technological opportunity.

[1] A. Moharana, AW et al., Sci. Adv.11, eado4285 (2025)

MA 29.2 Wed 10:00 POT/0112

Chiral Molecule-Induced Magnetic Anisotropies — •Simon Sochiera[1], Ashish Moharana[1], Yael Kapon[2], Fabian Kammerbauer[1], Shira Yochelis[2], Mathias Kläui[1], Yossi Paltiel[2], and Angela Wittmann[1] — [1]Johannes Gutenberg University, Mainz, Germany — [2]Hebrew University of Jerusalem, Jerusalem, Israel

The chiral-induced spin selectivity effect promises novel spintronic devices. Despite numerous interdisciplinary experiments revealing its implications and trends, this phenomenon challenges our theoretical understanding of the interplay between spin and chirality, particularly regarding apparent time-reversal symmetry breaking. This symmetry breaking can be observed by measuring a magnetic thin film's anisotropy upon chiral-molecule adsorption. We quantify this phenomenon by measuring the magnetic anisotropy through electrical magnetotransport measurements. Upon chiral-molecule adsorption, we observe a 35% change in out-of-plane hard-axis anisotropy. This approach enables sensitive probing of magnetic property changes induced by different chiral molecular systems on various conductive or insulating magnetic thin films. Correlating molecular properties, such as spin-orbit coupling, with their impact on magnetic anisotropy will be crucial for understanding the fundamental mechanisms of chiral-induced spin selectivity and for facilitating the design of spintronic devices that require a precisely tuned anisotropy.

MA 29.3 Wed 10:15 POT/0112

Generation, Transmission, and Conversion of Orbital Torque by an Antiferromagnetic Insulator — •Shilei Ding[1,2], Paul Noël[2], Gunasheel Kauwtilyaa Krishnaswamy[2], Niccolò Davitti[2], Giacomo Sala[2], Marzia Fantauzzi[3], Antonella Rossi[2,3], and Pietro Gambardella[2] — [1]School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371, Singapore — [2]Department of Materials, ETH Zürich, 8093 Zürich, Switzerland — [3]Dipartimento di Scienze Chimiche e Geologiche, Università degli Studi di Cagliari, Campus di Monserrato S.S. 554, Italy

Orbital currents and orbital torques have recently emerged as powerful tools for controlling magnetization, yet their transport has been studied almost exclusively in metals. We report the first demonstration of orbital generation, transport, and conversion through an insulating antiferromagnet CoO. By inserting CoO between Cu* and Co, we show that orbital transport is preserved and the orbital-torque efficiency is strongly enhanced. Temperature-dependent measurements indicate that orbital transport above the Néel temperature is mediated by thermal fluctuations, while antiferromagnetic order and exchange bias provide additional transport channels at low temperature. These results identify insulating antiferromagnets as effective mediators of orbital angular momentum and highlight transition-metal oxides with unquenched orbital moments as promising materials for efficient spin-orbitronic technologies.

MA 29.4 Wed 10:30 POT/0112

Modern theory of the Orbital Hall effect from Wannier Representation — •Mirco Sastges[1,2], Insu Baek[3], Hojun Lee[3], Hyun-Woo Lee[3], Yuriy Mokrousov[1,2], and Dongwook Go[4] — [1]Peter Grüunberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany — [3]Department of Physics, Pohang University of Science and Technology, Pohang, Kyungbuk 37673, South Korea — [4]Department of Physics, Korea University, Seoul 02841, South Korea

In the field of orbital dynamics and orbital transport a particularly important quantity is the so-called orbital Hall conductivity (OHC), which is expressed in terms of operators of velocity and orbital angular momentum (OAM). To overcome the difficulties in treating the unbounded position operator, very often the so-called atom-centered approximation (ACA) is used. However, while being very practical, this approach captures only some local contributions to the OAM operator. Here, we will report on developing a new approach to quantify the OAM operator in the basis of Wannier functions, which is based on the modern theory of orbital magnetization. This method allows us to capture both local and itinerant contributions to the OHC. By performing first principles calculations for selected transition metals we show that a significant correction to the OHC due to non-local contributions arises, while the local effects are captured in accordance to the ACA. Our approach is very promising since it improves our understanding of OAM and allows for a precise estimation of the OHC.

MA 29.5 Wed 10:45 POT/0112

Chirality-induced orbital Edelstein effect in an analytically solvable model — •Lennart Schimpf, Börge Göbel, and Ingrid Mertig — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg

Chirality-induced spin selectivity (CISS), a phenomenon wherein chiral structures selectively determine the spin polarization of electron currents flowing through the material, has garnered significant attention due to its potential applications in areas such as spintronics, enantioseparation, and catalysis. The underlying physical effect is the Edelstein effect that converts charge to angular momentum. Besides a spin contribution, there exists a contribution based on the orbital angular momentum but the precise mechanism for its generation remains yet to be understood. Here, we introduce the minimal model for explaining the phenomenon based on the orbital Edelstein effect [1]. We consider nonlocal intersite contributions to the current-induced orbital angular momentum and reveal the underlying mechanism by analytically calculating the Edelstein susceptibilities in a tight-binding and Boltzmann approach. While the orbital angular momentum is directly generated by the chirality of the crystal, the spin contribution of each spin-split band pair relies on spin-orbit coupling. Using tellurium as an example, we show that the orbital contribution surpasses the spin contribution by orders of magnitude.

[1] B.Göbel, L. Schimpf, I. Mertig, Phys. Rev. Res. 7, 033180 (2025)

15 min break

MA 29.6 Wed 11:15 POT/0112

Spin-charge and Orbital-charge Interconversion on SrTiO3-based Two-dimensional Electron Gases: A Semiclassical Approach — •Le Viet Duc Pham and Annika Johansson — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle (Saale), Germany

Two-dimensional electron gases (2DEGs) at SrTiO3-based oxide interfaces display large, gate-tunable Rashba-like spin-orbit coupling (SOC) that enables spin-charge interconversion via the spin Edelstein effect [1, 2]. It has also been demonstrated that the orbital Edelstein effect, i.e, current-induced orbital magnetization, is larger than the spin Edelstein effect by more than one order of magnitude [3]. Yet, most transport studies assume a constant relaxation time [1, 3], potentially underestimating the role of anisotropic relaxation times and scattering-in contributions. Here, we systematically study charge-spin and charge-orbital conversion in SrTiO3-based 2DEGs, combining the Boltzmann semiclassical transport theory and various ansatzes for the scattering terms, such as constant relaxation time, momentum relaxation time, as well as scattering on various impurity potentials. Comparing different scattering approaches, we gain insights into the influence of impurity scattering on charge-spin and charge-orbital interconversion phenomena.

[1] Vaz, Diogo C., et al. Nature Materials 18.11 (2019): 1187-1193. [2] Caviglia, A. D., et al. Physical Review Letters 104.12 (2010): 126803. [3] Johansson, Annika, et al. Physical Review Research 3.1 (2021): 013275.

MA 29.7 Wed 11:30 POT/0112

Quantum geometry for orbital magnetization and spintronics from parallel transport of Bloch states — •Johannes Mitscherling, Jan Priessnitz, and Libor Šmejkal — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

Quantum geometry emerges as a unifying, quantitative guiding principle for the linear and nonlinear response functions of quantum matter. Going beyond current-current responses [1,2], we identify the generator of parallel transport of Bloch states, given by the commutator of the band projector and its momentum derivative, as a further essential building block of quantum geometry [3]. I will show that orbital magnetism arises from the non-commutativity of adiabatic transport in orthogonal directions. We will see that the spin Berry curvature and the spin quantum metric, which control the linear spin conductivity, are not fundamentally geometric but yield three geometric contributions of distinct physical origin. Our theory enables efficient numerical and analytical evaluations for general Bloch Hamiltonians with an arbitrary number of potentially degenerate bands. I will exemplify the results in application to altermagnets [4] and p-wave magnets [5].

[1] Avdoshkin*, Mitscherling*, and Moore, PRL 135, 066901 (2025). [2] Mitscherling*, Avdoshkin*, and Moore, PRB 112, 085104 (2025). [3] Mitscherling and Šmejkal, to be submitted. [4] Šmejkal, Sinova, and T. Jungwirth, PRX 12, 031042 (2022). [5] Birk Hellenes, Jungwirth, Jaeschke-Ubiergo, Chakraborty, Sinova, and Šmejkal, arXiv:2309.01607v3.

MA 29.8 Wed 11:45 POT/0112

Signatures of magnon dispersion in spin transport — •Sebastian Sailler, Denise Reustlen, Michaela Lammel, Sebastian T. B. Goennenwein, and Richard Schlitz — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

The spin Hall magnetoresistance (SMR) provides electrical access to the magnetization of a magnetically ordered material. It recently became clear that changes in the net magnetization due to magnon creation and annihilation can be observed in the SMR. However, the number of magnons - and thus the magnetization - can also be modified by changing the energy of the system. In this work, we experimentally demonstrate that the changes of magnon occupation due to magnetic fields and crystal orientation sensitively modify the SMR response. Higher magnetic fields reduce the magnon population by pushing the magnon manifold to higher energies, leading to an increase of magnetization and thus the SMR. In turn, the influence of the anisotropic magnon gap in yttrium iron garnet films leads to a crystal orientation dependence of the SMR. The magnetic field and orientation dependence can be rationalized in terms of the changing magnon occupation. Our results showcase that magnetoresistive effects not only probe the properties of the static magnetization, but also reveal information about the dynamics, i.e., the magnons.

MA 29.9 Wed 12:00 POT/0112

Non-reciprocal spin-orbital-charge interconversion via magnon transport in nonlocal devices — •Jose Omar Ledesma-Martin[1], Sachin Krishnia[1], Edgar Galindez-Ruales[1], Duc Tran[1], Marcel Gasser[1], Dongwook Go[1,2], Gerhard Jakob[1], Yuriy Mokrousov[1,2], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Mainz, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany

In magnetic systems, angular momentum is carried by electrons' spin and orbital angular momentum. We use devices based on Pt nanowires on insulating magnets to study angular-momentum transport mediated by magnons, enabling angular-momentum information to propagate without charge flow. In these systems, magnons are generated by spin accumulation from the Spin Hall Effect (SHE) and detected via the inverse Spin Hall Effect (iSHE). In conventional Pt-YIG nonlocal geometries, this spin-charge interconversion is fully reciprocal: interchanging the injector and detector yields equal efficiencies. We further confirm that this power-to-power efficiency remains reciprocal when the thickness of one Pt wire is varied. However, when Ru is used as a source and detector of orbital currents via the orbital Hall effect (OHE) and inverse OHE, the reciprocity is broken. In our devices, the combined SHE + OHE-driven magnon generation, followed by detection through the iSHE, becomes ~35% more efficient than the reverse process, demonstrating nonreciprocity in the system. (1)

(1) J.O. Ledesma-Martin, Nano Lett. 2025, 25, 8, 3247-3252

MA 29.10 Wed 12:15 POT/0112

Giant orbital magnetoresistance in orbital magnets — •Sachin Krishnia[1], Christin Schmitt[1], Edgar Galindez Ruales[1], Takashi Kikkawa[2], Timo Kuschel[1], Eiji Saitoh[2], Olena Gomonay[1], Yuriy Mokrousov[1], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg-University Mainz, Mainz, Germany — [2]Department of Applied Physics, The University of Tokyo, Tokyo, Japan

Generation and transport of large orbital angular momentum (OAM) currents have recently emerged as a key research area in the field of orbitronics. In contrast to spin currents, whose generation depends on weak spin-orbit coupling, OAM currents arise directly from the coupling between crystal momentum and electronic OAM even in light and environmentally friendly materials (Cu, Al, Cr)[1]. A major challenge has been to exploit these giant orbital currents in magnetic systems, where static magnetization is dominated by spin. We show that this limitation can be overcome by employing magnetic materials in which OAM contributes significantly to the static magnetization. Using these orbital magnets, we demonstrate two orders of enhancement of orbital Hall magnetoresistance, compared to the spin counterpart. This enhancement originates from the interaction of the dynamic OAM generated in light metals with the static orbital moments of the orbital magnet. Our results establish a pathway to harness giant OAM currents for device functionalities that cannot be achieved with conventional spin-dominated magnets[2]. [1] S. Ding et al, PRL 125, 177201 (2020). [2] C. Schmitt, S. Krishnia et al. (under review).

MA 29.11 Wed 12:30 POT/0112

Spin-Current Sensitivity in $CuSeO_3$ Across the Antiferromagnetic Transition — •Ankita Nayak[1], Mathew James[1], Maxim Mostovoy[2], and Aisha Aqeel[1] — [1]University of Augsburg, 86135Augsburg, Germany — [2]Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands

Antiferromagnets are promising materials for next-generation spintronics due to their robustness against magnetic fields and ultrafast dynamics. Spin Hall magnetoresistance (SMR) provides a sensitive method to probe spin transport at normal-metal–antiferromagnetic-insulator interfaces. In antiferromagnets, SMR can detect Néel-vector reorientation, spin-flop behaviour, and short-range correlations above the ordering temperature, as shown in systems such as NiO and α-Fe_2O_3.

Here, we use SMR in a Pt/$CuSeO_3$ bilayer to investigate spin transport in the unconventional antiferromagnet $CuSeO_3$. An AC current in the Pt Hall bar generates a transverse spin accumulation, whose interface reflection modulates the Pt resistance and enables electrical detection of the magnetic state.

$CuSeO_3$ consists of Cu(1) spin dimers and Cu(2) spins that order antiferromagnetically below 8 K. SMR measurements between 5 and 100 K with magnetic-field rotation in three planes reveal clear SMR signals, including a finite response above the Néel temperature, indicating persistent spin correlations. The plane-dependent SMR amplitude also reflects the intrinsic magnetic anisotropy of $CuSeO_3$.

MA 30: Functional Antiferromagnetism

Time: Wednesday 9:30–12:45 Location: POT/0151

MA 30.1 Wed 9:30 POT/0151

Electric Current Control of Helimagnetic Chirality from a Multidomain State — •Yuta Kimoto[1], Hidetoshi Masuda[1], Jun-ichiro Ohe[2], Shoya Sakamoto[1], Takeshi Seki[1,3], and Yoshinori Onose[1,3] — [1]Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan — [2]Department of Physics, Toho University, Funabashi 274-8510, Japan — [3]Center for Science and Innovation in Spintronics (CSIS), Core Research Cluster, Tohoku University, Sendai 980-8577, Japan

In helimagnets, magnetic moments form a helical spin order possessing chirality. In centrosymmetric crystals, two helical states with opposite handedness are degenerate; thus, chiral domains can coexist and form domain walls. Here, we study the domain wall dynamics under electric current in the helimagnet $MnAu_2$. We found that the threshold current required for the transition from the multidomain state to a single-chiral domain state in a magnetic field is much lower than that for chirality reversal from a single-chiral domain within certain ranges of temperature and magnetic field. The chirality after the transition depends on whether the magnetic field and electric current were parallel or antiparallel. Numerical calculations based on the Landau-Lifshitz-Gilbert equation reproduce our observations. These results indicate that the domain walls are highly mobile in the helimagnet, reflecting a pinning potential much smaller than the domain-nucleation energy. They also suggest that helimagnetic domain walls could serve as efficient information carriers, opening new avenues for spintronic applications, such as racetrack-type memory devices.

MA 30.2 Wed 9:45 POT/0151

Multistate probabilistic computing in the chiral kagome antiferromagnet Mn3Sn — •Prajwal Rigvedi[1], Jae-Chun Jeon[1], Kevin Callahan-Coray[2], Kerem Y. Camsari[2], and Stuart S.P Parkin[1] — [1]Max-Planck Institute of Microstructure Physics, Halle (Saale), Germany — [2]Department of Electrical and Computer Engineering, University of California, Santa Barbara, CA, USA

Chiral kagome antiferromagnets such as Mn3Sn are promising candidates for spintronic applications due to their ultrafast spin dynamics and negligible stray

fields. Their magnetic ground state exhibits six-fold degeneracy, which naturally supports multistate information processing. In this work, we investigate ultra-thin W/Mn3Sn bilayers and demonstrate spin-orbit torque-driven multistate probabilistic switching. Above a critical current density, stochastic fluctuations in the anomalous Hall resistance (Rxy) emerge, and their probability distribution can be continuously tuned with nanosecond electrical pulses. This tunability results in a sigmoidal response of Rxy to the applied current, enabling electrically controlled antiferromagnetic probabilistic bits with multiple accessible states. Leveraging experimentally obtained state statistics, we implement a graph coloring task, an NP-hard optimization problem. These results constitute the first experimental realization of multistate probabilistic switching in an antiferromagnet and demonstrate its applicability to non-deterministic computing tasks. Our findings position non-collinear antiferromagnets as a promising material platform for multibit spintronics, highlighting their potential for unconventional computing architectures.

MA 30.3 Wed 10:00 POT/0151

Antiferromagnetic Writing by Magneto-electric Field in Cr_2O_3 — Nikolai Khokhlov[1], •Aleksandr Buzdakov[2], Timur Gareev[1], Anatoly Zvezdin[3], Sergey Artyukhin[2], and Aleksei Kimel[1] — [1]Radboud University Nijmegen, Institute for Molecules and Materials, Nijmegen 6525 AJ, The Netherlands — [2]Istituto Italiano di Tecnologia, Via Morego 30, Genova 16163, Italy — [3]Moscow, Russia

Antiferromagnetic (AFM) spintronics is a promising platform for next-generation storage, offering high domain wall velocities and immunity to stray fields. However, a bottleneck remains: the lack of a low-power method to write arbitrary domains without high-density currents and Joule heating. Here, we demonstrate full, non-volatile control of AFM domains in magnetoelectric Cr_2O_3 at room temperature. Utilizing an electrically charged needle to "draw" domains under a magnetic bias, we find that approaching the Néel temperature is critical. In this regime, domain walls lose their elastic "rubber band" behavior, allowing complex shapes to stabilize. We rationalize this via the Larkin length, establishing that reliable storage requires a Larkin length smaller than the bit size. Our findings provide a model for domain writability in insulating antiferromagnets, paving the way for low-energy, electrically controlled AFM memory.

MA 30.4 Wed 10:15 POT/0151

Magnetic-phase-entangled orbital anisotropy in the van der Waals antiferromagnet $CrPS_4$ revealed by resonant inelastic X-ray scattering — •Zhijia Zhang[1], Yuan Wei[1], Carlos William Galdino[1], Cedomir Petrovic[2], and Thorsten Schmitt[1] — [1]Centre for Photon Science, Paul Scherrer Institut, Villigen PSI 5225, Switzerland — [2]Shanghai Advanced Research in Physical Sciences, Shanghai 201203, P.R. China

The emergence of exfoliable magnetic van der Waals (vdW) materials with weak inter-layer correlations enables physicists to study magnetism directly in two dimensions (2D). Their sustained magnetic order and other novel magnetic properties down to the 2D limit make them promising candidates for spintronic applications. $CrPS_4$ is an A-type antiferromagnetic vdW material with strong correlations between spin, orbital, and structural degrees of freedom, and its highly unusual magnetic properties has been the subject of considerable scientific and practical interests. In this talk, I will present our temperature-dependent X-ray absorption spectroscopy (XAS) and resonant inelastic X-ray scattering (RIXS) measurements on bulk $CrPS_4$ crystals. Both the XAS and RIXS spectra display significant linear dichroism. In particular, the linear-dichroic RIXS intensity of one of the orbital excitations shows an order-parameter-like temperature dependence below the Néel temperature; and the dichroism entirely disappears in the paramagnetic phase. This evidence strongly supports the role of the orbital anisotropy as the shaping agent of the magnetic states in $CrPS_4$.

MA 30.5 Wed 10:30 POT/0151

Impact of deposition parameters on magnonic properties of α-Fe_2O_3 thin films. — •Katharina Müller[1,2], Tobias Herrlich[1,2], Monika Scheufele[1,2], Matthias Opel[1], Hans Huebl[1,2,3], Rudolf Gross[1,2,3], Akashdeep Kamra[4], Matthias Althammer[1,2], and Stephan Geprägs[1] — [1]Walther-Meißner-Institut, BAdW, Garching, Germany — [2]TUM School of Natural Sciences, Munich, Germany — [3]Munich Center for Quantum Science and Technology, Munich, Germany — [4]Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau, Kaiserslautern, Germany

Magnons in magnetic insulators are promising spin information carriers in future spintronic devices. For such applications, investigating and understanding the magnonic properties of thin films is crucial. Among the antiferromagnetic insulators, α-Fe_2O_3 is a prime example to study. Upon cooling, it features a Morin transition at 263 K from an antiferromagnetic easy-plane to an easy-axis phase below the Néel temperature. We obtain the magnetic anisotropy, the Dzyaloshinskii-Moriya interaction, as well as the magnon decay length from the magnon Hanle effect in all-electrical magnon transport experiments [1]. We study the dependence of these properties on the deposition parameters of α-Fe_2O_3 thin films grown on differently oriented Al_2O_3-substrates. Starting from a multi-domain state and driving the system with an external magnetic field, we use spin Hall magnetoresistance measurements to assess how the monodomainization field is influenced by the deposition parameters. [1] M.Scheufele *et al.*, APL Mater. **11**, 091115 (2023).

MA 30.6 Wed 10:45 POT/0151

Investigation of magnetic symmetries and domain imaging in antiferromagnetic Mn_2As via methods of electron microscopy — •Oleksandr Zaiets[1,2], Kamil Olejník[3], Filip Křížek[3], Jose Angel Castellanos-Reyes[4], Jan Rusz[4], Darius Pohl[2], and Axel Lubk[1,2] — [1]IFW Dresden, Germany — [2]TU Dresden, Germany — [3]Institute of Physics of the Czech — [4]Uppsala University, Sweden

Antiferromagnets are promising candidates for spintronic applications due to their ultrafast dynamics, low magnetic susceptibility, and lack of stray fields. Their switching behaviour is determined by the undisturbed antiferromagnetic ordering, the distribution of magnetic defects (notably domain walls) and their pinning to structural defects of the underlying crystal structure.

In this work we investigate antiferromagnetic Mn_2As thin films epitaxially grown on GaAs via methods of transmission electron microscopy, in particular high resolution imaging and electron diffraction. The antiferromagnetic ordering of Mn_2As entails a doubled magnetic unit cell compared to the structural one. This allows us to study purely magnetic Bragg reflections. The analysis of these reflections suggests the presence of a previously unknown antiferromagnetic phase. We furthermore reveal the presence of an antiferromagnetic domain structure by mapping the intensity of these reflections. We discuss stabilization mechanisms of this new AF ordering with the help of ab-initio methods. The strength of the antiferromagnetic signal is sufficient for domain mapping with sub-nanometer scale.

15 min break

MA 30.7 Wed 11:15 POT/0151

Creation of antiferromagnetic skyrmions by edge manipulation — •Aleksey Berg, Tim Matthies, and Elena Vedmedenko — University of Hamburg

Novel magnetic storage technologies rely on ferromagnetic topological objects to represent information. These objects can be created, propelled and annihilated by electric currents in racetracks. We have recently demonstrated theoretically that arbitrary sequences of coexisting ferromagnetic skyrmions and antiskyrmions can be processed via local rotations of magnetic moments at the edge of a rectangular slab, eliminating the need for global charge or spin currents [1]. This local manipulation can be achieved experimentally using rotating local magnetic fields or currents. Here, we demonstrate that edge rotation can be effectively applied to antiferromagnetic skyrmions, too. Furthermore, antiferromagnetic quasiparticles can be created and propelled without rotating the edge magnetisation, but rather by switching the local magnetisation at the racetrack edge. This low-energy manipulation of stable antiferromagnetic topological quasiparticles via local excitation would be highly advantageous in the field of antiferromagnetic spintronics. 1. P. Siegl et al., Phys. Rev. B 106, 014421 (2022)

MA 30.8 Wed 11:30 POT/0151

Field-induced spin-reorientation transitions in collinear antiferromagnet Cr_2O_3 — •Paulina J. Prusik[1,2], Igor Veremchuk[1], Florin Radu[3], Pavlo Makushko[1], Jürgen Fassbender[1,2], Kirill D. Belashchenko[4], Denys Makarov[1], and Oleksandr V. Pylypovskyi[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., 01328 Dresden, Germany — [2]Dresden University of Technology, Dresden 01062, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin 12489, Germany — [4]University of Nebraska-Lincoln, Lincoln, NE 68588, USA

We classify collinear antiferromagnets (AMFs) by presence in their σ-model of a term of exchange origin that couples the external magnetic field and gradients of the Néel vector. One representative material is the magnetoelectric, room-temperature, collinear AFM Cr_2O_3, which is promising for spintronics applications [1,2] as well as for fundamental research [3,4]. In Cr_2O_3 this term leads to a texture-induced magnetization with a finite component along the crystallographic c axis. By analyzing the field-induced spin-reorientation transitions, we find the appearance of a phase in which a field-induced domain wall lies in the basal plane at fields below the spin-flop field. The theoretical predictions are supported by X-ray magnetic linear dichroism measurements, which show that the transition field in thin films is reduced by nearly half compared to the single crystal. [1] Hedrich et al., Nat. Phys. 17, 574 (2021) [2] Rickhaus, Prusik et al., Nano Letters 24, 13172 (2024) [3] Makushko et al., Nat. Comm. 13, 6745 (2022) [4] Pylypovskyi et al., Phys. Rev. Lett. 132, 226702 (2024)

MA 30.9 Wed 11:45 POT/0151

Direct Observation of Hidden Excitonic States via Exciton-Magnon Coupling in CrSBr — Sophie Bork[1], •Richard Leven[1], Vincent Wirsdörfer[1], Alessandro Ferretti[2], Rafael Rojas Lopez[1], Mattia Benini[1], David Maximilian Janas[1], Umut Parlak[3], Alberto Brambilla[2], Alexey Scherbakov[1], and Mirko Cinchetti[1] — [1]Department of Physics, TU Dortmund University, 44227 Dortmund, Germany — [2]CNR-IFN Dipartimento di

Fisica, Politecnico di Milano, 20133 Milan, Italy — [3]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany

Two-dimensional van der Waals magnets exhibit strong exciton binding and intrinsic magnetic order, enabling exciton-magnon coupling that links collective spin excitations with excitonic states. However, detecting dark excitons and their coupling remains challenging. Here we employ broadband transient reflectivity on CrSBr, a quasi-two-dimensional antiferromagnetic semiconductor, to probe excitonic structures across 1.25 - 1.65 eV under varying magnetic fields. We identify two excitonic resonances: a bright 1s exciton at 1.36 eV and a dark exciton near 1.46 eV, the latter revealed solely through exciton-magnon interactions. The detected GHz magnon mode exhibits magnetic-field-dependent frequency shifts and coupling signatures with both excitons. High-energy excitation modifies magnon dispersion and enhances exciton-magnon hybridization. These findings provide direct insight into exciton-magnon coupling in CrSBr and demonstrate that ultrafast optical probes can uncover hidden excitonic states, advancing understanding of hybrid quasiparticles in van der Waals magnets.

MA 30.10 Wed 12:00 POT/0151

Rocket-like dynamics of ferrimagnetic domain walls in graded magnets — •Pietro Diona[1,2], Sergey Artyukhin[2], and Luca Maranzana[2,3] — [1]Scuola Normale Superiore di Pisa, Pisa, Italia — [2]Istituto Italiano di Tecnologia, Genova, Italia — [3]Università di Genova, Genova, Italia

The domain wall motion underpins emerging spintronic technologies, such as high-speed racetrack devices and THz logic. Spatially nonuniform magnetic exchange and anisotropy in ferromagnets can pin or accelerate domain walls [1,2]. In ferrimagnets, where Walker breakdown is suppressed, domain walls can therefore approach the magnon speed [3]. Here we show that in non-uniform ferrimagnets such gradients not only exert a net force on the ferrimagnetic domain walls, but also modify the effective mass of the wall, enabling an entirely new acceleration mechanism. As a domain wall travels through regions of varying exchange or anisotropy, it can shed or gain effective mass leading to a "rocket effect" as in variable-mass systems. This phenomenon becomes increasingly pronounced as the wall approaches the magnon velocity [3], providing a natural route to ultrafast domain-wall propulsion. Our analytical theory, supported by micromagnetic simulations, suggests strategies for mass control in racetrack devices. These results establish variable-mass domain walls as a new paradigm for efficient, high-velocity spintronics and THz-frequency magnetic technologies.

[1] F. N. Tan et al., Scient. Rep., 9, 7369 (2019).
[2] P. Diona et al., IEEE Trans. on Elec. Dev., 69(7), 3675 (2022).
[3] P. Diona et al., Adv. Func. Mat., e22549 (2025).

MA 30.11 Wed 12:15 POT/0151

Revealing Magnetic Chirality in Non-Collinear Kagome Antiferromagnets through Spin-Seebeck Measurements — •Feodor Svetlanov Konomaev, Mithuss Tharmalingam, and Kjetil Magne Dørheim Hals — Department of Engineering Sciences, University of Agder, 4879 Grimstad, Norway

Non-collinear antiferromagnets (NCAFMs) are appealing for antiferromagnetic spintronics, as they combine the advantages of collinear antiferromagnets with novel emergent phenomena stemming from their complex spin structures. These phenomena are often associated with the intrinsic spin chirality, which characterizes the handedness of the ground-state spin configuration. Here, we investigate a kagome NCAFM interfaced with a normal metal and demonstrate that the groundstate vector spin chirality can be probed through measurements of the spin Seebeck effect (SSE). Starting from a microscopic spin Hamiltonian, we derive the corresponding bosonic Bogoliubov-de-Gennes Hamiltonians for the two chiral configurations. Using linear response theory, we obtain a general expression for the spin current thermally pumped into the normal metal by the SSE. We show that a sizable in-plane spin current emerges exclusively in the negative-chiral state, providing a direct signature for real-time detection of chirality switching in kagome NCAFMs. In addition, we find a field-dependent out-of-plane spin current whose magnitude differs between the two chiralities, reflecting their distinct magnon band structures

MA 30.12 Wed 12:30 POT/0151

Strain engineering of antiferromagnetic $LaFeO_3$ films for magneto-optical investigations — •Antonia Rieche, Wolfgang Hoppe, Chis Körner, Aurora Diana Rata, Andreas Herklotz, and Kathrin Dörr — Martin-Luther-Universität Halle-Wittenberg

$LaFeO_3$ is a representative member of the orthoferrites. This antiferromagnet exhibits a high Néel temperature of 740 K. A weak net magnetization is created due to a small tilting of the magnetic moments. $LaFeO_3$ is considered to be a promising candidate for antiferromagnetic spintronics.

While the magneto-optical Kerr effect (MOKE) has been used to investigate bulk crystals, only a single study has reported MOKE data for $LaFeO_3$. [1]

Our work demonstrates the magnetic switching behavior of coherently strained $LaFeO_3$ films. The strain states were generated using different substrates and helium implantation. [2] The films were grown using pulsed laser deposition (KrF 248 nm), and their strain state was analyzed by X-ray diffraction.

Longitudinal MOKE hysteresis and microscopy measurements revealed a strain-dependent orientation of the magnetization axis, which is consistent with predictions from density functional theory. [3] Further single-domain remanence has been confirmed.

[1] J. Alaria et al., Chem. Sci. 5, 1599 (2014)
[2] A. Herklotz et al., Adv. Science, 5, 1800356 (2018)
[3] A. J. Mao et al., RSC Adv. 6, 100526 (2016)

MA 31: Frustrated Magnets II (joint session MA/TT)

Time: Wednesday 9:30–12:45 Location: POT/0361

MA 31.1 Wed 9:30 POT/0361

Finite-size spectral signatures of order by quantum disorder: A perspective from Anderson's tower of states — •Subhankar Khatua[1], Griffin C. Howson[2], Michel J. P. Gingras[2], and Jeffrey G. Rau[3] — [1]IFW Dresden, Germany — [2]University of Waterloo, Canada — [3]University of Windsor, Canada

In frustrated magnetic systems with a subextensive number of classical ground states, quantum zero-point fluctuations can select a unique long-range ordered state, a celebrated phenomenon referred to as order by quantum disorder (ObQD). While ObQD is well understood in the semiclassical, large spin length limit, its behavior in quantum spin-1/2 systems is less clear. As exact analytical solutions are scarce for frustrated systems, numerical approaches are essential. We show that ObQD can be identified from exact diagonalization (ED) calculations through an analysis akin to the Anderson tower of states associated with spontaneous symmetry breaking. By defining an effective quantum rotor model, we describe the competition between ObQD-induced localization of the rotor and its tunneling between symmetry-related ground states, identifying the crossover lengthscale from the finite-size regime where the rotor is delocalized, to the infinite system-size limit where it becomes localized. This rotor model relates the characteristic splittings in the ED energy spectrum to the ObQD selection energy scale, providing an estimate that can be compared to spin wave calculations. We demonstrate the general applicability of this approach in one-, two- and three-dimensional frustrated spin models that exhibit ObQD.

MA 31.2 Wed 9:45 POT/0361

Magnetic resonance experiments on the quantum spin liquid candidate $YbCuSe_2$ — Madhurima Biswas[1], •Marlis Schuller[3], Khokan Bhattacharya[1], Yoshifumi Tokiwa[2], Mamoun Hemmida[3], Hans-Albrecht Krug von Nidda[3], Norbert Büttgen[3], István Kézsmárki[3], and Mayukh Majumder[1] — [1]Department of Physics, Shiv Nadar Institution of Eminence, IN — [2]Advanced Science Research Center, Japan Atomic Energy Agency, JPN — [3]EPV, Institut of Physics, University of Augsburg, DE

Frustrated magnetism in triangular-lattice delafossites offers a fertile route to realising quantum spin liquids (QSL) beyond conventional ordered phases. Among these materials a new candidate, $YbCuSe_2$, stands out as a QSL candidate from the present study. Magnetisation and ESR measurements on high-quality single crystals of $YbCuSe_2$ reveal easy-plane anisotropy. Furthermore, heat-capacity measurements down to 400 mK and μSR measurements down to 30 mK show no signatures of long-range magnetic ordering, establishing this compound as a promising QSL candidate. To probe the low-energy spin dynamics, we performed ^{63}Cu (I = 3/2) NMR measurements down to 20 mK. We document in-plane and out-of-plane spin-lattice relaxation T_1 as a function of temperature in an applied field of approximately 4 T. A dynamical phase separation was observed below 0.7 K, where one phase corresponds to the disorder-induced state, whereas the temperature evolution of the relaxation rate of the other phase exhibits a power-law divergence indicative of some quantum-critical spin fluctuations due to the proximity to a field-induced ordered state.

MA 31.3 Wed 10:00 POT/0361

Fluctuation driven phases in the triangular lattice — •P. Peter Stavropoulos[1], Roser Valentí[1], and Johannes Knolle[2] — [1]Goethe University, Frankfurt, Germany — [2]Technical University of Munich, Garching, Germany

The triangular lattice has proven to be a model platform of frustrated magnetism, with a rich landscape of emergent phases. It is also an experimentally accessible platform, with many family of materials showing quasi-2D triangular arrangements of magnetic ions. Motivated by this, we revisit magnetic exchange models

on the triangular lattice. We discuss phases that are stabilized by order by disorder mechanisms, and comment on their observable signatures.

MA 31.4 Wed 10:15 POT/0361

Frustrated spin-1/2 chains in a correlated metal Ti4MnBi2 — •Xiyang Li and Meng Lyu — No.8, 3rd South Street, Zhongguancun, Haidian District, Beijing, China, 100190

Electronic correlations lead to heavy quasiparticles in three-dimensional(3D) metals, and their collapse can destabilize magnetic moments. It is an open question whether there is an analogous instability in one-dimensional (1D) systems, unanswered due to the lack of metallic spin chain materials. We report neutron scattering measurements and density matrix renormalization group calculations establishing spinons in the correlated metal Ti4MnBi2, confirming that its magnetism is 1D. Ti4MnBi2 is inherently frustrated, forming near a quantum critical point that separates different phases at temperature T = 0. One-dimensional magnetism dominates at the lowest T, and is barely affected by weak interchain coupling. Ti4MnBi2 is a previously unrecognized metallic spin chain in which 3D conduction electrons become strongly correlated due to their coupling to 1D magnetic moments.

MA 31.5 Wed 10:30 POT/0361

Low-temperature spin-freezing in frustrated zirconates $Tb_2Zr_{2-x}Ti_xO_7$ — •Frederik Leon Carstens[1], Sujata Singh[2], C. S. Yadav[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]School of Physical Sciences, IIT Mandi, India

We report on magnetic studies of polycrystalline $Tb_2Zr_{1-x}Ti_xO_7$ ($x = 0, 0.5$). The zironates possess significant cationic disorder due to similar radii of the cations which introduces magnetic frustration. The materials are investigated by means of low-temperature ac and dc magnetization measurements in magnetic fields up to 7 T and down to 400 mK. Long-range magnetic order is not found down to $T = 400$ mK. However, in small magnetic fields, we observe a low-temperature spin-frozen state below $T = 1.4$ K and a slow spin relaxation regime which is significantly enhanced in static magnetic fields, e.g. to 15 K at $B = 2$ T. A similar behavior has been previously reported for the related rare-earth zirconate $Ho_2Zr_2O_7$ and in the hafnate $Tb_2Hf_2O_7$ [1,2].

[1] A. Elghandour et al., Phys. Rev. B **110**, 064408 (2024)

[2] V. K. Anand et al., Phys. Rev. B **97**, 094402 (2018)

MA 31.6 Wed 10:45 POT/0361

Magnetization plateaus, spin-canted orders and field-induced transitions in a spin-1/2 Heisenberg antiferromagnet on a distorted diamond-decorated honeycomb lattice — •Katarina Karlova and Jozef Strecka — Pavol Jozef Safarik University in Kosice, Slovakia

We investigate the spin-1/2 Heisenberg antiferromagnet on a distorted diamond-decorated honeycomb lattice in an external magnetic field. Using density-matrix renormalization group, sign-problem-free quantum Monte Carlo, exact diagonalization, and an effective lattice-gas approach based on localized-magnon physics, we determine the ground-state phase diagram and analyze the finite-temperature magnetization process.

The model hosts a rich variety of frustration-induced quantum phases, including Lieb-Mattis ferrimagnetic states, spin-canted regimes, monomer-dimer and dimer-tetramer phases, and dimensional-crossover states with 0D or 1D character. Depending on the lattice distortion, we identify robust magnetization plateaus at 0, 1/4, 1/2, and 3/4 of the saturation value, originating from competing local singlet clusters, composite spins, and flat-band localized magnons. Finite-temperature QMC data show how thermal fluctuations progressively smear the plateau structure, while the effective lattice-gas description reliably captures the corresponding low-temperature trends.

Funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V04-00403.

15 min break

MA 31.7 Wed 11:15 POT/0361

Effect of Ca-doping on the exotic quantum spin liquid states of Y3Cu2Sb3O14 — •Muhammad Usama Akbar[1], Hans-Albrecht Krug von Nidda[1], Mamoun Hemmida[1], Avinash Mahajan[2], and Saikat Nandi[2] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, D-86135 Augsburg, Germany — [2]Department of Physics, Indian Institute of Technology, Mumbai, 400076, India

The three-dimensional spin S = 1/2 compound Y3Cu2Sb3O14 was recently identified as a promising candidate for novel quantum spin liquid (QSL) behavior, with two inequivalent Cu2+ sites in edge-sharing triangles and no long-range order observed in multiple experiments [1]. NMR detects a transition near 120 K, associated with partial singlet formation, while muSR and DFT indicate frustrated antiferromagnetic interactions around both Cu+2 sites. ESR shows a Lorentzian line (g = 2.16) above 120 K that splits into two components on cooling, with only a part of spins being ESR-active. In the current work, we extend this investigation to Ca-doped Y3-xCaxCu2Sb3O14 (x = 0.05, 0.10, 0.25), to examine how chemical substitution at the Y site influences the spin dynamics of the compound.

[1] S. Nandi et al. (2025), arXiv:2509.15835 [cond- mat.str-el]

MA 31.8 Wed 11:30 POT/0361

Synthesis and H-T phase diagram of $Cu_2(OH)_3HCOO$ — •Issei Niwata[1,2], Kaushick K. Parui[1], Maxim Avdeev[3], Anton A. Kulbakov[1], Dmytro S. Inosov[1], and Darren C. Peets[1] — [1]TU Dresden, Dresden, Germany — [2]Hokkaido University, Sapporo, Japan — [3]ANSTO, Sydney, Australia

$Cu_2(OH)_3X$ (X = monovalent anion) consists of quasi one-dimensional (1D) ferromagnetic (FM) and antiferromagnetic (AFM) chains which alternate to form two-dimensional triangular layers, which are stacked along the c axis. As the interchain interactions are frustrated and interlayer interactions are weak, the system can be regarded as weakly coupled 1D FM and AFM chains. In bulk measurements, these compounds typically show AFM behavior with a Néel temperature (T_N) below 10 K. Because of the coexistence of FM and AFM chains, exotic magnetic excitations are expected. As a matter of fact, for $X = Br^-$, inelastic neutron scattering revealed magnon excitations and a gapped spinon continuum in the same energy range. In addition, for $X = NO_3^-$, the realization of a Tomonaga-Luttinger-liquid state in the AFM chain was suggested in magnetic fields around 20 T, where the magnetization shows a half saturation indicating full polarization of the FM chains. Recently, we grew single crystals of the $X = HCOO^-$ compound. Magnetization measurements showed $T_N = 5.4$ K and a half saturation below 5 T, much lower than $X = NO_3^-$. This suggests that we can explore the excitation structure in relatively low magnetic fields. I will discuss the phase diagram obtained by physical properties measurements.

MA 31.9 Wed 11:45 POT/0361

H–T Phase Diagram of the Frustrated Quantum Magnet Antlerite, $Cu_3SO_4(OH)_4$ — •Darren C. Peets[1], Nikolai S. Pavlovskii[1], Roman Gumeniuk[2], Sergey Granovsky[1], and Dmytro S. Inosov[1] — [1]IFMP, TU Dresden, Germany — [2]IEP, TU Bergakademie Freiberg, Germany

The magnetic copper sites in antlerite, $Cu_3SO_4(OH)_4$, are arranged in three-leg triangular-lattice ladders, a unique magnetic lattice. In the ground state, the outer legs are ferromagnetic and antialigned, while the central leg is antiferromagnetic. This material has four distinct magnetic states in zero field alone, and we show that the phase diagram in applied fields is also remarkably rich.

MA 31.10 Wed 12:00 POT/0361

Magnetic structure of a geometrically frustrated Mn3V2Ge3O12 garnet oxide — •Sagar Mal Kumawat[1], Tsai-Ling Liu[1], Chin-Wei Wang[2], Jia-Xiang Hsu[1,3], En-Pei Liu[3], Wei-Tin Chen[3,4,5], and Chien-Lung Huang[1] — [1]Department of Physics and Center for Quantum Frontiers of Research & Technology (QFort), National Cheng Kung University, Tainan 701, Taiwan — [2]National Synchrotron Radiation Research Center, Hsinchu 30076, Taiwan — [3]Center for Condensed Matter Sciences, National Taiwan University, Taipei 10617, Taiwan — [4]Center of Atomic Initiative for New Materials, National Taiwan University, Taipei 10617, Taiwan — [5]Taiwan Consortium of Emergent Crystalline Materials, National Science and Technology Council, Taipei 10622, Taiwan

We investigated the low-temperature magnetic structure and thermodynamic properties of Mn3V2Ge3O12 (MVGO) using neutron diffraction, magnetic, and heat capacity measurements. MVGO crystallizes in a cubic Ia-3d structure with a minor MnV2O4 impurity. Two successive transitions at TN1 = 4 K and TN2 = 2.4 K indicate noncollinear antiferromagnetic ordering of the frustrated V3+ and Mn2+ sublattices. Field-dependent heat capacity shows suppression of the TN1 anomaly and a shift of TN2, consistent with magnetic frustration and spin reorientation. The total magnetic entropy reaches approximately 51 J/mol K above 20 K, accounting for ~81% of the theoretical entropy for the full spin system. Temperature-dependent measurements reveal noncollinear antiferromagnetic order below TN2, with peak broadening up to TN1 indicating strong spin frustration.

MA 31.11 Wed 12:15 POT/0361

Crystallographic and magnetic structure of Pr_2PdSi_3: a single crystal neutron diffraction study — •Matthias Frontzek — Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

The intermetallic compound series R_2PdSi_3 (R = rare earth metal) exhibits intriguing magnetic properties, including giant magnetoresistance, pronounced anisotropy in its electronic behavior, and a generic field-induced phase. The magnetic structures are complex, with large magnetic unit cells arising from the delicate interplay between competing crystal electric-field effects, magnetic exchange interactions, and geometric frustration. Recently, the discovery of a Skyrmion lattice in Gd_2PdSi_3 has renewed interest in the magnetic properties of this series.

In our contribution, we present a detailed neutron single crystal diffraction study using the WAND^2 diffractometer at the High-Flux Isotope Reactor (HFIR) at ORNL. In heavy rare earth members, Pd/Si ordering lowers the symmetry from hexagonal to monoclinic; in contrast, the Pr_2PdSi_3 compound adopts an

orthorhombic structure with a $2 * a, 2 * b, 4 * c$ unit cell relative to the primitive hexagonal cell. Magnetic order setting in at $T_N = 2.1$K is preceded by broad diffuse scattering around the nuclear reflections, and below T_N a long-wavelength spin-density wave is observed coinciding with the short-range order evidenced by the diffuse scattering.

MA 31.12 Wed 12:30 POT/0361

Dynamical heterogeneity and fractal subdiffusive transport in spin-ice — •Malte Bieringer[1], Gianluca Teza[1,2], Claudio Castelnovo[3], and Roderich Moessner[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany — [2]Department of Physics, University of Trieste, Strada Costiera 11, 34136 Trieste, Italy — [3]TCM Group, Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK

Spin ice is a paradigmatic model that, despite its simplicity, enables the exploration of rich and robust emergent phenomena in topological magnets. Here we uncover a novel set of spin-ice phenomenology typically associated with vitrification processes in disordered systems.

We identify a pronounced peak in dynamical heterogeneity in a classical spin-ice model on the three-dimensional pyrochlore lattice, in the complete absence of disorder and - remarkably - in thermal equilibrium. At low temperatures, additional dynamical constraints emerge that confine the motion of magnetic monopole excitations to three-dimensional percolation clusters. This gives rise to ergodic subdiffusion, opposing conventional emergent hydrodynamics. The observed dynamical heterogeneity arises without disorder or ergodicity breaking, distinguishing it from conventional glasses and systems with Hilbert space fragmentation, suggesting a generic feature of topological magnets hosting deconfined quasiparticles.

Our results motivate the search for materials and artificial spin-ice realizations of this physics and propose higher-order dynamical correlations as a distinctive experimental signature of topological magnetism.

MA 32: Excursion: Current and Future High-Field THz User Facilities at HZDR

As part of the Focus Session "Chiral phonons and crystals coupled to magnetic order" and open to all interested potential users, we offer a tour of the high-field THz user facilities at Helmholtz-Zentrum Dresden-Rossendorf (HZDR) and an introduction to the planned Dresden Advanced Light Infrastructure (DALI). The superconducting accelerator-based THz beam lines TELBE and FELBE currently provide extreme THz and mid-infrared pulse energies at high repetition rates for international users from around the globe. In 2025, DALI was announced as one of the 9 shortlisted priority research infrastructures in Germany. It has been selected as a world-leading THz facility by the Federal Ministry for Research, Technology, and Space (BMFTR) to secure and enhance Germany's long-term research capabilities for the next decades. The guided tour includes a bus transfer to the Rossendorf site, lab visits at the current ELBE facilities and an introduction to DALI.

As the number of participants is limited, registration is required latest by 6 March 2026, using the following link https://events.hifis.net/e/DPG-2026_HZDR-excursion. The meeting point will be provided after registration.

Contact: Sebastian F. Maehrlein, s.maehrlein@hzdr.de

Time: Wednesday 14:00–17:30 Location: HZDR

Excursion

MA 33: Altermagnets IV

Time: Wednesday 15:00–18:30 Location: HSZ/0002

MA 33.1 Wed 15:00 HSZ/0002

Magnon transport and surface effects in an altermagnetic toy model — •Moumita Kundu[1], Rabea Schmidhuber[2], Marian Duelli[1], and Ulrich Nowak[1] — [1]Fachbereich Physik, Universität Konstanz, Konstanz, Germany — [2]Ludwig-Maximilians-Universität München, Geschwister-Scholl-Platz 1, 80539 München, Germany

Altermagnets are a recently discovered class of magnetic materials that show non-relativistic spin-splitting of the magnon bands and on exposure to a thermal gradient can carry a net magnetization unlike conventional antiferromagnets. Here, we present a simplistic toy model of an altermagnet having asymmetric exchange interactions in a checkered antiferromagnetic lattice. Using atomistic spin dynamic simulations based on the stochastic-LLG equation we obtain the spin dynamics. The altermagnetic phase is confirmed from magnon dispersions under a steady thermal excitation revealing chiral spin splitting as expected along one of the high-symmetry directions [110] and directions orthogonal to it. Surface effects are a direct outcome from these calculations, showing an orientation dependent surface magnetization detected for each cut of the sample. The spin Seebeck and spin Nernst effects are investigated both showing unique orientation dependent net magnetization and magnon accumulations following the lattice symmetries. Owing to the nondegenerate magnons branches, the group velocities of the corresponding magnons vary leading to distinct propagation lengths of the RH- and LH- modes predominant along different directions. The robustness to external magnetic fields is explored revealing preferential band liftings with an additional gap at the Γ point.

MA 33.2 Wed 15:15 HSZ/0002

Skyrmion dynamics in altermagnets — •Nicolai Timon Bechler and Jan Masell — Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Altermagnetism is a new type of magnetic order that combines the time-reversal symmetry breaking nature of ferromagnetism with the stray-field free nature of antiferromagnetism. [1] Altermagnets can host skyrmions - whirling magnetic textures that are characterized by an integer real-space topological winding number. In d-wave altermagnets, the skyrmions in both sublattices are elliptical, related by lattice symmetries, and the total winding number vanishes as the contributions of each sublattice cancel each other. In this talk, we explore the motion of skyrmions in d-wave altermagnets, driven by either spin transfer torque (STT) or a magnon current. We combine an analytical collective-coordinate approach with high-precision micromagnetic simulations. Our findings predict that the anisotropic skyrmion profile yields a genuine Hall response beyond conventional Zhang-Li STT. In turn, standard Zhang-Li STT yields no Hall-signal but large artifacts in simulations which were previously misinterpreted as a physical Hall effect. [2] Furthermore, we show that for a system driven by a magnon current, the anisotropic scattering cross-sections immediately lead to a skyrmion Hall effect.

[1] L. Šmejkal et al., Emerging Research Landscape of Altermagnetism. Phys. Rev. X 12, 040501 (2022). [2] Z. Jin et al., Skyrmion hall effect in altermagnets. Phys. Rev. Lett. 133, 196701 (2024).

MA 33.3 Wed 15:30 HSZ/0002

Unconventional Magnetism in Fe-Based Materials — Reuel Dsouza[1], Andreas Kreisel[1], Brian M. Andersen[1], Daniel Agterberg[2], and •Morten H. Christensen[1] — [1]Niels Bohr Institute, University of Copenhagen, 2200 Copenhagen, Denmark — [2]Department of Physics, University of Wisconsin-Milwaukee, Milwaukee, Wisconsin 53201, USA

Odd-parity magnetism constitutes an intriguing phase of matter which breaks inversion symmetry while preserving time-reversal symmetry. Here we demonstrate that the Fe-based superconductors exhibiting coplanar magnetic order realize an odd-parity magnetic state by combining low-energy modeling with density-functional theory. In the absence of spin-orbit coupling, the electronic spins are polarized along the k_z-direction and the splitting of the up and down states exhibits an h- wave form-factor. The magnitude of the splitting depends sensitively on specific parameters of the low-energy model, including specific out-of-plane hopping parameters and the Fermi energies of the hole- and electron-pockets. Interestingly, despite this state breaking inversion symmetry and exhibiting a finite out-of-plane Berry curvature and non-linear anomalous Hall effect, the Edelstein effect vanishes. Incorporating spin-orbit coupling tilts the momentum-space electronic spins into the (k_x, k_y)-plane and imparts finite

in-plane components to the Edelstein response. Our findings highlight the Fe-based superconductors as platforms for exploring odd-parity magnetism both on its own and coexisting with unconventional superconductivity.

MA 33.4 Wed 15:45 HSZ/0002

Optical investigations of electron-doped $FeSb_2$ — Renjith Mathew Roy[1], •Maxim Wenzel[1], Maksim Povolotskiy[1], Christian Prange[1], Artem Pronin[1], Yujie Xie[2], Tiantian Zhang[2], Vignesh Sundaramurthy[3], Maximilian van de Loo[4], Jule Kirschke[4], Andreas Kreyssig[4], Anna Böhmer[4], and Martin Dressel[1] — [1]1. Physikalisches Institut, Universität Stuttgart — [2]Institute of Theoretical Physics, Chinese Academy of Science, 100190 Beijing, China — [3]Max-Planck-Institute for Solid State Research, 70569 Stuttgart — [4]Experimental Physics IV, Ruhr Universität Bochum

While the marcasite-structured semiconductor $FeSb_2$ is nonmagnetic, theoretical predictions suggest that hole or electron doping can stabilize an altermagnetic order with a substantial non-relativistic spin splitting of approximately 0.2 eV [1].

Here, we investigate a series of Co-doped $FeSb_2$ samples using optical spectroscopic techniques including broadband infrared spectroscopy, Müller-matrix ellipsometry, and Raman scattering. Combined with density-functional theory calculations, we discuss the effects of electron doping and the consequent magnetic ordering on the electronic structure and optical phonon modes. In particular, we address the possibility of an emerging altermagnetic state for dopings above $x = 0.12$.

[1] I. I. Mazin, K. Koepernik, M. D. Johannes, R. González-Hernández, L. Šmejkal, PNAS **118**, e2108924118 (2021)

MA 33.5 Wed 16:00 HSZ/0002

Realization of epitaxial thin films of CrSb altermagnetic candidate material — •Edouard Lesne and Claudia Felser — Max-Planck-Institute für Chemische Physik fester Stoffe

CrSb belongs to a newly identified class of antiferromagnetically ordered materials coined altermagnets, whose spin-sublattices arrangement breaks time-reversal symmetry, giving rise to alternating spin-split bands with lifted Kramers degeneracy throughout the Brillouin zone. CrSb crystallizes in the hexagonal NiAs-type structure ($P6_3/mmc$) and exhibits a high antiferromagnetic ordering temperature (700-710 K), making it an ideal altermagnetic candidate material for room-temperature studies and prospective technological use in antiferromagnetic spintronic architectures.

We resort to a combination of X-ray diffraction, SQUID magnetometry and electrical magnetotransport techniques to investigate the intertwined structural, magnetic, and electronic transport properties of CrSb epitaxial thin films. We explore the growth of CrSb crystalline films by magnetron sputtering on a variety of crystalline seed layers and underlying single-crystalline substrates with hexagonal or cubic symmetry, which allows the stabilization of different crystallographic orientations of CrSb, while also tuning epitaxial strain. This work, while providing a testbed for the fundamental study of altermagnets and their structure-properties relationship, also opens avenues for the use of altermagnetic CrSb for antiferromagnetic devices with new functionalities relying on the manipulation of charge, orbital and spin degrees of freedom.

MA 33.6 Wed 16:15 HSZ/0002

Emergent d-Wave Order from Altermagnetic Symmetry in Cuprate and Nickelate Superconductors — •Tom G. Saunderson[1], James F. Annett[2], and Samir Lounis[1] — [1]Institute of Physics and Halle-Berlin-Regensburg Cluster of Excellence CCE, Martin-Luther-University Halle-Wittenberg, Halle(Saale) 06120, Germany — [2]H. H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8-1TL, United Kingdom

Since the discovery of cuprate high-T_c superconductivity, numerous theoretical frameworks have been proposed to explain its mechanism. Anderson's RVB picture [1] and U(1) gauge theory [2], for example, motivate a minimal one-band description that largely integrates out the role of oxygen. By contrast, 'altermagnetism' [3] produces a d-wave like k-space magnetic texture originating from alternatingly rotated *nonmagnetic* cages. In this talk, we take the central ideas of altermagnetism and apply them to both cuprate and nickelate families of superconductors. We show that the in-plane oxygen sublattice of CuO_2/NiO_2 layers, ubiquitous in these materials, intrinsically realizes the same symmetry. By imposing an *oxygen-centered*, staggered s-wave pairing, one obtains a d-wave gap with perfect C_4 symmetry, demonstrated self-consistently in $NdNiO_2$ from first principles. This description of superconductivity enables a direct mapping between a real-space order parameter and a lattice-based picture, opening the possibility of treating superconductivity and Hubbard-model physics on the same footing. [1] Science **235**, 1196 (1987); [2] Phys. Rev. Lett. **76**, 503 (1996); [3] Phys. Rev. X **12**, 031042 (2022).

15 min break

MA 33.7 Wed 16:45 HSZ/0002

Medium-Throughput Evaluation of Topological Transports for Altermagnets — •Fu Li[1], Bo Zhao[1], Shengqiao Wang[2], Chen Shen[1], Hao Wang[1], and Hongbin Zhang[1] — [1]Institute of Materials Science,Technical University of Darmstadt, 64287 Darmstadt, Germany — [2]School of Materials Science and Engineering, Jilin University, Changchun, 130012, China

The recent surge of interest in altermagnetism, distinct from both ferromagnetism and antiferromagnetism, highlights its potential for a wide range of technological applications. Quantifying their topological transport properties can provide essential guidance on the characterization of such materials while assessing their suitability for spintronic and optical applications. In this work, we collect around 200 known altermagnets (including also those with odd parity) based on symmetry arguments and perform medium-throughput density functional theory calculations to evaluate their topological transport properties such as anomalous Hall conductivity, magneto-optical Kerr effect, and shift current. Focusing on cases with broken inversion symmetry (i.e., polar altermagnets and odd-parity magnets), it is observed that the shift current can be large, making them promising for bulk photovoltaic applications. Furthermore, taking ferroelectric Fe2Mo3O8 as an example, it is demonstrated that its shift current can be controlled by external electric fields. Our results provide significant features characterizing altermagnets, and the obtained electronic structure can be starting point to investigate other intriguing physical properties.

MA 33.8 Wed 17:00 HSZ/0002

Electronic Raman spectroscopy in altermagnet MnTe — •Garima Garima[1,2,3], Thomas Böhm[1,3], Rudi Hackl[3], Bernd Büchner[1,3], and Jochen Geck[1,2] — [1]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01062 Dresden, Germany — [3]Leibniz Institute for Solid Sate and Materials Research Dresden, Helmholtzstrasse 20, D-01069 Dresden, Germany

Altermagnets, the new class of magnets, are promising candidates to realize spintronic and spin-information processing devices. The new magnetic state is characterized by broken time-reversal symmetry, resulting in spin-split bands in momentum space and hence provides a basis to foster chiral magnetic excitations. Here, we utilize electronic Raman scattering to investigate chirality in the hexagonal altermagnet MnTe. In consistency with RIXS experiments [1], our polarization-resolved results reveal optical signatures of 2-magnon excitations, appearing below the magnetic transition temperature of 310 K in the chiral A_{2g} channel. [1] Jost, D., et al. Chiral altermagnon in MnTe. arXiv preprint arXiv:2501.17380.

MA 33.9 Wed 17:15 HSZ/0002

Optically tunable spin transport in bilayer altermagnetic Mott insulators — Niklas Sicheler[1], Roberto Raimondi[2], Giorgio Sangiovanni[1], and •Lorenzo Del Re[1] — [1]Würzburg University — [2]Roma Tre

Altermagnets are a class of materials in which antiferromagnetic order coexists with non-relativistic spin splitting (NRSS), offering a promising route to spintronic functionalities without relying on strong spin*orbit coupling. In this work, we study a two-dimensional bilayer Mott insulator that realizes an altermagnetic phase shaped by the interplay between spin and layer degrees of freedom. This coupling produces a rich symmetry-breaking structure in which magnetic order is intertwined with inter-layer excitonic correlations. The layer polarization*tunable through an external gate voltage*acts as a key control parameter for this excitonic altermagnetic state. We demonstrate that an in-plane electric field applied with opposite signs across the layers generates a polarization current, which in turn drives a spin current within each layer. While the polarization current itself is isotropic, the induced spin current is highly anisotropic and can be reversed by tuning the photon energy. These results identify a mechanism for electrically and optically manipulating spin transport in correlated altermagnets, and highlight the central role of excitons in enabling controllable spin responses.

MA 33.10 Wed 17:30 HSZ/0002

Microscopic origin of the magnetic interactions and their experimental signatures in altermagnetic La2O3Mn2Se2 — •Laura Garcia-Gassull[1], Aleksandar Razpopov[1], Panagiotis P. Stavropoulos[1], Igor I. Mazin[2], and Roser Valentí[1] — [1]Goethe-Universität Frankfurt, Germany — [2]George Mason University, Fairfax, USA

Our analysis on the altermagnetic candidate La2O3Mn2Se2, realized on an inverse Lieb lattice, combines ab initio calculations, analytical modeling and spin-wave theory. We resolve a contradiction within the existing literature, where the GKA rules for half-filled orbitals have been applied, instead of the high-spin configuration ones. By studying the exchange pathways we show that the antiferromagnetic nearest-neighbor dominates over the next-nearest-neighbor coupling, since both direct exchange and superexchange cooperatively stabilize the magnetic ground state.

Going beyond static interactions, we compute the magnon spectrum within linear spin-wave theory and identify experimental signatures of the altermag-

netic exchange, a characteristic chiral splitting of magnon bands driven the inequivalent second-neighbor exchanges.

Our work not only clarifies the microscopic origin of altermagnetism, but also offers concrete predictions for its experimental verification, reinforcing La2O3Mn2Se2 as a model system for studying altermagnetic physics. You can find more details at: https://arxiv.org/pdf/2506.21661.

We thank the (DFG) through the TRR 288 (project B05).

MA 33.11 Wed 17:45 HSZ/0002

Altermagnetic Magnons in MnTe Probed by CD-RIXS — Daniel Jost[1,2], Resham B. Regmi[3,4], Eder G. Lomeli[5,1], Samuel Sahel-Schackis[6,2,7], •Monika Scheufele[8,9], Marcel Neuhaus[2], Rachel Nickel[10], Flora Yakhou[10], Kurt Kummer[10], Nicholas B. Brookes[10], Lingjia Shen[2], Georgi L. Dakovski[2], Nirmal J. Ghimire[3,4], Stephan Geprägs[8], and Matthias F. Kling[6,2,11] — [1]Stanford Inst. for Material and Energy Science, SLAC, USA — [2]Linac Coherent Light Source, SLAC, USA — [3]Dept. of Physics and Astronomy, Univ. of Notre Dame, USA — [4]Stravropoulos Center for Complex Quantum Matter, Univ. of Notre Dame, USA — [5]Dept. of Materials Science and Engineering, Stanford Univ., USA — [6]Stanford PULSE Inst., SLAC, USA — [7]Dept. of Physics, Stanford Univ., USA — [8]Walther-Meißner-Inst., BAdW, Germany — [9]TUM School of Natural Sciences, Physics Dept., TUM, Germany — [10]ESRF, France — [11]Dept. of Applied Physics, Stanford Univ., USA

Altermagnetism has emerged as a novel magnetic order combining features of both ferro- and antiferromagnetism. Despite their compensated spin structure, altermagnets exhibit symmetry-induced momentum-dependent splitting of magnon bands with well-defined chirality. This splitting must reflect the material's point-group symmetry. Here, we demonstrate the chiral character of these magnons by circular-dichroism resonant inelastic X-ray scattering (CD-RIXS) on altermagnetic α-MnTe [1]. We reveal momentum-dependent dichroism, indicating the polarization-dependent magnon splitting consistent with a g-wave symmetry. [1] D. Jost *et al.*, arXiv:2501.17380v2 (2025).

MA 33.12 Wed 18:00 HSZ/0002

Robust spin splitting and optical control in a layered altermagnet — •Alessandro De Vita[1,2], Chiara Bigi[3], Davide Romanin[4], Ralph Ernstorfer[1,2], Ilija Zeljkovic[5], Younghun Hwang[6], Matteo Calandra[7], Jill A. Miwa[8], and Federico Mazzola[9] — [1]Institut für Physik und Astronomie, Technische Universität Berlin — [2]Fritz Haber Institut der Max Planck Gesellshaft — [3]Synchrotron SOLEIL — [4]Université Paris-Saclay, CNRS — [5]Department of Physics, Boston College — [6]Electricity and Electronics and Semiconductor Applications Ulsan College — [7]Department of Physics, University of Trento — [8]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University — [9]Dipartimento di Fisica e Astronomia Galileo Galilei, Padova

Altermagnetism defies conventional classifications of collinear magnetic phases, with its unique combination of spin-dependent symmetries, net-zero magnetization, and anomalous Hall transport. Although altermagnetic states have been realized experimentally, their integration into functional devices has been hindered by the structural rigidity and poor tunability of existing materials. First, through cobalt intercalation of the superconducting 2H-NbSe2 polymorph, we induce and stabilize a robust altermagnetic phase and, via angle- and spin-resolved photoemission spectroscopy (spin-ARPES), we directly observe the lifting of Kramers degeneracy. Then, using ultrafast laser pulses, we demonstrate how a low-temperature phase can be quenched. Our findings open pathways to spin-based technologies and lay a foundation for advancing the emerging field of altertronics.

MA 33.13 Wed 18:15 HSZ/0002

Odd-parity-wave spin-polarized multiferroics — •Jan Priessnitz, Johannes Mitscherling, and Libor Šmejkal — Max Planck Institute for Physics of Complex Systems, Dresden, Germany

Combining ferroelectricity with spin polarization in ferromagnets is difficult due to the poor compatibility of insulating band structures and ferromagnetism. Recently, an alternative strategy based on combining time-reversal-broken spin polarization in altermagnetic insulators and ferroelectricity into type-I multiferroics was suggested [1]. Here we propose a different strategy based on time-reversal-symmetric odd-parity-wave spin polarization, which we demonstrate in type-II multiferroics induced by noncollinear magnetism [2,3]. Via state-of-the-art spin group theory and first-principle calculations, we demonstrate the spin polarization in $GdMn_2O_5$, a type-II multiferroic material combining coplanar p-wave magnetic order with ferroelectric order. Furthermore, we propose the antialtermagnetoelectric effect – cross-coupling between ferroelectric and odd-parity-wave time-reversal-symmetric spin polarization. The calculated switching path, influenced by exchange fields and spin-orbit coupling, and consistent with previous studies of ferroelectricity in this material, connects two distinct magnetic states with opposite signs of both electric and spin polarization.

[1] L. Šmejkal, arXiv:2411.19928.

[2] A. Birk Hellenes et al., arXiv:2309.01607v3.

[3] A. Chakraborty et al., Nat Commun 16, 7270 (2025).

MA 34: Computational Magnetism I

Time: Wednesday 15:00–18:30 Location: HSZ/0004

MA 34.1 Wed 15:00 HSZ/0004

GPU acceleration of atomistic spin dynamics simulations — Mariia Mohylna[1], Anders Bergman[2], Arkadijs Slobodkins[2], Olle Eriksson[2], Anna Delin[1], and •Johan Hellsvik[1] — [1]KTH Royal Institute of Technology, Stockholm, Sweden — [2]Uppsala University, Uppsala, Sweden

The Uppsala Atomistic Spin Dynamics (UppASD) [1,2] code implements algorithms for modelling magnetic materials on microscopic and mesoscopic length scales. In our recent implementation, kernels for magnetic field calculation for bilinear spin-spin pair interaction and one numerical integrator have been implemented with the CUDA programming model for use on NVIDIA GPUs, and the HIP programming model for AMD GPUs. Benchmarks for the simulation of bulk bcc Fe and the spin glass CuMn establish firmly the proposition of high speed-up for magnetization dynamics simulation on GPU hardware. The superior performance of the GPU implementations highlights the compatibility of spin-related problems with GPU architecture.

[1] The UppASD code https://github.com/UppASD/UppASD [2] Atomistic spin-dynamics; foundations and applications, O. Eriksson, et al. (Oxford University Press, 2017).

MA 34.2 Wed 15:15 HSZ/0004

Spin waves in double-layered antiferromagnets: insights from chain models and application to CrN — Seo-Jin Kim[1], Zdeněk Jirák[2], Jiří Hejtmánek[2], Karel Knížek[2], Helge Rosner[1], and •Kyo-Hoon Ahn[2] — [1]Max Planck Institute for Chemical Physics of Solids, D-01187 Dresden, Germany — [2]Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, 162 00 Praha 6, Czechia

The stability and magnonic properties of double-layered antiferromagnets are examined using two model systems, the linear chain (LC) and the railroad trestle (RT) geometry, and compared with the behavior of the real solid CrN. In the LC, the spin-paired order ($\cdots++--\cdots$) requires alternating ferromagnetic and antiferromagnetic (AFM) exchanges, whereas in the RT geometry an analogous order remains stable even with purely AFM interactions under specific analytical conditions. In CrN, the rock-salt structure causes strong magnetic frustration because each Cr atom has twelve symmetry-equivalent AFM nearest neighbors. Below T_N = 287 K, however, a magnetostructural transition to an orthorhombically distorted phase generates four distinct Cr-Cr distances and, consequently, a broad distribution of exchange strengths. This diversification suppresses frustration and stabilizes the double-layered AFM order. We trace this behavior to the competition between Cr–Cr direct exchange and 90° Cr–N–Cr superexchange, both exhibiting characteristic power-law dependencies on the interatomic distances. Finally, using *ab initio* exchange parameters, we derive the magnon spectrum and the temperature evolution of the ordered moments.

MA 34.3 Wed 15:30 HSZ/0004

Magnetoelastic behavior calculations in tetragonal systems — •Jakub Sebesta and Dominik Legut — IT4Innovations, VSB-TU Ostrava, 17.listopadu 2172/15, 708 00 Ostrava-Poruba, Czech Republic

In modern devices, various energy conversion effects are used for efficient operation. One of these effects represents magnetoelasticity – the conversion between the magnetic and mechanical energy. It is widely used in sensors or actuators *e.g.* force or torque sensors, fuel injectors, micro-pump, etc. So far, high symmetry systems, such as ferromagnetic 3d elements or rare-earth-based Laves phases, have been studied especially. In contrast ,here we provide a theoretical investigation of magnetoelastic behavior in tetragonal systems, focusing on the determination of the magnetoelastic properties influenced by the magnetic structure, and investigating the source of the observed modification. Eventually, we discussed a simple theoretical model for the magnetoelasticity in the considered systems.

[1] J. Sebesta et al. Magnetoelasticity - magnetic structure interrelation - tetragonal MnPt system study, Arxiv 2503.14693

MA 34.4 Wed 15:45 HSZ/0004

Ontology-driven Metadata for Multiscale Magnetism: The mammos-entity tool — •Andrea Petrocchi[1], Swapneel Amit Pathak[1], Martin Lang[1], Samuel J. R. Holt[1], Wilfried Hortschitz[2], Santa Pile[2], Martin Dobiasch[2], Thomas Schrefl[2], and Hans Fangohr[1] — [1]MPSD, Hamburg, Germany — [2]UWK, Krems, Austria

In science numerical values are interpretable only when their units and semantic meanings are known. Ontologies are able to identify physical quantities (i.e. using unique labels) and the provenance of data (i.e. the source and process creating it). The magnetic materials ontology is developed within the MaMMoS project and defines magnetic material properties and their interrelationships across various length scales.

In this talk, we present the core capabilities and limitations of mammos-entity, a Python package focused on one essential subset of information (called entity) needed for reliable data exchange: value, unit, and ontology label. This package facilitates working with entities programmatically, streamlines reading and writing data enriched with units and ontology identifiers as metadata and improves FAIRness of data. The aim is to make semantic annotation of data simple enough for everyday use. The mammos-entity package emerges from the magnetism community but supports all quantities defined in the EMMO (https://emmc.eu/emmo/).

Acknowledgements: Supported by the EU Horizon Europe programme under grant agreement No. 101135546 (MaMMoS).

MA 34.5 Wed 16:00 HSZ/0004

Prediction of Iron Atom Magnetic Moments in Fe-Al Alloys via SOAP-based Neural Network Models — •Vojtěch Ráliš[1,2], Martin Friák[1], Jan Fikar[1], and Aleš Horák[2] — [1]Institute of Physics of Materials, v.v.i., Czech Academy of Sciences, Brno, Czech Republic — [2]Faculty of Informatics, Masaryk University, Brno, Czech Republic

We investigate neural network approaches for predicting local magnetic moments of iron atoms in Fe-Al disordered alloys using a dataset of 227 unit cells (27–216 atoms) with Al concentrations of 0–60%, totaling 6880 Fe atoms (mean: 2.013 μ_B, std: 0.424 μ_B) from DFT calculations.

Local environments are encoded using SOAP descriptors with a cutoff capturing the first three coordination shells, yielding rotation- and translation-invariant features. Our feedforward neural network achieves MAE = 0.0436 μ_B on the test set, significantly outperforming a first-neighbor baseline (MAE = 0.121 μ_B) and CHGNet (MAE = 0.215 μ_B), while requiring far less memory and compute time.

These results demonstrate the effectiveness of SOAP-based neural networks for fast, accurate prediction of electronic properties in metallic alloys, with implications for large-scale computational screening and local magnetic phenomena studies.

MA 34.6 Wed 16:15 HSZ/0004

Material Parameter Determination with Deep Learning — •Jack Smith[1,2], Dieter Suess[1], and Florian Slanovc[2] — [1]University of Vienna, Vienna, Austria — [2]Silicon Austria Labs, Villach, Austria

Measuring a set of material parameters from stray field measurements presents a challenging inverse problem. In this work, we introduce a data-driven approach for this task using a probabilistic neural network.

A standard regression approach can fail to capture the non-uniqueness of this task, leading to unphysical predictions. To mitigate this, we model the conditional probability distribution of the material parameters and measured stray field. We use a mixture density network (MDN)[1], which combines a neural network with a mixture density model, to model this conditional probability distributions. To capture spatial correlations, we employ a convolutional neural network feature extractor that projects the stray field map into a high-dimensional latent space before probabilistic decoding with the MDN.

We demonstrate that this method can extract ground-truth parameters with high accuracy, even for visually indistinguishable stray fields. It also provides a quantifiable uncertainty, identifying regimes where the stray field solution is non-unique and traditional inversion methods would fail.

[1] C. M. Bishop, Mixture density networks (1994).

MA 34.7 Wed 16:30 HSZ/0004

Automated Magnetism Analysis via Tensorial Interacting Spins — •Haichang Lu[1,2] and Stefan Blügel[3,4] — [1]Fert Beijing Institute, MIIT Key Laboratory of Spintronics, School of Integrated Circuit Science and Engineering, Beihang University, Beijing, 100191, China — [2]Engineering Department, Cambridge University, Cambridge CB2 1PZ, UK — [3]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [4]Institute for Theoretical Physics, RWTH Aachen University, 52062 Aachen, Germany

Analyzing and describing magnetism in materials with localized moments requires accurate and generalizable spin models that go beyond conventional scalar or vector exchange interactions. Here we present *AMATIS*: an automated computational workflow that systematically incorporates tensorial spin interactions (non-relativistic and relativistic) into the effective Hamiltonian. Grounded in quantum spin properties and group theoretical analysis, tensorial components are extracted from the constrained least-squares fitting, ensuring fidelity to *ab initio* data. An integrated Monte Carlo module allows for the simulation of finite-temperature magnetic thermal equilibrium properties. We demonstrate the utility of this workflow on a series of two-dimensional magnetic materials and a van der Waals heterostructure, revealing the full spectrum of relevant tensorial interactions and their impact on magnetic properties. This approach offers a robust, high-throughput pathway from atomic structure to magnetic behavior, advancing the predictive design of novel magnetic materials.

15 min break

MA 34.8 Wed 17:00 HSZ/0004

Forestalled phase separation as the precursor to stripe order and superconductivity — •Aritra Sinha and Alexander Wietek — Max Planck Institute for the Physics of Complex Systems

Stripe order is a key feature of the cuprate phase diagram and appears as the ground state of the two-dimensional Fermi-Hubbard and t-J models in relevant regimes. With increasing temperature, stripe and superconducting orders give way to the strange metal and pseudogap phases, whose microscopic origins remain unclear. Using advanced tensor-network simulations, we try to identify the real-space mechanisms behind this evolution. iPEPS reveals a strong peak in the uniform charge susceptibility above the stripe phase near hole doping p=0.1, sharpening on cooling. METTS simulations on finite cylinders trace this peak to fluctuating charge clusters, resembling incipient phase separation into hole-rich and hole-poor regions-ultimately prevented by stripe order at low temperature. In the doped Mott regime of the t-t'-J model, we find that fluctuating domain walls of doped holes act as precursors to superconductivity. At low T, transient mergers of hole-rich regions create larger clusters containing superconducting condensates, which gradually phase-lock upon cooling into a coherent, stripe-aligned d-wave superconductor. Together, these results suggest a unified picture where charge and pairing fluctuations evolve into stripe order and superconductivity, clarifying their intertwined roles in strongly correlated systems.

MA 34.9 Wed 17:15 HSZ/0004

Anisotropic Ligand-Mediated Magnetic Interactions in Strongly Correlated Layered Antiferromagnet $GdTe_3$ — •Sergii Grytsiuk[1], Patrik Thunström[2], Mikhail I. Katsnelson[1], and Malte Rösner[1] — [1]Radboud University, Institute for Molecules and Materials, Nijmegen, The Netherlands — [2]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

In this study, we investigate the magnetic properties of $GdTe_3$ through first-principles calculations and spin-dynamics simulations. We reveal that its complex phase diagram arises from the interplay between the antiferromagnetic isotropic exchange of Gd localized f- and delocalized d-states and the substantial anisotropic exchange with Te ligand-conducting p-states. Despite the half-filled nature of Gd-f states suggesting a lack of magnetocrystalline anisotropy (MCA), we identify that the anisotropic coupling of it with ligand states serves as the primary source of MCA. This coupling is significantly influenced by the magnetic ordering of neighboring localized spins and is sensitive to charge density waves (CDW). It can also be tuned via magnetic field, temperature, and pressure. By linking the ligand spin-orbit coupling and induced magnetic moments to the effective interactions among localized spins, we successfully reproduce the experimental magnetic susceptibility across varying temperatures, magnetic fields, and pressures.

MA 34.10 Wed 17:30 HSZ/0004

operator Lanczos approach enabling neural quantum states as real frequency impurity solvers — •Jonas Rigo[1] and Markus Schmitt[1,2] — [1]Forschungszentrum Jülich GmbH, Peter Grünberg Institute, Quantum Control, 52425 Jülich, Germany — [2]University of Regensburg

To understand the intricate exchange between electrons of different bands in strongly correlated materials, it is essential to treat multi-orbital models accurately. For this purpose, dynamical mean-field theory (DMFT) provides an established framework, whose scope crucially hinges on the availability of efficient quantum impurity solvers. Here we present a real-frequency impurity solver based on neural quantum states (NQS) combined with an operator-space Lanczos construction. NQS are an asymptotically unbiased variational ground-state ansatz that employs neural networks to capture long-range correlations on complicated graph structures. We leverage this ability to solve complex multi-orbital impurity problems using a systematically improvable segmented commutator operator Lanczos (SCOL) construction. Our benchmarks on both the single-orbital Anderson model and the multi-orbital Hubbard–Kanamori impurity Hamiltonian reveal excellent ground state precision and the capacity to resolve key features of zero temperature spectral functions and self-energies. These promising results open avenues for extending DMFT to more challenging problems.

MA 34.11 Wed 17:45 HSZ/0004

Theoretical study of doping and pressure effects in organic magnets — Rohit Pathak[1,2], Isabella Rudengren[1,2], Torbjörn Wigren[1], Anna Delin[2,3], Olle Eriksson[1,2], Niklas Wahlström[1,2], and •Vladislav Borisov[1,2] — [1]Uppsala University, Sweden — [2]Wallenberg Initiative Materials Science for Sustainability, Sweden — [3]KTH Royal Institute of Technology, Stockholm, Sweden

Technologically important permanent magnets used nowadays rely on rare-earth elements and are associated with negative environmental impact and high energy costs, when produced. On the other hand, organic magnets are known, which can solve these problems, but their applications are limited due to low ordering temperature and coercivity. In this work, we aim to explore further the class of organic magnets to find ways of improving their magnetic properties, which would allow their applications and potentially even partial replacement of inorganic magnets. Also, fundamental aspects of organic magnets are studied in terms of delocalized nature of magnetism. Using first-principles electronic structure theory and atomistic spin dynamics (UppASD code [1]), we model magnetic properties of different compounds including the effects of chemical doping and mechanical pressure to understand the structural and chemistry-related trends. Machine-learning models for property prediction and structure reverse engineering will be applied to make the search for new magnets feasible.

1. B. Skubic, J. Hellsvik, L. Nordström, and O. Eriksson, A method for atomistic spin dynamics simulations: implementation and examples, J. Phys.: Condens. Matter. 20, 315203 (2008).

MA 34.12 Wed 18:00 HSZ/0004

Ground-state phases and excitation spectra of dipole conserving spin-half chain — •Prabhakar Prabhakar[1], Soumya Bera[1], and Giuseppe De Tomasi[2] — [1]Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India — [2]CeFEMA-LaPMET, Departamento de Fisica, Instituto Superior Tecnico, Universidade de Lisboa, Portugal

We explore the ground state phase diagram of a translationally invariant, non-integrable one-dimensional spin chain with dipole conservation. The model is typically realized in quantum simulators, such as cold-atom setups, in the presence of a large, tilted electric field. Despite the strong kinetic constraints imposed by dipole conservation, which prevent the propagation of isolated spin excitations and suppress single-spin order, the system stabilizes an antiferromagnetic dipole-ordered ground state. However, at a large Ising interaction strength, the model shows a phase transition to a spin-ordered phase. Using exact diagonalization along with density matrix renormalization group simulations, we examine the associated phases with different antiferromagnetic order parameters, the entanglement spectrum, and the dynamical spectral function.

MA 34.13 Wed 18:15 HSZ/0004

Implementation of spin-current density functionals in VASP — •Fabien Tran, Marie-Therese Huebsch, and Martijn Marsman — VASP Software GmbH, A-1090, Vienna, Austria

The implementation of spin-current density functionals (SCDF) in VASP is reported. SCDFs, which depend on the spin kinetic-energy density and spin current density, are intended for non-collinear calculations and can capture a non-zero local exchange-correlation spin torque. Results obtained with various SCDFs, namely TDRU [Tancogne-Dejean *et al.*, Phys. Rev. B **107**, 165111 (2023)], nc-mSCAN [Desmarais *et al.*, Phys. Rev. Lett. **134**, 106402 (2025)] and HTM [Huebsch *et al.*, arXiv:2501.04124 (2025)] will be presented.

MA 35: Spintronics (other effects) (joint session MA/TT)

Time: Wednesday 15:00–18:00 Location: POT/0112

Invited Talk MA 35.1 Wed 15:00 POT/0112

Magneto-optic Kerr effects of higher order in magnetization in thin films of different crystal orientations — •Timo Kuschel — Johannes Gutenberg University Mainz, Germany

The magneto-optic Kerr effect (MOKE) is an important tool to study magnetic properties of thin films. While the MOKE contribution linear in magnetization (LinMOKE) is mainly used for Kerr imaging, Kerr spectroscopy, time-resolved MOKE, and vectorial magnetometry of ferromagnetic thin films [1], the MOKE contributions quadratic in magnetization (QMOKE) [2] have been used for investigations of antiferromagnetic materials, spin-orbit torques, and structural order of Heusler compounds [3]. Recently, we have identified MOKE contributions of third order in magnetization (cubic MOKE, CMOKE) [4] and studied its dependence on the structural domain twinning of Ni(111) thin films.

In this talk, I will introduce these MOKE effects of higher order and describe their angular dependencies with respect to the crystal orientations of the thin films. While it is quite simple to find CMOKE in (111)-oriented films, it is not straightforward to identify it in (001)-oriented samples. I will discuss the reasons. Furthermore, I will report on the material systems that have shown CMOKE so far and mention potential applications.

[1] T. Kuschel et al., J. Phys. D: Appl. Phys. 44, 265003 (2011)
[2] R. Silber, TK et al., Phys. Rev. B 100, 064403 (2019)
[3] R. Silber, TK et al., Appl. Phys. Lett. 116, 262401 (2020)
[4] M. Gaerner, TK et al., Phys. Rev. Applied 22, 024066 (2024)

MA 35.2 Wed 15:30 POT/0112

Ignition of spin-triplet supercurrent in a ballistic S/F/S Josephson junction with precessing magnetization — •Elizaveta Andriyakhina, Miad Mansouri, Maxim Breitkreiz, and Piet Brouwer — Freie Universität Berlin, Germany

We develop a theory for a ballistic Josephson junction with a ferromagnetic (including half-metallic) interlayer whose uniformly precessing magnetization generates a controllable equal-spin (triplet) supercurrent. In a co-rotating frame, the driven junction maps to an effective static problem that can be treated with a scattering-matrix approach to obtain Andreev bound states and the dc Josephson current.

A key result is that steady precession produces a spin-dependent non-equilibrium occupation in the rotating frame, yielding a finite dc supercurrent. In the half-metal limit the junction is "off" without precession, but becomes "on" when a finite precession angle induces phase-sensitive Andreev levels and a triplet current.

For small precession angles, the induced current is approximately sinusoidal in phase and the critical current scales quadratically with the precession angle (and with drive parameters), enabling microwave-controlled switching via ferromagnetic resonance.

MA 35.3 Wed 15:45 POT/0112

Magnetic Domain Wall Motion under Microwave Excitation — •Lukas Fischer[1], Rouven Dreyer[2], Jae-Chun Jeon[1], Georg Woltersdorf[2], and Stuart Parkin[1] — [1]Max-Planck Institute of Microstructure Physics, Halle (Saale), Germany — [2]Martin-Luther-University Halle-Wittenberg, Halle (Saale), Germany

Chiral domain walls (DWs) and their synchronous motion via current pulses in magnetic conduits (so-called magnetic racetracks) are of enormous interest due to their fast speed, non-volatility, and capability of creating high bit-density for advanced memory and logic technologies. Most experimental and numerical studies have focused on the motion of the DWs by spin-orbit torque using nanosecond-long current pulses which are not efficient in coupling to magnetization precessions of the magnetic material, typically occurring in the GHz regime.

Here we present that the microwave excitation of chiral Néel DWs in a magnetic microwire with perpendicular magnetic anisotropy significantly impacts the DW motion. We use either magnetic fields or electrical currents at RF-frequencies to explore the pronounced impact on the DW motion. Firstly, we directly visualize the high-frequency response of the DW by using the Super-Nyquist sampling magneto-optical Kerr effect. We then determine the effect of this excitation on the DW motion. When the DW is excited in the presence of a static, transverse magnetic field, it exhibits unidirectional self-propulsion. Moreover, the resonant excitation in a static, longitudinal field leads to a current-triggered, sustained DW motion over micrometer distances, which dramatically increases the effective DW displacement.

MA 35.4 Wed 16:00 POT/0112

Assembly of Magnetic Heterostructures with Chiral Nanographenes — •Chi Fang, Wenhui Niu, Jitul Deka, and Stuart Parkin — Max Planck Institute of Microstructure Physics, Halle(Saale) 06120, Germany

Chirality-induced spin selectivity (CISS) is an emergent phenomenon whereby chiral molecules act as efficient spin filters, selectively transmitting electrons of a particular spin orientation. A central challenge in advancing CISS-based spintronics lies in experimentally verifying spin filtering in structurally defined, laterally extended molecular systems, using standard solid-state device techniques that yield reproducible and robust spin-dependent transport signals. Here, we present direct experimental evidence of the CISS effect in helical nanographenes (NGs), using magnetoresistance (MR) measurements in magnetic heterostructures. The device architecture included a bottom electrode ferromagnetic con-

tact, orthogonally patterned and electrically isolated by an AlOx layer to confine current to the junctions. NG, a synthetically tailored chiral molecule, was spin-coated to form a thin, uniform layer serving as a spin-filter interface. Different from previous works, the ferromagnet layer grown directly on the substrate offers a better performance of the magnetic properties. Both enantiomeric devices showed MR values around 1 % at room temperature, with minimal variation over the 10*400 K temperature range, indicating robust and reproducible spin selectivity. [1] B. Bloom et al. Chem. Rev. 124(4), 2014;[2] S. Ham et al. Micromachines 15(4), 528, 2024;[3] S. Yang et al., Nat. Rev. Phys. 3, 328, 2021.

MA 35.5 Wed 16:15 POT/0112

Alloying-Driven Modifications of the Magnetic Properties in Transition-Metal Iodides — •Paulina Jureczko[1,2] and Martin Gmitra[1,3] — [1]Institute of Experimental Physics, Slovak Academy of Sciences, 04001 Košice, Slovakia — [2]Institute of Physics, University of Silesia in Katowice, 41-500 Chorzów, Poland — [3]Institute of Physics, Pavol Jozef Šafárik University in Košice, 04001 Košice, Slovakia

Single-layer transition-metal dihalides have recently emerged as a platform for exploring two-dimensional magnetism and topology. Using density-functional theory, we investigate the electronic and magnetic properties of MI_2 monolayers and alloyed $M_{1-x}N_xI_2$ systems, where M and N represent Mn, Fe, Co, Ni. We analyze how chemical substitution modifies exchange interactions and spin-orbit-driven topological features by computing the Berry curvature and Chern numbers. The results reveal that alloying provides an efficient route for tuning magnetic anisotropy and topological phases in transition-metal iodides, underscoring their potential relevance for 2D spintronics.

This work has been funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I05-03-V02-00071.

15 min break

MA 35.6 Wed 16:45 POT/0112

Spintronic THz Frequency Conversion Mediated by Ferromagnetic/Oxide Interfaces — •Kang Jin[1], Ruslan Salikhov[1], Stefan Kober[2], Igor Ilyakov[1], Jan-Christoph Deinert[1], Aleksandra Lindner[1], Jürgen Fassbender[1,3], Sebastian F. Maehrlein[1,3], Zhe Wang[2], and Jürgen Lindner[1] — [1]HZDR — [2]TU Dortmund — [3]TU Dresden

Frequency conversion is a key nonlinear phenomenon for communication and data processing technologies. Exploring this phenomenon at terahertz (THz) frequencies is of particular interest, as the high carrier frequency enables faster data transfer and higher operational speeds. Previous experiments have revealed that THz frequency conversion could serve as a distinctive probe for THz-light-induced ultrafast spin-transfer currents (STCs) at Ferromagnetic (FM)/Non-Magnetic (NM) interfaces. Building on these findings, we report THz frequency conversion using cost-effective NM materials (such as SiO2 and Al2O3 films) and demonstrate their origin from the interfacial inverse Rashba-Edelstein effect. We compare conversion efficiencies and characteristics of different samples, revealing that FM interfaces, featuring off-stoichiometric SixOy and AlxOy, achieve conversion efficiencies comparable to heavy metal capping layers (i.e. Ta). The deposition sequence and the oxidation level of the samples were found to critically influence the sign of the spin-charge conversion. The observed THz second harmonic generation represents a spintronic foundation for developing THz frequency mixers and rectifying components.

MA 35.7 Wed 17:00 POT/0112

Magnetic hyperfine fields in solids without inversion symmetry induced by an external electric field — •Alberto Marmodoro[1,2,3,4], Hubert Ebert[1], Sergiy Mankovsky[1], and Jan Minar[3] — [1]LMU Munich, Munich, DE — [2]Inst. of Physics of the Czech Acad. of Sci., Prague, CZ — [3]University of West Bohemia, Pilsen, CZ — [4]Czech Technical University., Prague, CZ

An electric field induces in a solid without inversion symmetry spin and orbital magnetization - a phenomenon called Edelstein effect. This induced magnetization has to have its counterpart in an induced magnetic hyperfine field seen by nuclear magnetic moments. Corresponding NMR experiments have been performed recently on Te with success [1]. Using Kubo's linear response formalism implemented on the basis of the relativistic Korringa-Kohn-Rostoker Green function technique a description for the field induced hyperfine field (EFI-HFF) has been developed in analogy to that for the spin and orbital Edelstein effect [2]. The EFI-HFF drastically differs from that induced by an external magnetic field as the later one does not need missing inversion symmetry. Making use of a Gordon decomposition of the electronic current a splitting of the EFI-HFF into its spin and orbital parts is achieved [3]. This allows to discuss them in relation to their counterparts concerning the magnetization as well as the role of the spin-orbit coupling for them. Corresponding numerical results are presented for Te.

[1] T. Furukawa et al., Phys. Rev. Res., **3**, 023111 (2021). [2] S. Wimmer et al. Phys. Rev B, **103**, 024437 (2021). [3] M. Battocletti and H. Ebert, Phys. Rev. B, **64**, 094417 (2001).

MA 35.8 Wed 17:15 POT/0112

Theoretical description of the optical activity and directional dichroism of chiral solids — •Hubert Ebert and Sergiy Mankovsky — Ludwig Maximilian University of Munich, Munich, DE

A scheme to deal with the optical activity and directional dichroism of solids on the basis of Kubo's linear response formalism is presented. Accounting for the $\vec{q}$-dependence of the radiation field implies that the corresponding optical transitions described in $\vec{k}$-space are no more vertical. More important, one is led to corrections to the electric dipole matrix element due to the electric quadrupole and magnetic dipole interaction. The scheme is implemented making use of the relativistic Korringa-Kohn-Rostoker Green function (KKR-GF) formalism. Corresponding applications to chiral Te that has time reversal ($\mathscr{T}$) but no inversion ($\mathscr{I}$) symmetry led to a $\vec{q}$-dependent optical conductivity tensor with off-diagonal elements caused by the interference of the electric dipole and its correction terms giving rise to optical activity. In the case of anti-ferromagnetic Cr_2O_3 without $\mathscr{T}$-symmetry the correction terms lead to directional dichroism that strongly depends on whether a magnetic configuration with or without $\mathscr{I}$-but with combined $\mathscr{I}\mathscr{T}$-symmtetry is considered.

MA 35.9 Wed 17:30 POT/0112

Intrinsic and Proximity-Enhanced Spin-Orbit Torques in Fe_3(Ge,Ga)Te_2 and WTe_2 Heterostructures — •Gusthavo Brizolla[1], Stepan Tsirkin[2], Yaroslav Zhumagulov[2], and Jaroslav Fabian[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]EPFL, Lausanne, Switzerland

Spin-orbit torques (SOTs) in 2D magnets and their heterostructures offer a route to ultra-thin, energy-efficient memories where currents can switch magnetization without external magnetic fields. Materials such as Fe_3GeTe_2 (FGT) and Fe_3GaTe_2 (FGaT), and their interfaces with low-symmetry WTe_2, are especially promising, but the angular dependence and microscopic origin of their SOTs are still not fully understood. Here we compute SOTs in FGT, FGaT and WTe_2-proximitized heterostructures using first-principles (DFT) calculations and compare two protocols for mapping the angular dependence: self-consistent magnetization rotation and rigid rotation of a fixed exchange field. They agree when spin-orbit mixing is weak, but differ strongly near in-plane alignment, where interband hot spots and evolving spin-orbit hybridization amplify the torkances. In WTe_2 heterostructures, broken symmetry and Te-Te interfacial hybridization further boost torques with out-of-plane spin polarization. These results provide design rules for field-free current control in 2D magnets and show that the angle dependence of spin-orbit coupling must be treated explicitly to obtain reliable SOT angular maps.

MA 35.10 Wed 17:45 POT/0112

Spin vacuum switching — •Eddie Harris-Lee[1,2], John Kay Dewhurst[2], Samuel Shallcross[1], and Sangeeta Sharma[1,3] — [1]Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Berlin, Germany. — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany. — [3]Institut für Theoretische Physik, Freie Universität Berlin, Berlin, Germany.

While physical mechanisms underpinning spin switching are established for nano- to pico-second time scales, here we present a physical route to magnetization toggle control at < 100 femtoseconds. A minority spin current injected into a ferromagnet is shown to create a minority "spin vacuum" that then drives rapid charge redistribution from the majority channel and spin switching. We demonstrate this mechanism reproduces many of the features of recent sub-picosecond switching of ferromagnetic Co/Pt multilayers, and provide simple practical rules for the design of materials to optimize "spin vacuum" control over magnetic order.

Harris-Lee *et al.*, Sci. Adv. **10**, eado6390 (2024). DOI:10.1126/sciadv.ado6390

MA 36: Molecular Magnetism and Magnetic Particles / Clusters I

Time: Wednesday 15:00–18:30 Location: POT/0151

MA 36.1 Wed 15:00 POT/0151

A Combined Theoretical and Experimental Study of Oxygen Vacancies in Co_3O_4 for Liquid-Phase Oxidation Catalysis — Amir Omranpour[1], •Lea Kämmerer[2], Catalina Leiva–Leroy[1], Anna Rabe[2], Takuma Sato[3], Soma Salamon[2], Joachim Landers[2], Benedikt Eggert[2], Eugen Weschke[4], Jean Pascal Fandré[5], Ashwani Kumar[5], Harun Tüysüz[5,6], Martin Muhler[1], Heiko Wende[2], and Jörg Behler[1] — [1]University of Duisburg-Essen and CENIDE — [2]Ruhr-University Bochum — [3]Max Planck Institute for Chemical Energy Conversion — [4]Helmholtz-Zentrum Berlin für Materialien und Energie — [5]Max-Planck-Institut für Kohlenforschung — [6]IMDEA Materials Institute, Spain

We combined Density Functional Theory (DFT) and experimental techniques to investigate oxygen vacancies (V_O) in bulk Co_3O_4 and during liquid-phase ethylene glycol oxidation. DFT calculations show that a V_O reduces two adjacent Co^{3+} ions to stable, high-spin Co^{2+} in distorted octahedral sites, simultaneously narrowing the band gap. Comparison of experimental O K-edge X-ray absorption spectra with DFT calculated spectra reveal that the fresh catalyst resembles the vacancy-containing calculation, but the post-reaction catalyst shifts toward the ideal Co^{3+} state, strongly suggesting that Co_3O_4 becomes more oxidized under liquid-phase ethylene glycol oxidation by refilling preexisting oxygen vacancies, a finding supported by increased conversion at higher O_2 pressures and the catalyst's stability and activity over multiple cycles. We gratefully acknowledge the DFG funding by CRC/TRR 247 (Project ID: 388390466) projects A01, A10, and B02.

MA 36.2 Wed 15:15 POT/0151

KNB mechanism in convex polygon molecular magnets: bipartite entanglement transfer with the aid of electric field. — •Zhirayr Adamyan[1,2], Vadim Ohanyan[1,2], Ani Chobanyan[1], Hamid Arian Zad[3], Jozef Strecka[3], Azadeh Ghannadan[4], and Saeed Haddadi[4,5] — [1]Laboratory of Theoretical Physics, Yerevan State University, 1 Alex Manoogian, 0025 Yerevan, Armenia — [2]CANDLE, Synchrotron Research Institute, 31 Acharyan Str., 0040 Yerevan, Armenia — [3]Department of Theoretical Physics and Astro- physics, Faculty of Science, P. J. Safarik University, Park Angelinum 9, 041 54 Kosice, Slovak Republic — [4]Saeeds Quantum Information Group, P.O. Box 19395-0560, Tehran, Iran — [5]Faculty of Physics, Semnan University, P.O. Box 35195-363, Semnan, Iran

The unique properties exhibited by single molecular magnets (SMMs) have led to their integration into hybrid devices, emphasizing their quantum nature. We examine models of 1/2-spin molecular magnets arranged in a convex polygon configuration, utilizing a Katsura-Nagaosa-Balatsky (KNB) mechanism to couple the spin degrees of freedom to an external electric field. This KNB mechanism enables extensive control over quantum entanglement through both the magnitude and direction of the electric field. By employing a rotating configuration of the KNB-coupled electric field, where the field's magnitude remains constant while its direction changes, we demonstrate the controllable transfer of bipartite entanglement between different pairs of spins in the model.

MA 36.3 Wed 15:30 POT/0151

Magneto-optical properties of ferromagnetic liquid crystals — •Tom Rehfeldt[1], A. Jarosik[1], D. Lisjak[2], A. Eremin[1], and H. Nádasi[1] — [1]Institute of Physics, Otto von Guericke University, Universitätsplatz 2, 39106 Magdeburg, Germany — [2]Jožef Stefan Institute, Jamova cesta 39, Ljubljana SL-1000, Slovenia

Ferromagnetic nematic liquid crystals (FNLCs) combine the orientational order of nematic liquid crystals with the spontaneous magnetization of ferrimagnetic nanoplatelets.

In this work, the dynamic magneto-optical behavior of FNLCs is investigated by changing the parameters of the external dynamic magnetic field.

MA 36.4 Wed 15:45 POT/0151

Making molecular changes visible using near-surface transport of micron-sized magnetic particles — •Yahya Shubbak, Nikolai Weidt, Arne Vereijken, Rico Huhnstock, and Arno Ehresmann — Institute of Physics and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), University of Kassel, Heinrich-Plett-Strasse 40, 34132 Kassel, Germany

Transport of magnetic particles (MPs) in liquid close to the surface of a flat substrate containing a periodic magnetic domain pattern is a promising lab-on-a-chip (LOC) technology for detecting MP-bound analytes, even when their size is negligible compared to the MP size. As proof of principle, we show that simple observation of MP motion via optical microscopy is sufficient to distinguish MPs of the same nominal size, but surface-functionalized with two different functional groups. The different surface chemistry changes the liquid-mediated MP-to-substrate forces acting during close-to-surface transport, resulting in significant variations in the experimentally observable MP velocity. More specifically, superparamagnetic MPs measuring 2 micrometre in diameter with a polymer coating of solely carboxyl (COOH) end groups, or a mixture of carboxyl and amino (NH2) groups, respectively, have been studied. Transport of these MPs above a magnetic stripe domain pattern in double-distilled water showed a remarkable difference in their average velocities, rendering the COOH-functionalized MPs almost twice as fast as the NH2 counterparts for otherwise identical experimental parameters. This result enables the magnetophoretic separation of MPs based on their surface properties.

MA 36.5 Wed 16:00 POT/0151

Magnetic cuboidal particles as field sensors for microscaled magnetic stray field landscapes — •Jonas Bugase, Christian Janzen, Arne Vereijken, Yahya Shubbak, Nikolai Weidt, Rico Huhnstock, and Arno Ehresmann — Institute of Physics , University of Kassel, 34132 Kassel

Recently, magnetic domain patterns engineered in thin-film systems have been widely used in data storage, spintronics, and magnetic imaging. Characterizing the micron-scale magnetic stray fields emerging from these patterns remains a topical but challenging task [1]. We present a non-mechanical, optically trackable method to visualize effective magnetic field directions using anisotropically shaped magnetic particles. These particles are fabricated via 2-photon polymerization lithography and magnetic exchange-biased layer deposition to achieve custom shapes and anisotropies. When positioned in the field landscape of a periodically patterned substrate [2] within a quiescent liquid, the particles spontaneously orient and reorient in response to local micron-scale stray fields. This enables efficient characterization of complex magnetic domain patterns. We further explore probing local field variations with superimposed external fields facilitating diagnostic and biomedical microfluidic applications [3].

[1] Nistico *et al.* (2020), Inorganics, 8(1):6.
[2] Holzinger *et al.* (2013), J. Appl. Phys, (114): 013908.
[3] Ehresmann *et al.* (2015), Sensors, (15): 28854.

MA 36.6 Wed 16:15 POT/0151

Metal-free magnetism and organic 2D crystals — •Hongde Yu and Thomas Heine — TU Dresden, Dresden, Germany

Organic 2D crystals with metal-free magnetism have attracted considerable research interest owing to their promising applications in organic spintronics and quantum information technologies. However, achieving stable spin-polarization and controlling magnetic interactions in these systems remains challenging due to strong electronic coupling and the closed-shell nature of most organic monomers. In this talk, I will present a strategy to induce spin-polarization and tailor magnetic interactions in organic 2D crystals. By assembling triangulene monomers into dimers and extended 2D polymers, we theoretically explore strategies to control magnetic interactions and electronic structures. We showed substantial magnetic coupling (J) up to -198 meV through rational chemical design of triangulene dimers. Furthermore, triangulene-based 2D crystals exhibit unique electronic features, including a Dirac point flanked by twin flat bands. By tuning the Fermi level, we predict metal-free ferromagnetism with Curie temperatures of ~260 K and half-metallic behavior. Furthermore, we proposed a mixed-topology design strategy enabling purely organic 2D FM semiconductors with J values up to 127 meV and Curie temperatures exceeding 500 K. Beyond conventional FM and AFM, I will also present a simple approach to achieve metal-free altermagnetism.

MA 36.7 Wed 16:30 POT/0151

Modelling the Spin States of Frustrated Nanographenes and Their Dimers: Challenges & Insights — •Helen Preiss, Hongde Yu, and Thomas Heine — Dresden University of Technology, Germany

Metal-free magnetism is an emerging field with promising applications especially in quantum computing. Fundamentally, metal atoms are replaced by organic radicals as spin-carriers, which can be extended to 1D or 2D networks via suitable coupling reactions while possibly maintaining a long-range magnetic order. One class of such radical building blocks are the topologically frustrated nanographenes. For these, it is impossible to pair all π-electrons into alternating single and double bonds, resulting in an open-shell system. A prominent example is the recently synthesised Clar's goblet, a biradical with a singlet ground-state according to Lieb's theorem. We will show that BS-DFT fails to quantitatively predict the magnetic coupling in this molecule, and to describe its dimer even qualitatively, owing to the delocalised nature of the spin centres and their inherent multi-reference character, while higher level ab initio methods struggle with the sheer size of the systems. Alternatively, Clar's goblet may be thought of as two olympicenyl radicals fused together by a six-membered ring. Sublattice-balanced and C-C-linked olympicenyl dimers thus offer themselves as a comparable yet simpler system to study. By comparing both types of nanographene, we gain insights into the limitations of modelling the magnetic states and both inter- and intramolecular coupling of organic molecules with BS-DFT.

15 min break

MA 36.8 Wed 17:00 POT/0151

Tuning chiral-induced unidirectional spin-charge conversion via molecular organization — •Ashish Moharana[1], Zhitian Ling[2], Hao Wu[2], Tomasz Marszalek[2], and Angela Wittmann[1] — [1]Institut für Physik, Johannes-Gutenberg-Universität Mainz, 55099 Mainz, Germany — [2]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128, Mainz, Germany

The observation of spin-dependent transmission of electrons through chiral molecules has led to the discovery of chiral-induced spin selectivity (CISS). The high efficiency of the spin filtering effect in chiral molecules has recently gained significant interest due to the high potential for novel hybrid molecule magnetic spintronics applications. However, the fundamental mechanisms underlying the CISS effect at the molecule-metal interface remain an open challenge. In our work, we explore spin-to-charge conversion at hybrid chiral helical nanographene and heavy metal interfaces. We demonstrate that spin-to-charge conversion in hybrid chiral heterostructures can be tuned by controlling the ordering, and crystallinity of helical nanographene molecules at the interface. We show a more than two-fold increase in interfacial CISS efficiency with increasing molecular crystallinity. Quantifying the impact of spin to charge as a function of the molecular structure reveals the role of the molecular design and organization in the spin filtering effect, paving the path toward the three-dimensional engineering of hybrid interfaces.

MA 36.9 Wed 17:15 POT/0151

Revealing molecular alignment in thin films of DyCu5 single-molecule magnets via XMCD — •David Anthofer, Ashish Moharana, Alexander Hagenow, Dominik Laible, Tristan Fischer, Eva Rentschler, Hans-Joachim Elmers, and Angela Wittmann — Johannes-Gutenberg Universität Mainz, Deutschland

Single-molecule magnets (SMMs) have recently gained significant interest due to their ability to retain magnetic information at the molecular level, offering potential applications in ultra-compact and high-density data storage devices. A crucial challenge hindering their application in technology is the integration with thin-film devices. To tackle this, we probe the magnetic properties of DyCu5 SMMs deposited by dip-coating on a gold surface, where layer thickness is controlled by rinsing or not rinsing the sample. Using X-ray magnetic circular dichroism combined with sum-rule analysis for 4f elements, we extract the spin and orbital moments of the central Dy3+ ion. Rotating the sample relative to the incident beam reveals magnetic anisotropy in the thin layer, indicating preferential molecular alignment at the interface. In thicker films, this anisotropy vanishes, suggesting that the molecules are ordered on top of the gold surface, but have a random orientation with increasing coverage. While engineering ordered molecular assemblies on surfaces is generally challenging, our results demonstrate that a readily accessible dip-coating protocol can induce ordered alignment in the low-coverage regime, providing a practical route toward incorporating SMMs into thin-film devices.

MA 36.10 Wed 17:30 POT/0151

Probing the magnetic behavior of the metastable high-spin state achieved by light-induced excited spin-state trapping in Fe (II) spin-crossover complexes — •Sangeeta Thakur[1], Marcel Walter[1], Tarek Al Said[2], Eike F. Kuhlemann[3], Clara W. A. Trommer[3], Torben Adam[3], Karsten Holldack[2], Felix Tuczek[3], and Wolfgang Kuch[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [3]Institut für Anorganische Chemie, Christian-Albrechts Universität zu Kiel, 24098 Kiel, Germany

The magnetic behavior of the metastable high-spin (HS) state of the Fe (II) complexes mononuclear [Fe(bpz)$_2$(bipy)]; (bpz = dihydrobis(pyrazolyl)borate) and dinuclear [(Fe(bpz)$_2$)$_2\mu$-(ac(bipy)$_2$)] (ac(bipy)$_2$ = bridging ligand) was investigated at 5 K by frequency-domain Fourier transform electron paramagnetic resonance (EPR) spectroscopy in a magnetic field of 1-10 T. The magnetic field map of the EPR measurements indicates a large value (70-90 cm^{-1}) of zero-field splitting (ZFS) for the dinuclear and mononuclear complexes. Comparatively, the HS-locked complexes [Fe(H$_2$B(pz)$_2$)$_2$(4,7-Me$_2$-phen)] and [Fe(tris(3-Methylpyrazolyl)borate)$_2$] exhibit values of ZFS around around 10-17 cm^{-1}. The large ZFS obtained for the dinuclear and mononuclear complexes could be due to the contribution of spin-orbit coupling (SOC). To the best of our knowledge, this is the first time the spin Hamiltonian parameters for Fe (II) SCO complexes were investigated in the metastable HS state.

MA 36.11 Wed 17:45 POT/0151

Insights into magnetic and magnetocaloric features of 3d-4f nonanuclear Gd3Cu6 complex from a mixed spin-(7/2, 1/2) Heisenberg diamond cluster — •Jozef Strecka and Katarina Karlova — Pavol Jozef Safarik University, Kosice, Slovakia

Low-temperature magnetization curves and magnetocaloric features of 3d-4f molecular complex [Gd3Cu6L6(OH)6(CH3OH)6(H2O)6]Cl3.5H2O (LH2 = 1,1,1-trifluoro-7-hydroxy-4-methyl-5-aza-hept-3-en-2-one) to be further abbreviated as Gd3Cu6 are examined within the framework of exact diagonalization method as well as the cluster-based mean-field theory. The magnetic compound Gd3Cu6 reveals in low-temperature magnetization curves an intermediate magnetization plateau at 21.27 Bohr magnetons, which is far below the saturated magnetization value of 27 Bohr magnetons expected for three spin-7/2 Gd3+ and six spin-1/2 Cu2+ magnetic ions per magnetic molecule. The crystal structure of the Gd3Cu6 complex is built from three condensed cubane-like moeties Gd2Cu2, which are from the magnetic point of view equivalent with three corner-sharing diamond motifs. The nonanuclear coordination compound Gd3Cu6 thus affords an intriguing experimental realization of the mixed spin-(7/2, 1/2) Heisenberg diamond chain composed from three unit cell. The magnetic compound Gd3Cu6 displays at sufficiently low temperatures an enhanced magnetocaloric effect, which is due to a geometric spin frustration quite superior with respect to that one of paramagnetic salts built from Gd3+ magnetic ions.

This work was supported by the grant APVV-24-0091.

MA 36.12 Wed 18:00 POT/0151

Suppressing geometric frustration in triangular dysprosium cluster encapsulated in fullerenes — •Matheus Barbosa, Wei Yang, Noel Israel, Fupin Liu, Bernd Büchner, Stanislav Avdoshenko, and Alexey Popov — Leibniz Institute for Solid State and Materials Research, Dresden/Germany

Nitride clusterfullerenes are compounds in which a metallic cluster is encapsulated within a fullerene cage, exhibiting diverse magnetic properties that depend on the composition and geometry of the endohedral cluster. For the case of $Dy_3N@C_{80}$, the presence of the central nitrogen ion induces a strong uniaxial Ligand Field contribution, locking the magnetic moments of dysprosium centers in a triangular arrangement. Such geometry avoids simultaneous ferromagnetic alignment of the moments between the dysprosium ions, leading to ground state frustration and exhibiting rather efficient spin reorientation through the Quantum Tunneling channel. Their magnetic and geometric frustration is harmful for the Single Molecule Magnetism, resulting in closed hysteresis loops in zero-field and at 2 K. We here report the suppression of this frustration by functionalization of the fullerene cage. The photochemical reaction of $Dy_3N@C_{80}$ with adamantane aziridine produced the monoadduct $Dy_3N@C_{80}$-Ad. This additional space inside the fullerene has direct influence on the cluster, elongating the atomic distance in the Dy-N bond towards the modified fragment (breaking the spatial symmetry) and substantially increasing the Dy*Dy coupling constants. As a result, the monoadduct $Dy_3N@C_{80}$-Ad exhibits suppression of the geometric frustration and enhanced Single Molecule Magnetism.

MA 36.13 Wed 18:15 POT/0151

Orientation of Magnetic Anisotropy Axes in Single Molecule Magnets by Inelastic Neutron Scattering: A Case Study on Mn_2Y_2 — •Yifan Wang[1], Christoper E. Anson[2], Zayan A. Ali[1], Annie K. Powell[2], and Oliver Waldmann[1] — [1]Physikalisches Institut, Universität Freiburg, Germany — [2]Institut of Inorganic Chemistry, Karlsruhe Institute of Technology (KIT), Germany

Single molecule magnets (SMMs) are molecular systems that exhibit slow magnetic relaxation and well-defined spin states arising from strong magnetic anisotropy. These features give them potential for future information storage and have attracted much research interest. However, determining the magnetic parameters experimentally, especially the anisotropy orientations, remains challenging. In this work, we demonstrate, with regard to this point, the capability of inelastic neutron scattering (INS) on powder samples through a case study on the dimeric molecular spin cluster Mn_2Y_2. This complex belongs to a family of SMMs and consists of two magnetic spin-2 Mn^{III} ions coupled by antiferromagnetic exchange. The recorded INS spectrum on Mn_2Y_2 displays three cold transitions corresponding to singlet-triplet excitations. The transition energies enable a precise determination of the exchange coupling and the anisotropy magnitudes of the Mn^{III} centers. Most interestingly, a detailed analysis of the peak intensities is shown to yield, in addition, information on the orientation of the Mn^{III} magnetic anisotropy axes. The approach can be generally extended to related SMM families and provides a valuable addition to the range of experimental techniques.

MA 37: Non-Skyrmionic Magnetic Textures

Time: Wednesday 15:00–17:15 Location: POT/0351

MA 37.1 Wed 15:00 POT/0351

Regularized micromagnetic theory for Bloch points — •Vladyslav M. Kuchkin[1], Andreas Haller[1], Andreas Michels[1], Thomas L. Schmidt[1], and Nikolai S. Kiselev[2] — [1]Department of Physics and Materials Science, University of Luxembourg — [2]Peter Grünberg Institute, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Magnetic singularities, known as Bloch points, pose a significant challenge for the micromagnetic theory due to the divergence of the effective field at these points. In this talk, we present a recently developed regularized micromagnetic model that does not assume a fixed magnetization length, but treats magnetization as an order parameter on the $\mathbb{S}^3$ sphere, thus allowing it to vary in length from zero up to a threshold value. Such an extension of micromagnetics respects the fundamental properties of local spin expectation values in quantum systems. Relying on the $\mathbb{S}^3$ order parameter, we derive Landau-Lifshitz-Gilbert and Thiele equations and apply them to the dynamics of several spin textures: domain walls in nanowires, chiral bobbers, and magnetic dipole strings. The results demonstrate how the extended formalism accounts for the dynamics of Bloch points observed experimentally and open up prospects for modeling complex spin structures, including the nucleation and annihilation of topological states such as skyrmions and hopfions.

MA 37.2 Wed 15:15 POT/0351

Magnetoelastic Fingerprints in Dysprosium Iron Garnet Thin Films: Inversion of Effective Local Anisotropy within Domain Walls — •Lukas D. Ćavar[1], Julian Skolaut[2], Olena Gomonay[1], Miela J. Gross[3], Khang Vi Becker[1], Simon J. Sochiera[1], Dirk Backes[4], Caroline A. Ross[3], and Angela Wittmann[1] — [1]Johannes Gutenberg Universität, Mainz, DE — [2]Christian-Albrechts-Universität zu Kiel, DE — [3]Massachusetts Institute of Technology, Cambridge, MA, USA — [4]Diamond Light Source, Oxfordshire, UK

A promising direction for future computing devices is to embed topological spin textures in compensated collinear magnetic systems. Yet in the absence of significant stray fields, these textures must be stabilized unconventionally. While we observe a wide variety of topological textures in magnetoelastic systems, including the altermagnet α-Fe2O3 ('hematite') and the ferrimagnet dysprosium iron garnet (DyIG), their specific origin is not clear. Here, we compare Néel vector mapping via x-ray magnetic linear dichroism photoemission electron microscopy and stray-field imaging by scanning nitrogen vacancy center magnetometry to show that the DyIG 360° domain wall profile exhibits significant deviations from the classical domain wall profile. These are consistent with an inversion of the effective local anisotropy, i.e. the easy and hard axes trading places within the domain wall body. Thereby we obtain quantitative insight into the mechanism, scale, and energetics of the magnetoelastic stabilization of topological textures in thin films with strong magneto-elastic coupling and uncover a new degree of straintronic freedom for next-generation spin devices.

MA 37.3 Wed 15:30 POT/0351

Hopfions in Symmetry-Transformed Magnetic Models — •Sandra Chullipparambil Shaju, Maria Azhar, and Karin Everschor-Sitte — Faculty of Physics and CENIDE, University of Duisburg-Essen

Three-dimensional (3D) topological spin structures continue to attract significant interest due to their rich physics and potential for future information technologies. We present a systematic framework of continuously transformed models that enables the stabilisation of topologically non-trivial 3D spin configurations. By applying this approach, we construct an effective model that hosts Hopfions embedded in a ferromagnetic background, with distinct energetic and dynamical characteristics. Our results provide new routes for investigating the formation, stability, and dynamics of three-dimensional topologically non-trivial textures.

MA 37.4 Wed 15:45 POT/0351

Fractional Hopfions in Composite Magnets — •Sanjay Ashok and Jan Masell — Karlsruhe Institute of Technology (KIT), Karlsruhe

Hopfions are three dimensional magnetization textures studied due to their unique physical-, topological properties and their functionalization prospects [1]. These textures are usually doughnut shaped and classified by their integer topological winding number called Hopf index. In our work, we demonstrate that hopfions with fractional Hopf index, called fractional hopfions [2, 3], can be stabilized in composite magnets. We identify a two-slab composite magnet with slab-dependent Dzyaloshinskii-Moriya interaction (DMI) as a suitable material platform for stabilizing fractional Hopfions. We further distinguish the role of Bloch-, Neel- and Antiskyrmion-type DMI in composite magnets and their effect on the winding of fractional hopfions [4]. By studying the phase diagram of fractional hopfions we predict the range of external magnetic field and uniaxial anisotropy where these textures can be found.

[1] Zheng et al., Nature 623, 7988 (2023); [2] Knapman et al., Comm. Phys. 7, 1 (2024); [3] Yu et al., Adv. Mat. 35, 20 (2023); [4] Ashok and Masell, *in preparation*

MA 37.5 Wed 16:00 POT/0351

Acoustically-driven manipulation of magnetic textures in epitaxial ferromagnetic thin-films — •João Pedro Leite Gomes, Jens Herfort, and Alberto Hernández-Mínguez — Paul-Drude-Institut für Festkörperelektronik - Leibniz-Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117 Berlin, Germany

Recent advances in information technology have driven the research towards more reliable storage devices, while striving for ever higher memory densities. One drawback of current spintronic technologies for information recording is the need for large spin-polarized currents to access/write information in magnetic materials, leading to less energy-efficient devices. An alternative proposal to achieve controlled magnetization switching is to make use of the magnetoelastic (ME) interaction, for example, through the excitation of surface acoustic waves (SAW) in piezoelectric substrates.

In this contribution, we report SAW-driven manipulation of domain walls (DWs) in epitaxial ferromagnetic thin-films with both cubic and uniaxial magnetic anisotropies along well-defined crystalline directions. Micromagnetic simulations model the physical mechanism by which the tickling magnetic field generated by the strain modulation, via the ME interaction, can result in the local switching of the DWs. We discuss how much SAWs are a feasible approach to achieve magnetization switching and/or promote DW pinning in single crystal ferromagnetic thin-films.

MA 37.6 Wed 16:15 POT/0351

Control of helix orientation in chiral magnets via lateral confinement — •Maurice Colling[1], Mariia Stepanova[1], Mario Hentschel[2], Erik Lysne[1], Kasper Hunnestad[1], Naoya Kanazawa[3], Yoshinori Tokura[3,4], Jan Masell[4,5], and Dennis Meier[1] — [1]Department of Materials Science and Engineering, NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]Physics Institute and Research Center SCoPE, University of Stuttgart, Stuttgart, Germany — [3]Department of Applied Physics, University of Tokyo, Tokyo, Japan — [4]RIKEN Center for Emergent Matter Science (CEMS), Wako, Japan — [5]Institute of Theoretical Solid State Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany

Helimagnetic materials offer a versatile platform for spin-based device concepts due to their long-range, tunable spiral order. This talk demonstrates control of the helimagnetic propagation vector q via geometrical confinement, using FeGe as a model DMI-driven chiral magnet. Micromagnetic simulations based on the nonlinear sigma model show that open boundaries generate a chiral surface twist that acts as an effective surface anisotropy selecting the helix orientation. This behavior is captured well by an analytical model derived from the DMI boundary condition. Magnetic force microscopy on focused ion beam structured FeGe confirms the predicted orientation and establishes geometry-controlled helimagnetic order as a robust mechanism for steering DMI-stabilized spin-spiral states. The concept provides a route to device-level control of chiral magnetic textures.

MA 37.7 Wed 16:30 POT/0351

Magnetization dynamics of twists in (anti-)ferromagnetic insulators — Patricia Oehrl[1,2], Mathew James[3], Luca Maranzana[4], Andreas Bauer[2], Denis Mettus[2], Christian Pfleiderer[2], Christian Back[2], Sergey Artyukhin[4], Hans Huebl[1,2], and •Aisha Aqeel[3] — [1]Walther-Meißner-Institut, 85748 Garching, Germany — [2]Technical University of Munich, 85748 Garching, Germany — [3]University of Augsburg, 86159 Augsburg, Germany — [4]Quantum Materials Theory, Italian Institute of Technology, Via Morego 30, Genoa, Italy

Magnetic insulators hosting noncollinear spin textures display a remarkable variety of static and dynamic phenomena. In chiral systems such as Cu2OSeO3, the lack of inversion symmetry gives rise to helices and skyrmions stabilized by Dzyaloshinskii-Moriya interactions [1]. By contrast, in centrosymmetric compounds like CuSeO3, complex antiferromagnetic spiral states can emerge purely from competing symmetric exchange interactions, providing an intriguing platform to explore magnetism without intrinsic chirality. In this talk, I will present our preliminary results on dynamic excitation of these textures in chiral Cu2OSeO3 and centrosymmetric CuSeO3 magnets using magnetic resonance spectroscopy [2].

References: [1] S. Mehboodi, V. Ukleev, C. Luo, R. Abrudan, F. Radu, C. H. Back, A. Aqeel, Sci. Technol. Adv. Mater 26(1) 2532366 (2025) [2] Aisha Aqeel, Jan Sahliger,... Christian H Back, Phys. Rev. Lett. 126, 017202 (2021)

MA 37.8 Wed 16:45 POT/0351

Extraordinary return point memory in ferrimagnetic materials — •Tamer Karaman[1], Kai Litzius[1], Aladin Ullrich[1], Riccardo Battistelli[1], Manas Patra[1,2], Raluca Boltje[1], Miela Gross[2], Steffen Wittrock[2], Krishnanjana Joy[1], Daniel Metternich[2], Sebastian Hoffman[1], Timo Schmidt[1], Daniel Perez[3], Manuel Valvidares[3], Sebastain Wintz[2], Manfred Albrecht[1], and Felix Büttner[1,2] — [1]University of Augsburg, Germany — [2]Helmholtz-Zentrum Berlin, Germany — [3]ALBA Synchrotron Light Source, Spain

Magnetic domains and domain walls are promising information carriers, widely explored for racetrack memory [1] and other mobility applications [2]. In this study, we demonstrate deterministic magnetic-domain nucleation in rare-earth transition-metal (RE-TM) ferrimagnetic systems. Remarkably, the as-grown domain configuration serves as an intrinsic template that reappears with 100% return-point memory after repeated out-of-plane magnetic-field cycling. Even more surprisingly, the full domain pattern can be toggle switched using extremely small in-plane fields near 0 mT, while the overall domain morphology remains unchanged. These findings point to new opportunities in cryptography and other technologies requiring deterministic pattern reproducibility, and they highlight the importance of further exploring properties of RE-TM ferrimagnets. References: 1.Parkin, S. et al. Nat. Nano. 10, 195-198 (2015) 2.Venkat, G. et al. J. Phys. Appl. Phys. 57, 063001 (2024).

MA 37.9 Wed 17:00 POT/0351

Microscale coexistence of magnetic phases compatible with the Kagome spin-ice rule in HoAgGe — •Manuel Zahn[1,2], Kan Zhao[3], Philipp Gegenwart[1], Sándor Bordács[4], and István Kézsmárki[1] — [1]Center for Electronic Correlation and Magnetism, University of Augsburg, Augsburg, Germany — [2]Norwegian University of Science and Technology, Trondheim, Norway — [3]School of Physics, Beihang University, Beijing, China — [4]Department of Physics, Budapest University of Technology and Economics, Budapest, Hungary

HoAgGe realizes kagome spin-ice with a series of fractionalized magnetization plateau states for applied in-plane magnetic fields [1]. Corresponding magnetoresistance and Hall effect reveal a hysteresis at the plateau states, indicating field-history dependent occupation of magnetic domains with opposite chirality and Berry curvature [2].

In the presented study, we investigate the microscale magnetic patterns, using low-temperature atomic force microscopy to visualize possible phase coexistence. By studying different crystal cuts and varying magnetic fields using a vector magnet, we reconstruct the full 3D magnetic texture of phase coexistence. Our results provide insights into the interplay of geometrical, topological and frustrated properties of spin ice materials and demonstrate pathways for external manipulation of magnetic textures in highly-frustrated systems.

[1] K. Zhao *et al.*, Science **367**, 1218 (2020). [2] K. Zhao *et al.*, Nat. Phys. **20**, 442 (2024).

MA 38: Ultrafast Magnetization Effects II

Time: Wednesday 15:00–18:45 Location: POT/0361

MA 38.1 Wed 15:00 POT/0361

Ultrafast light-induced spin and orbital moment in nonmagnetic band insulators from RT-TDDFT — •Andri Darmawan, Markus E. Gruner, and Rossitza Pentcheva — Department of Physics, University of Duisburg-Essen

Recently dynamical multiferroicity was predicted in $SrTiO_3$ as well as $KTaO_3$ [1-2] and subsequently observed experimentally in $SrTiO_3$ [3], employing THz circularly polarized pulse. This is particularly intriguing as $SrTiO_3$ and $KTaO_3$ are nonmagnetic band insulators with d^0 occupation at Ti and Ta. Here, using real-time time-dependent density functional theory (RT-TDDFT) as implemented in the Elk code we employ optical circularly polarized laser pulses to investigate laser-induced spin and orbital moment in $SrTiO_3$ and $KTaO_3$. We study systematically the dependence on the laser parameters and find that duration and frequency of the pulse strongly influence the behavior of the light-induced spin and orbital magnetic moment in both $SrTiO_3$ and $KTaO_3$. While in $SrTiO_3$ the induced orbital momentum predominates, at certain frequencies $KTaO_3$ exhibits both substantial light-induced spin moment and orbital moment.

Funding by DFG within CRC1242 (project C02) and computational time at magnitUDE, amplitUDE are gratefully acknowledged.

[1] D. Juraschek et al., Phys. Rev. Mater. **1**, 014401 (2017)
[2] R. M. Geilhufe et al., Phys. Rev. Research **3**, L022011 (2021)
[3] M. Basini et al., Nature **628**, 534 (2024)

MA 38.2 Wed 15:15 POT/0361

Interfacial magnon generation drives ultrafast spin dynamics in Gd — •Corvin Krohn[1], Ekaterina Bobrova[1], Tim Amrhein[1], Dominic Lawrenz[1], Niko Pontius[2], Christian Schüssler-Langeheine[2], Martin Weinelt[1], and Nele Thielemann-Kühn[1,2] — [1]Freie Universität Berlin, Berlin, Germany — [2]Helmholtz-Zentrum Berlin, Berlin, Germany

Previous time-resolved photoemission [1] and x-ray magnetic circular dichroism (XMCD) [2] experiments investigating 4*f* magnetization dynamics in Gadolinium (Gd) showed conflicting results, with demagnetization timescales of 14 ps [1] and 0.7 ps [2], respectively.

Within an XMCD study at the FemtoSlicing facility, we could now show that intrinsic dynamics in Gd is slow. For a thin Gd film, however, where the pump laser directly excites the non-magnetic substrate as well, generation of magnons at the metal-substrate interface drives the ultrafast demagnetization.

In the next step we aim to identify magnons as m_s state excitations within the Gd 4*f* electronic ground level, using time-resolved x-ray absorption spectroscopy.

Revealing signatures of magnetic dynamics in the electronic structure will provide insights into the correlated electronic and magnetic structure of 4*f* metals.

[1] B. Frietsch *et al.*, Nat. Commun. **6**, 8262 (2015).
[2] K. Bobowski *et al.*, J. Phys.: Condens. Matter **29**, 234003 (2017).

MA 38.3 Wed 15:30 POT/0361

Probing ultrafast dynamics of artificial antiferromagnets by soft-x-ray diffraction — •Jasmin Jarecki[1], Martin Borchert[1], Stefan Eisebitt[1,2], and Daniel Schick[1] — [1]Max-Born-Institut für Nichtlineare Optik & Kurzzeitspektroskopie, Berlin, Germany — [2]Institut für Optik & Atomare Physik, TU Berlin, Germany

Ordering phenomena in solids encode key information about microscopic interactions and subsystem coupling. In magnetic materials, magnetic and structural order can be strongly coupled, yet the corresponding periodicities may exhibit different characteristic lengths. This calls for methods capable of simultaneously probing lattice and spin degrees of freedom to disentangle phonon and spin dynamics.

Using on- and off-resonant ultrafast x-ray diffraction (UXRD) in the soft-x-ray regime, we investigate the coupled structural and magnetic dynamics of a Fe/Cr superlattice (SL), an artificial antiferromagnet in which adjacent Fe layers adopt alternating magnetization directions for the chosen Cr spacer thickness. By tracking the structural and magnetic SL Bragg peaks, we study photon-energy- and fluence-dependent dynamics via their transient peak positions and intensities. While the structural peak shift and the magnetic peak intensity follow the expected behavior, the magnetic peak shift deviates markedly from the structural response and, in particular, does not exhibit the anticipated linear fluence dependence. These findings highlight the strong intercoupling between depth-dependent sample dynamics and depth-dependent probing, underscoring the need for careful analysis and modeling to reliably extract microscopic dynamics from UXRD.

MA 38.4 Wed 15:45 POT/0361

Double-pulse all-optical magnetization re-switching of GdFe — Rahil Hosseinifar[1], Felix Steinbach[2], Ivar Kumberg[1], José Miguel Lendínez[3], Sangeeta Thakur[1], Sebastien E. Hadjadj[1], Jendrik Gördes[1], Chowdhury S. Awsaf[1], Mario Fix[4], Manfred Albrecht[4], Florian Kronast[5], Unai Atxitia[3], Clemens von Korff Schmising[2], and •Wolfgang Kuch[1] — [1]Freie Universität Berlin, Berlin, Germany — [2]Max-Born-Institut, Berlin, Germany — [3]ICMM-CSIC, Madrid, Spain — [4]Universität Augsburg, Augsburg, Germany — [5]Helmholtz-Zentrum Berlin, Berlin, Germany

The reversible helicity-independent switching of the magnetization direction of ferrimagnetic materials like GdFe by individual sub-ps optical laser pulses bears the potential to accelerate magnetic data storage. We present a systematic Kerr-microscopy domain-imaging study of a 10 nm $Gd_{26}Fe_{74}$ film after excitation with two laser pulses with a certain time delay in between. Our results show that when the fluence of the first pulse is adjusted just above the threshold of single-pulse switching, a second pulse with about 60% of the fluence of the first pulse, arriving only 4 ps later, can already switch the magnetization back [1]. Atomistic spin dynamics simulations reproduce the experimental results and show that under these conditions the magnetizations of the Fe and Gd sublattices have already moved sufficiently away from zero when the second pulse hits the sample, a prerequisite for fast re-switching.

[1] R. Hosseinifar *et al.*, Phys. Rev. B **112**, 174406 (2025).

MA 38.5 Wed 16:00 POT/0361

Light-induced ultrafast magnetization dynamics driven by chiral phonons — •Shiqi Hu and Sangeeta Sharma — Max-Born Institute for Nonlinear Optics and Short Pulse Spectroscopy,Berlin,Germany

The pursuit of high-speed, low-power information processing is driving advanced research into ultrafast laser control of magnetic order. Going beyond conventional approaches that rely on heterojunctions for spin-current injection, this work demonstrates direct manipulation of magnetism in bulk materials

through intrinsic interactions. Using circularly polarized laser excitation, we generate THz chiral phonons in the non-collinear antiferromagnet Mn3Sn with a Kagome lattice. The angular momentum of these phonons produces an effective magnetic field, inducing coupled in-plane and out-of-plane spin precession that reorients the magnetic octupole. This reorientation, in turn, modulates the topological properties of Weyl points. Spin*orbit coupling and the rotational motion of chiral phonons are shown to be essential to this mechanism. We attribute the observed spin dynamics to a competition between the phonon-induced effective field*favoring ferromagnetic alignment*and the intrinsic antiferromagnetic spin interactions in the Kagome lattice. These findings open a new pathway for controlling magnetic topology.

MA 38.6 Wed 16:15 POT/0361

Exploring the ultrafast change of antiferromagnetic and ferromagnetic order in a Mn_2Au/Py bilayer — •Jendrik Gördes[1], Markus Weissenhofer[1,2], Sangeeta Thakur[1], Chowdhury S. Awsaf[1], Marcel Walter[1], Lorenzo Grilli[1], Deeksha Gupta[3], Niko Pontius[3], Christian Schüssler-Langeheine[3], Peter M. Oppeneer[2], Martin Jourdan[4], and Wolfgang Kuch[1] — [1]Freie Universität Berlin, Berlin, Germany — [2]Uppsala University, Uppsala, Sweden — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [4]Johannes Gutenberg-Universität Mainz, Mainz, Germany

Antiferromagnetic (AFM) materials are promising candidates for future data storage devices. One noteworthy material is Mn_2Au, a metallic collinear AFM that can be electrically switched [1]. We report on the time-resolved change of AFM and ferromagnetic (FM) order of a Mn_2Au/permalloy (Py) bilayer after excitation with 800 nm fs laser pulses by X-ray magnetic linear and circular dichroism (XMLD and XMCD) in resonant soft X-ray reflectivity at the Mn and Fe L_3 edges. We observe an ultrafast loss and an exceptionally fast recovery of the AFM order within a few ps, much faster than the recovery of the adjacent FM order. Local and non-local mechanisms are considered in simulations using an atomistic spin model. The presented research highlights the fast dynamics of AFM layers for spintronic applications. [1] J. Železný, H. Gao, K. Výborný et al., PRL 113, 157201 (2014)

MA 38.7 Wed 16:30 POT/0361

Intrinsic timescales of ferro- and antiferromagnets in ultrafast demagnetisation — •Tobias Dannegger[1], Stephan Wust[2], Paul Herrgen[2], Martin Aeschlimann[2], Benjamin Stadtmüller[3], and Ulrich Nowak[1] — [1]Fachbereich Physik, Universität Konstanz, Konstanz, Germany — [2]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, Kaiserslautern, Germany — [3]Experimentalphysik II, Institute of Physics, University of Augsburg, Germany

For small deviations from the ground state, the spin dynamics of a magnetically ordered material can be described within linear spin-wave theory. There is a well known difference between the intrinsic timescales, given by the eigenfrequencies, of ferro- and antiferromagnets, the latter being approximately two orders of magnitude faster. Here, we present a systematic investigation, based on atomistic spin dynamics simulations, of how ferro- and antiferromagnetic ordering affects the intrinsic timescales of the magnetic order parameter far away from equilibrium, such as in ultrafast light-induced quenching experiments. We find that the speed advantage of antiferromagnets persists in the strongly non-equilibrium regime, but with some striking qualitative differences for very large excitations, where antiferromagnets slow down while the ferromagnetic quenching efficiency increases again.

15 min break

MA 38.8 Wed 17:00 POT/0361

Field-tuning of ultrafast magnetization fluctuations in $Sm_{0.7}Er_{0.3}FeO_3$ — •Julius Schlegel[1], Marvin Alexander Weiss[1], Daniel Anić[1], Emil Steiner[1], Franz Stefan Herbst[1], Makoto Nakajima[2], Takayuki Kurihara[3], Alfred Leitenstorfer[1], Sebastian T.B. Goennenwein[1], and Ulrich Nowak[1] — [1]Department of Physics, University of Konstanz, Germany — [2]Institute of Laser Engineering, Osaka University, Japan — [3]Department of Basic Science, The University of Tokyo, Japan

The missing stray field and the vanishing net magnetization make it challenging to investigate antiferromagnetic dynamics experimentally. Nevertheless, thermal magnetization fluctuations persist in antiferromagnets and can be exploited to gain insights into their dynamics [1].

In this work, we investigate these fluctuations in the canted antiferromagnet $Sm_{0.7}Er_{0.3}FeO_3$ under the influence of an external magnetic field [2]. Using femtosecond noise-correlation spectroscopy combined with atomistic spin-dynamics simulations, we examine the spin noise in the vicinity of the magnetic reorientation transition.

We demonstrate that the external magnetic field suppresses characteristic features of critical fluctuations, such as a diverging noise amplitude. Moreover, it enhances the quasi-ferromagnetic magnon frequency near the reorientation transition. Our results offer a means to tune ultrafast spin fluctuations via experimentally accessible external parameters.

[1] M. A. Weiss et al., Nat. Commun. 14, 7651 (2023).
[2] M. A. Weiss et al., arXiv:2509.26084 (2025)

MA 38.9 Wed 17:15 POT/0361

Large strain contribution to the laser-driven magnetization response of magnetostrictive $TbFe_2$ — •Constantin Walz[1], Fried-C. Weber[1,2], Steffen-P. Zeuschner[1], Karine Dumesnil[3], Alexander von Reppert[1], and Matias Bargheer[1,2] — [1]Institut für Physik und Astronomie, Universität Potsdam, Potsdam, Germany — [2]Helmholtz-Zentrum Berlin, Berlin, Germany — [3]Institut Jean Lamour, Université de Lorraine, Nancy, France

Rare Earth-Iron compounds ($REFe_2$ with $RE = \mathrm{Tb}, \mathrm{Dy}, \mathrm{Tb_{0.3}Dy_{0.7}}$) are well known for their giant (inverse) magnetostriction, exhibiting lattice-constant changes exceeding 10^{-3} at saturation. While they are widely used as ultrasonic transducers in the MHz regime, their ultrafast magnetization dynamics remain less explored.

We investigate the strain-driven magnetization dynamics in $TbFe_2$ using time-resolved magneto-optical Kerr effect (trMOKE) and optical reflectivity measurements. The delayed strain response in the trMOKE signal indicates a true magnetic origin of these features, ruling out instantaneous changes of the optical constants. In addition, we show that glass-capped sample structures efficiently transduce unipolar strain pulses, which we use to calibrate the contribution of quasi-static-strain-induced magnetization dynamics to the total signal. Modeling with a Landau-Lifshitz-Gilbert equation including a time-dependent magneto-elastic field reproduces the observations and demonstrates that strain can even provide the dominant contribution to the laser-driven magnetization dynamics.

MA 38.10 Wed 17:30 POT/0361

All-optical stochastic switching of magnetisation textures in Fe3Sn2 — •Andras Kovacs[1], Jonathan Weber[2], Michalis Charilaou[3], Rafal Dunin-Borkowski[1], and Sascha Schaefer[2] — [1]Ernst Ruska-Centre, Forschungszentrum Jülich, Germany — [2]Regensburg Center for Ultrafast Nanoscopy, University of Regensburg, Regensburg, Germany — [3]Department of Physics, University of Louisiana at Lafayette, USA

We utilize femtosecond optical pulses to alter the helicity of the magnetic spin configuration in dipolar skyrmions formed in the kagome magnet Fe3Sn2 in the absence of an external magnetic field and at room temperature. In situ Lorentz transmission electron microscopy is used to visualise the light-induced stochastic switching process of chiral Néel caps, while the internal Bloch component of the dipolar skyrmions remains unchanged. To corroborate the spin states and the light-induced magnetisation dynamics, micromagnetic modelling and simulations of the resulting electron phase shift maps are conducted to elucidate the spin rearrangement induced by individual femtosecond optical pulses [1]. We acknowledge the scientific support to D. Kong, L. Prodan, V. Tsurkan, A. Schroder, N. Kiselev, I Kezsmarki, A. Tavabi and the financial support to EU grant No. 856538. [1] A. Kovacs etal, Comm. Mater. 6, 223 (2025)

MA 38.11 Wed 17:45 POT/0361

Nonlinear spin and orbital Rashba–Edelstein effects induced by a femtosecond laser pulse: Simulations for Au(001) — Oliver Busch, •Franziska Ziolkowski, Börge Göbel, Ingrid Mertig, and Jürgen Henk — Martin-Luther-Universität Halle-Wittenberg, 06099 Halle, Germany

Rashba-type spin-orbit coupling gives rise to distinctive surface and interface phenomena, such as spin-momentum locking and spin splitting. In nonequilibrium conditions, it manifests e.g., as the Rashba–Edelstein effect, where an electric current generates a net spin or orbital polarization perpendicular to the current direction. While the steady-state behavior of these effects is well studied, their dynamics on ultrafast timescales remain largely unexplored.

We theoretically investigate the ultrafast spin and orbital Edelstein effects on an Au(001) surface, induced by femtosecond laser excitation [1]. These effects are intrinsic and inherently nonlinear. We simulate the ultrafast electron dynamics in response to the laser pulse by using a real-space tight-binding model combined with unitary time evolution of the density matrix.

Our results reveal pronounced differences between the spin and orbital responses and quantify the resulting charge, spin, and orbital currents, including laser-induced spin and orbital Hall effects. These findings provide insights into ultrafast angular momentum transfer mediated by the light-matter interaction and offer guidance for the design of next-generation spintronic and orbitronic devices.

[1] Busch *et al* PRR **7**, 043023 (2025)

MA 38.12 Wed 18:00 POT/0361

Impact of Structural Imperfections on the Ultrafast Orbital Hall Effect in Metallic Nanoribbons — •Theresa Albrecht, Franziska Ziolkowski, Börge Göbel, Ingrid Mertig, Jürgen Henk, and Samir Lounis — Institut für Physik, Martin-Luther-Universität, D-06099 Halle

The ultrafast orbital Hall effect (UOHE) arises when a femtosecond laser pulse drives a transient orbital current. We investigate how structural defects affect the UOHE in a Cu nanoribbon [1]. Using Evolve, a real-space tight-binding framework for finite systems [2], we simulate the laser-induced electron dynamics and

compute the orbital angular momentum (OAM) and its associated currents with atomic resolution. Defects significantly alter the OAM landscape: while defect-free ribbons exhibit pronounced edge accumulation, imperfections redistribute OAM toward defect sites and progressively suppress edge signatures as their number increases. Furthermore, we analyze the phase relation between the p- and d-orbital contributions to the OAM in interface geometries. Our results reveal the pivotal influence of defects on ultrafast orbital transport and dynamics.

[1] O. Busch *et al.*, Physical Review Research **6**, 013208 (2024)
[2] F. Töpler *et al.*, New Journal of Physics **23**, 033042 (2021)

MA 38.13 Wed 18:15 POT/0361

Pump-induced out-of-equilibrium magnetism in the Mott insulator CuO — •Katja Sophia Moos[1,2], Yun Yen[2], Gian Parusa[1,2], Arnau C. Romaguera[3], Elia Razzoli[3], Hiroki Ueda[3], and Michael Schüler[1,2] — [1]Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland — [2]Center for Scientific Computing, Theory and Data, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland — [3]Center for Photon Science, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland

Understanding ultrafast magnetism requires tracking energy flow among coupled electronic, spin, and lattice subsystems. Using time-resolved resonant diffuse scattering combined with complementary X-ray techniques and quantum-kinetic simulations, we reveal microscopic pathways of pump-induced demagnetization in the antiferromagnetic Mott insulator CuO. Above-bandgap photoexcitation creates non-thermal magnons across the Brillouin zone within tens of femtoseconds, followed by magnon-magnon scattering driving quasi-thermalization within picoseconds. Magnetic recovery occurs via magnon-phonon coupling on nanoseconds, constrained by dispersion mismatches imposing intrinsic bottlenecks. Our momentum-resolved quantum Boltzmann simulations establish a hierarchical energy-transfer framework beyond phenomenological multi-temperature models, reproducing key features of the experiments. This approach provides design principles for controlling non-equilibrium magnetic states and highlights time-resolved resonant diffuse scattering as a power tool for ultrafast quantum materials research.

MA 38.14 Wed 18:30 POT/0361

Ultrafast spin and pure spin currents — •Deepika Gill, Sam Shallcross, and Sangeeta Sharma — Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Max-Born-Strasse 2A, 12489, Berlin, Germany

Pure spin currents, the flow of spin in the absence of charge flow, represent a promising route toward energy efficient next-generation electronics [1]. Creating such currents often involves designed nano-structures, which can be challenging to create in experiment. Here, relying only on intrinsic material properties, we shift the design to the light pulse via two schemes: (1) via anti-symmetric laser pulses [2] and (2) via composite light pulses that generate pure spin current by tailoring spin density occupation in momentum space [3]. We provide realistic material examples including WSe2 and calculate the ultra-fast spin current response both via state-of-the-art time density function theory as well as Wannier parameterized tight-binding calculations.

[1] S Sharma et al. Nature Communications 15 (1), 7579 (2024)
[2] D Gill et al. Nanoletters 25 (25), 9913-9917 (2025)
[3] D Gill et al. npj 2D Materials and Applications 9 (1), 49 (2025)

MA 39: Poster Magnetism II

Time: Wednesday 18:00–21:00 Location: P2

MA 39.1 Wed 18:00 P2

Observation of negative orbital torque from Vanadium — •Jose Omar Ledesma Martin[1], Nikhil Vijayan[1], Durgesh Kumar[1], Ao Du[1], Lei Gao[2], Zijie Xiao[2], Hai I. Wang[2], Rahul Gupta[1], Gerhard Jakob[1], Sachin Krishnia[1], Yuriy Mokrousov[1,3], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Germany — [2]Max Planck Institute for Polymer Research, Germany — [3]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany

Vanadium is predicted to exhibit a large orbital Hall effect. This effect is measured using ST-FMR, second-harmonic Hall, and THz emission, and all techniques reveal a negative orbital torque, in contrast to previous predictions and measurements that report a positive sign. The consistency in the results suggests the intrinsic origin of the OHE in our V samples. The torque magnitude depends strongly on the choice of ferromagnet: FeCoB/V, sensitive mainly to SHE-driven currents, shows only a weak response, whereas Ni/V, which efficiently converts OHE-driven currents, exhibits a torque nearly seven times larger. The torque increases with V thickness while remaining negative, and the extracted parameters indicate a large negative orbital Hall conductivity and long orbital diffusion length. Our results show that V generates strong orbital Hall currents with minimal spin Hall contribution and that itinerant interfacial orbital currents play a decisive role in determining both the efficiency and the sign of the torque (1).

(1) Vijayan, N. et al., arXiv:2508.16339 (2025).

MA 39.2 Wed 18:00 P2

Transport and spin torque in van der Waals heterostructures — •Nils Stüber[1], Sadeed Hameed[1], Aditya Kumar[1], Xinran Wang[1], Durgesh Kumar[1], Aravind Puthirath Balan[1], and Mathias Kläui[1,2] — [1]Institute of Physics, Johannes Gutenberg-Universität, Mainz, Germany — [2]Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, Trondheim, Norway

Graphene serves as an ideal spin-transport channel due to its long spin relaxation times and possible near-ballistic transport. In Ni/Gr heterostructures, the strength of the Spin Hall effect can be tuned via gate voltage, enabled by the Dirac-cone band structure.

In this work, we investigate spin-current generation in graphene induced by proximity-driven spin-orbit coupling (SOC) from epitaxially grown Ni(111). The SOC arises from hybridization between the graphene*s π-electrons and the Ni 3d orbitals.

We perform spin-torque ferromagnetic resonance (ST-FMR) to study the dependence of the spin-current signal on the Ni thickness and to identify the origin of the generated spin current. Additionally, THz emission experiments were carried out to detect the inverse Spin Hall effect in graphene, revealing a significantly different signal compared to CoFe/Gr heterostructures.

MA 39.3 Wed 18:00 P2

Tuning Spin-Charge Conversion at the hybrid heavy-metal/ organic semiconductor interface via Doping — Parul Devi[1], •Devamrutha I S[1], Zhitian Ling[2], Ashish Moharana[1], David Anthofer[1], Tomasz Marszalek[2], and Angela Wittmann[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Deutschland — [2]Max-Planck-Institut für Polymerforschung, Mainz, Deutschland

Spintronics, the way forward to device miniaturization, leverages electron spin rather than charge. Though inorganic materials were predominantly given more attention in spin transport studies, organic semiconductor (OSC)/magnetic hybrid interfaces are quickly gaining interest, owing to the flexibility, scalability, and structural tunability of organic materials. Here, we probe the role of the charge carrier concentration of the OSC on the spin injection and spin-charge conversion efficiency in hybrid heterostructures via spin pumping. For this, we probe the inverse spin Hall effect (ISHE) in a ferrimagnetic insulator/ heavy-metal/ OSC heterostructure and systematically dope the conjugated polymer PBTTT with F4-TCNQ. We observed that the ISHE amplitude in the heavy metal increases by a factor of 4 upon adsorption of the PBTTT layer while doping reduces the signal. These results open the door to charge doping as an effective tool to control spin injection across hybrid interfaces.

MA 39.4 Wed 18:00 P2

Chirality controlled quantum transport in kagome AV3Sb5 — •Li Cheng and Qun Yang — Max Planck Institute of Microstructure Physics

Kagome metals AV3Sb5 exhibit a rich interplay among charge-density waves (CDWs), structural chirality, unconventional superconductivity, and anomalous Hall transport. Recent theoretical progress shows that layer-dependent phase shifts between CDW wave vectors can generate helical stacking and chiral electronic structures, while experiments reveal strong correlations between chirality and anomalous charge transport. In parallel, distorted kagome compounds display intertwined CDW and magnetic orders with enhanced tunability under external stimuli.

Motivated by these developments, this project aims to establish a predictive first-principles framework that connects CDW chirality with spin/orbital polarization as well as anomalous transport, and to uncover the microscopic mechanisms driving anomalous Hall responses in kagome systems. We further propose to explore pressure, strain, and temperature as external knobs for switching chirality and controlling emergent electronic and magnetic functionalities.

MA 39.5 Wed 18:00 P2

Tunable Topological Spin Pump in the XXZ Chain via Incommensurate Boundary Drives. — •Anshuman Tripathi[1], Mircea Trif[2], and Thore Posske[1] — [1]I. Institute for Theoretical Physics, University of Hamburg, Hamburg, Germany — [2]International Research Centre MagTop, Institute of Physics, Polish Academy of Sciences, Warsaw, Poland

We investigate an interacting XXZ spin-1/2 chain driven quasiadiabatically at its boundaries by two incommensurate phase drives. The independently evolving

phases result in a quasi-periodic trajectory on a two-dimensional torus, which generates a robust topological spin pump in the ground state. We show that the pumped spin is determined by an effective Chern number defined over the drive-phase torus, whose value is set by the number of degeneracy points enclosed by the trajectory. These degeneracy points increase systematically with the chain length and can be tuned through the exchange anisotropy, providing direct control of the topological pumping strength. Our results demonstrate that incommensurate multi-tone driving enables a versatile and robust realization of topological pumps in interacting quantum spin chains.

MA 39.6 Wed 18:00 P2

Ab-initio calculated linear, quadratic and cubic magneto-optic Kerr effect spectra — •Martin Zeman[1], Maik Gaerner[2], Robin Silber[3], Martin Veis[1], Timo Kuschel[2,4], and Jaroslav Hamrle[1,5] — [1]Charles University Prague, Czech Republic — [2]Bielefeld University, Germany — [3]VSB - Technical University of Ostrava, Czech Republic — [4]Johannes Gutenberg University Mainz, Germany — [5]Czech Technical University, Prague, Czech Republic

The cubic magneto-optic Kerr effect originates from higher-order symmetry terms in cubic crystals. Using density-functional theory within WIEN2k, we calculate the linear, quadratic, and cubic MOKE contributions. First, the permittivity tensor is calculated for different magnetization orientations using the Kubo formula (linear response theory). Then, the individual contributions are separated using expected dependence on the magnetization direction, as predicted by the symmetry. Here we limit to ferromagnetic materials of cubic symmetry, bcc Fe, fcc Co, fcc Ni, and Heusler compounds Co_2FeSi and AuMnSb, whose magneto-optic response is described by principal spectra K, G_s, $2G_{44}$, and ΔH. Surprisingly, the strength of the cubic contribution ΔH is of similar order as the quadratic ones G_s, $2G_{44}$, which has also been confirmed by experimentally [1,2].

[1] M. Gaerner et al., Phys. Rev. Appl. **22**, 024066 (2024)
[2] R. Silber et al, Phys. Rev. B **100**, 064403 (2019)

MA 39.7 Wed 18:00 P2

Application of 3D Nano-Lithography in Magnetism — •Jana Kredl[1], Christian Denker[1], Cornelius Fendler[2], Julia Bethune[1], Nina Meyer[1], Theresa Brinker[1], Finn-F. Stiewe[1], Tobias Kleinke[1], Chris Badenhorst[1], Alena Rong[1], Robin Silber[3], Mark Doerr[1], Raghvendra Palanakar[1], Toni Hache[6], Neha Jah[1], Uwe T. Bornscheuer[1], Marcel Kohlmann[1], Hauke Lars Heyen[1], Michaela Lammel[4], Alexander Paarmann[5], Andy Thomas[4], Robert Blick[2], Jakob Walowski[1], Michaela Dalcea[1], and Markus Muenzenberg[1] — [1]University of Greifswald, Germany — [2]University of Hamburg — [3]VSB-Technical University of Ostrava, Czech Republic — [4]IFW Dresden, Gemany — [5]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [6]Helmholtz-Zentrum Dresden-Rossendorf, Germany

3D 2-Photon-Lithography, originally developed for 3D photonic crystals, opens a wide range of new possible applications in many fields, e.g. life sciences, microoptics and mechanics. We will present our recent applications of 3D 2-Photon-lithography and show 3D evaporation masks for in-situ device fabrication using different deposition angles, infra-red laser light focusing lenses directly fabricated on optical fibers, tunnel structures for guiding growth of neurons [1], pillars for investigation of cell mechanics and master-mold fabrication for Polydimethylsiloxane (PDMS) micro-fluidic channels. Based on our experience we will discuss possible applications in magnetism. [1] C. Fendler et al., Adv. Biosys. 5 (2019) doi: 10.1002/adbi.201970054

MA 39.8 Wed 18:00 P2

Mapping the Interaction Field in Artificial Spin Ices — •Brindaban Ojha, Matías P. Grassi, and Vassilios Kapaklis — Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

Artificial spin ice (ASI) consists of lithographically patterned nanomagnet arrays that interact through dipolar coupling. Although these interactions can be tuned by adjusting nanomagnet dimensions, periodicity, and thickness, their detailed distribution and influence on magnetization reversal remain incompletely understood. We study square ASI structures with nanomagnet widths corresponding to aspect ratios (length/width) of 3 and 4.5, while keeping the length fixed at ~450 nm, and probe their interaction fields using First-Order Reversal Curve (FORC) analysis. ASI with an aspect ratio of 4.5 shows a single central peak in the FORC distribution, whereas the aspect-ratio-3 system displays both a central peak and an asymmetric 'boomerang'-shaped feature. To understand these signatures, we perform micromagnetic simulations using MuMax. After relaxation from a random state, lower-aspect ratio ASI develops multidomain or vortex-like states, while higher-aspect-ratio ASI stabilizes in single-domain configurations due to enhanced shape anisotropy. The simulations confirm that the central FORC peak corresponds to single-domain switching in the higher-aspect ratio ASI, whereas the 'boomerang' feature arises from an intermediate S-shaped reversal mode in the lower-aspect ratio system. These results demonstrate how geometry governs interaction-field distributions and reversal mechanisms in ASI.

MA 39.9 Wed 18:00 P2

Element- and Depth-Selective Magnetometry of Buried Magnetic Layers by MCD-HAXPES at PETRA III — •Andrei Gloskovskii[1], Christoph Schlueter[1], and Gerhard Fecher[2] — [1]Photon Science / DESY, Hamburg — [2]Max Planck Institute for Chemical Physics of Solids, Dresden

Magnetic circular dichroism (MCD) in hard X-ray photoelectron spectroscopy (HAXPES) provides direct element-specific access to magnetization in deeply buried layers. The MCD signal follows a simple $\cos(\theta)$ dependence on the angle between the X-ray polarization vector and the sample magnetization. Depth-selective magnetic sensitivity is achieved by exploiting near-total-reflection and waveguide excitation geometries, where the depth resolution is controlled by shaping the spatial intensity profile of the incident hard X-ray field inside the multilayer structure. In both cases, the probing depth is tuned by redistributing the X-ray excitation field inside the sample rather than by changing the emission angle or the kinetic energy of the photoelectrons. Using Co-based alloys as model systems, we show that MCD-HAXPES provides element- and depth-resolved magnetic contrast in complex multilayer stacks. The method is particularly powerful for disentangling interface and bulk magnetization in buried heterostructures. In addition to the methodological aspects, this contribution also presents an overview of recent user activities at beamline P22 (PETRA III), where an increasing number of external user groups have successfully applied MCD-HAXPES for depth-resolved magnetic studies and have already published a broad range of high-impact results.

MA 39.10 Wed 18:00 P2

Interferometric measurements of Yittrium-Iron-Garnet cantilevers — Sumiya Saleem[1], •Richard Boucher[1], Seth Kaufman[1], and Georg Schmidt[1,2] — [1]Martin-Luther-Universität Halle-Wittenberg Insitut für Physik, Halle, Germany. — [2]Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany.

Interferometric effects provide a sensitive detection of displacement, including those related to the resonance oscillations of cantilevers. We fabricate Yttrium-Iron-Garnet (YIG) cantilevers using a room-temperature pulsed laser deposition of amorphous YIG, lift-off method, followed by an anneal in oxygen yielding single-crystal structures [1]. By combining these in an interferometer built on the basis of the work of Pernpeitner [2] and Jörg [3] we have looked at the resonance frequency dependence on YIG cantilever length in the micrometre range, which will be compared with the work of Seo [4], various theoretical models, and COMSOL simulations, showing excellent agreement with theoretical results. We further show that these cantilevers can be driven to a non-linear regime, indicated via a characteristic Duffing non-linearity at high driving powers.

[1] P. Trempler et al, APL, 117, 232401 (2019) [2] M. Pernpeitner PhD thesis, TUM. [3] P. Jörg Bachelor's thesis, TUM [4] Y-J. Seo, APL., 110, 132409 (2017)

MA 39.11 Wed 18:00 P2

Spin-lattice coupling as a source of chiral phonons in cubic magnets — •Yelyzaveta A. Borysenko, Daniel Schick, and Ulrich Nowak — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

Hybrid spintronic device concepts can be implemented based on angular momentum, as this can be transferred over significant distances and effectively exchanged between different quasiparticles. The understanding, control, and effective generation of angular momentum is crucial for such applications.

The creation and manipulation of chiral phonons introduces an additional degree of freedom, as they can couple to other quasiparticles in a chirality-selective manner as well as transfer angular momentum obtained from magnons. Chiral phonons mainly occur in materials with inversion-symmetry breaking, although recent works proved that they can be also generated in materials preserving this symmetry due to spin-lattice coupling [1], which was also experimentally demonstrated with ultrafast demagnetization in a nickel thin film [2].

In this work, we linearize the coupled equations of motion for the spin and lattice degrees of freedom assuming a coupling term of anisotropy type. We describe the appearance of chiral phonons induced by spin-lattice coupling comparing cubic ferromagnets and antiferromagnets, calculate angular momentum of the modes and discuss the chirality selective coupling of magnon and phonon bands.

[1] M. Weißenhofer et al., Phys. Rev. Lett. 135, 216701 (2025);
[2] S. R. Tauchert et al., Nature 602, 73 (2022);

MA 39.12 Wed 18:00 P2

Optical manipulation of spin based AC-nanooscillators — •Niklas Dornquast[1], Kevin Jäckel[1], Jakob Walowski[1], Tim Böhnert[2], and Markus Münzenberg[1] — [1]University of Greifswald, Germany — [2]The International Iberian Nanotechnology Laboratory (INL), Portugal

With the steady rise of artificial intelligence and the end of Moore's law, a novel approach for computational capabilities arises to fulfill the ever-increasing demand, while keeping energy consumption low. The research field of spintronics provides new possibilities for such energy-efficient technology by also utilizing the transport of electron spin in addition to charge transport, opening up operation processing in a higher Gigahertz frequency range. Devices

that realize such utilization of electron spin are, for example, spintronic AC-nanooscillators such as Spin-Torque-nanooscillators (STNOs) and Spin-Hall-nanooscillators (SHNOs). Additionally, these types of nanooscillators have the prospect of being used in a whole new computer architecture based on the human brain, called "neuromorphic computing". We investigate the effects of femtosecond laser pulses (<100 fs) of different polarities on such nanooscillators by optimizing the lasers' parameters to increase oscillation efficiency as well as manipulate the oscillation frequency optically.

MA 39.13 Wed 18:00 P2

Cubic magneto-optic Kerr effect in (001)-oriented thin films at grazing incidence of light — •Marius Krause[1], Maik Gaerner[1], Robin Silber[2], Jaroslav Hamrle[3], and Timo Kuschel[1,4] — [1]Bielefeld University, Germany — [2]VSB - Technical University of Ostrava, Czech Republic — [3]Charles University Prague, Czech Republic — [4]Johannes Gutenberg University Mainz, Germany

We investigate the cubic magneto-optic Kerr effect (CMOKE) in thin films of cubic crystal structures. CMOKE is proportional to third order in magnetization ($\propto M^3$) and was recently observed in Ni(111) thin films with 45° incidence of light [1]. At this angle of incidence, no CMOKE could be observed for (001)-oriented Ni thin films so far. However, we could observe a distinct CMOKE signal in Ni(001) at grazing incidence. Similar behaviour is found in other materials with (001)-oriented cubic crystal structure, indicating that grazing-incidence CMOKE is a more general feature of this crystal orientation. In this contribution, we present first experimental results of grazing-incidence CMOKE and discuss the incidence-angle dependence of CMOKE for different materials and crystal orientations. Our findings open new possibilities for CMOKE-based characterization of materials with (001)-oriented crystal structures.

[1] M. Gaerner et al., Phys. Rev. Appl. 22, 024066 (2024)

MA 39.14 Wed 18:00 P2

Generation of Floquet-like sidebands in spin-wave systems induced by surface accustic waves — •Tim Vogel, Matthias Wagner, Björn Heinz, and Philipp Pirro — Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU Kaiserslautern-Landau

The interaction between spin waves (SWs) and surface accoustic waves (SAWs) offers promising opportunities for advanced magnonic and spintronic applications. In this work, we investigate the generation of Floquet-like frequency combs in the GHz spin-wave spectrum with low-frequency SAWs in the MHz range as the Floquet-drive. We study the excitation of these states by coupling SAWs of different frequencies and incidence angles to SWs in both Damon-Eshbach and backward-volume geometry. We further explore these effects in multiple material systems to validate an analytical model describing the modified spin-wave dispersion under SAW driving. Our results contribute to a deeper understanding of magnon-phonon interactions and the conditions under which Floquet-like states emerge.

We acknowledge funding by the European Union via Horizon Europe project MandMEMS, Grant No. 101070536.

MA 39.15 Wed 18:00 P2

Growth and magnetic characterization of freestanding single-crystalline SrRuO3 /La0.7Sr0.3MnO3 oxide bilayers — •Diana Rata, Lilly Patschinsky, Elin Vocks, Alexander Much, Oleksandr Dolynchuk, Antonia Rieche, and Kathrin Dörr — Institute of Physics, Martin Luther University Halle*Wittenberg, 06099 Halle, Germany

We report the successful fabrication of freestanding epitaxial SrRuO3 /La0.7Sr0.3MnO3 (SRO/LSMO) heterostructures. LSMO and SRO layers were first prepared by PLD on a water-soluble sacrificial oxide Sr3Al2O6 (SAO), which was epitaxially grown on a SrTiO3 (100) substrate, followed by selective release and transfer of the membranes onto SiO2 wafers. The structure was characterized by X-ray diffraction. Our findings reveal that the epitaxial growth and strain of SAO layer is strongly affected by the subsequent growth condition (e.g., oxygen partial pressure) of upper oxide layers and influences strongly the quality and integrity of the oxide membranes. Magnetic characterization show that the freestanding SRO/LSMO membranes retain the key magnetic signatures of their corresponding bilayers. Notably, in the case of freestanding single-layer SrRuO3, we observe an enhancement of the magnetic response compared to its epitaxial single layer, suggesting strain relaxation and reduced substrate clamping as important factors. These results highlight the potential of freestanding oxide membranes for flexible integration and for exploring strain-decoupled magnetic phenomena in functional single-crystalline freestanding oxide bilayers.

MA 39.16 Wed 18:00 P2

Magnetic Anisotropy in Ordered and Disordered CoPd Alloys: A First-Principles Study — •Christian Maas, Michael Czerner, and Christian Heiliger — Institute for Theoretical Physics, Justus Liebig University Giessen

Understanding the magnetic anisotropy in magnetic materials is crucial for designing devices like sensors or data storage. In this work, we present ab initio density functional theory calculations of the magnetocrystalline anisotropy of $Co_xPd_{(1-x)}$ alloys with varying concentrations as well as $L1_0$ like $[CoPd]_x[PdCo]_{(1-x)}$ structures. We also show results for ordered layer structures with different thicknesses of Co and Pd layers. For our calculations, we employ the relativistic screened Korringa-Kohn-Rostoker Green's function method. The alloys are treated within the coherent potential approximation. Additionally, we explore the magnetic anisotropy of thin $Co_xPd_{(1-x)}$ films, considering both the magnetocrystalline and shape anisotropy.

MA 39.17 Wed 18:00 P2

Tailoring magnetic textures and investigation of magnetization processes in 3D via geometrical transformation — •Aman Singh[1], Timo Schmidt[2], Ivan Soldatov[1], Manfred Albrecht[2], Rudolf Schäfer[1], and Volker Neu[1] — [1]Leibniz IFW Dresden, D-01069 Dresden, Germany — [2]Institute of Physics, University of Augsburg, D-86159 Augsburg, Germany

Control over magnetic domains and domain walls is crucial for developing magnetic systems and devices. Here, we use a simple technique that uses a self-assembled reversible geometrical transformation from a flat 2D state to a rolled-up 3D state and back to the 2D state to create periodic up-down magnetization patterns in TbFe by applying a homogeneous magnetic field in the 3D state. We present how the magnetization patterns can be deterministically tailored simply by selecting the magnitude and direction of the applied magnetic field in the 3D state, which would otherwise require much more elaborate processes. This approach further provides a unique pathway to access and visualize magnetization processes in 3D by investigating the imprinted domains in the unrolled state of material magnetized at various fields in the 3D state. We further show that the overall 3D magnetization evolution can be reconstructed from recoil measurements in the 2D state when combined with the intrinsic anisotropy of the material. Finally, we discuss how this platform can be extended to investigate anisotropy changes in magnetostrictive materials, opening new possibilities for studying and engineering 3D magnetic states through reversible shape transformation.

MA 39.18 Wed 18:00 P2

Exploring spin reorientation and structural stability in distorted kagome metal — •Jayjit Kumar Dey[1], Tomke Glier[2], Sourav Chowdhury[1], Mouli Roy-Chowdhury[3], Subhajit Nandy[1], Amir-Abbas Haghighirad[4], Dmitry Reznik[2], and Moritz Hoesch[1] — [1]Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany — [2]University of Colorado Boulder, Boulder, CO, USA — [3]Université Grenoble Alpes, CEA, CNRS, Grenoble INP, SPINTEC, Grenoble, France — [4]Karlsruhe Institute of Technology, Karlsruhe, Germany

Distorted kagome metals have emerged as fertile platforms for investigating the interplay between geometrical frustration, magnetoelastic coupling, and exotic electronic states. In this work, we investigate the magnetic anisotropy and spin-reorientation behavior of TbAgGe and DyAgGe using X-ray magnetic circular dichroism (XMCD) and X-ray magnetic linear dichroism (XMLD) at the rare-earth M4,5-edges. XMCD reveals strong magnetocrystalline anisotropy and highlights the gradual evolution of 4f-moment orientation under applied magnetic field. Complementary XMLD measurements provide direct evidence of exchange-driven spin arrangement and local crystal field anisotropy. The robustness of the hexagonal crystal framework is evidenced by Extended X-ray absorption fine structure (EXAFS) and Raman spectroscopy, with no evidence of symmetry breaking despite noticeable shifts in bond angles and interlayer spacing. These results establish spin dynamics and structural stability in distorted kagome systems.

MA 39.19 Wed 18:00 P2

More is not always better: the case of $Mn_{0.56}Ge_{0.09}Sb_{0.23}Te$ — Tijmen Groot[1], Marie Tardieux[1], Laura T. Corredor[2,3], Manaswini Sahoo[4], Anja U.B. Wolter[4], and •Anna Isaeva[1,2,3] — [1]University of Amsterdam, The Netherlands — [2]TU Dortmund University, Germany — [3]Research Center Future Energy Materials and Systems, Germany — [4]Leibniz IFW Dresden, Germany

In the quest to optimize magnetic topological materials within the $(MnX_2Te_4)(X_2Te_3)_n$ family [1], Mn enrichment appears to be a viable strategy that enhances the ferrimagnetic ground state and the Curie temperature. We recently reported the most Mn-rich phases derived from $MnSb_2Te_4$, achieving T_C = 58-73 K [2-3], nearly satisfying one key requirement for potential applications.

Our further attempts to tune T_C show that not only Mn richness but also lattice symmetry plays a key role. Here we present the cubic, Mn-rich compound $Mn_{0.56}Ge_{0.09}Sb_{0.23}Te$ ($Fm\bar{3}m$, a = 5.9320(2) Å), as identified by powder and single-crystal XRD, SEM/EDX, and DC susceptibility. Due to the statistical disorder of Mn, Ge, and Sb over the cationic sites, it loses ferrimagnetic order in favor of an A-type antiferromagnetic arrangement with a low T_N = 25 K. This ground state is also supported by DFT+U calculations across a wide range of plausible compositions.

References: [1] National Science Review 11 (2024), nwad282; [2] Mater. Today Phys. 38 (2023), 101265; [3] Chem. Mater. 37 (2025), 1446-1456.

MA 39.20 Wed 18:00 P2

Magnetic Domain Structure of Erbium thin films — •Ujjval Mishra, Patrick Härtl, and Matthias Bode — University of Würzburg, Experimental Physics 2, Am Hubland, D-97074 Würzburg, Germany

Rare-earth metal (REM) films exhibit diverse magnetic behaviors governed by the indirect RKKY coupling of localized $4f$ moments, leading to complex long-range order. Building on prior studies of REM surface magnetism [1-5], we investigate the magnetic properties of epitaxial Erbium (Er) thin films. Er, a heavy rare-earth element with two unpaired $4f$ electrons, crystallizes in a hexagonal close-packed structure and remains paramagnetic above T_N = 85 K. Below T_C = 20 K, it adopts a conical ferromagnetic phase with the cone axis parallel to the c direction and a semi-cone angle of 29.6° at 6 K [6].

Spin-polarized scanning tunneling microscopy (SP-STM) reveals a complex domain structure in Er(0001) films epitaxially grown on W(110). At 4.5 K, domain walls are predominantly pinned to structural defects, while external magnetic fields around 2 T induce a maze-like contrast, confirming their magnetic origin. These findings highlight the intricate coupling between structural defects and magnetic domain evolution in Er(0001) thin films.

[1] P. Härtl et al., Phys. Rev. B **105**, 174431 (2022). [2] P. Härtl et al., Phys. Rev. Lett. **133**, 186701 (2024). [3] P. Härtl et al., Phys. Rev. B **110**, 184405 (2024). [4] P. Härtl et al., Phys. Rev. B **112**, 024416 (2025). [5] P. Härtl et al., Phys. Rev. B **112**, 174402 (2025). [6] W. C. Koehler et al., J. Appl. Phys. **36**, 1078 (1965).

MA 39.21 Wed 18:00 P2

First-principles study of Mn mono- and bilayers on the Ta(001) surface — •Leo Kollwitz, Tim Drevelow, and Stefan Heinze — Institute of Theoretical Physics and Astrophysics, Kiel University, Leibnizstraße 15, 24098 Kiel, Germany

The magnetic order in ultrathin $3d$ transition-metal films on surfaces can be strongly influenced by the substrate. A prominent example is a Mn monolayer on W(001), in which the prototypical antiferromagnetic Mn exhibits strong ferromagnetic exchange coupling [1]. Deposition of an additional Mn layer, however, leads to a checkerboard antiferromagnetic order in the surface layer, while the magnetic moment of the Mn interface layer is quenched moment [2]. Here, we study the magnetism in Mn mono- and bilayers on the Ta(001) surface by density functional theory (DFT) via the Fleur code [3]. Surprisingly, the Ta substrate leads to a very similar behavior of magnetic order in the Mn mono- and bilayer as on the W(001) surface, contrary to the trend observed for Fe monolayers [4]. Our DFT calculations show a strong dependence of the magnetic moments of the lower Mn layer on the interlayer distance as well as the magnetic configuration. Based on the DFT results we parameterize an atomistic spin Hamiltonian.

[1] P. Ferriani *et al.*, Phys. Rev. B **72**, 024452 (2005)
[2] S. Meyer *et al.*, Phys. Rev. Res. **2**, 012075(R) (2020)
[3] The Fleur project, www.flapw.de
[4] P. Ferriani *et al.*, Phys. Rev. Lett. **99**, 187203 (2007)

MA 39.22 Wed 18:00 P2

prospects of studying circularly polarised phonons in 2D magnetic materials — •Hanna Shirin Pulikkal Hamza[1], Lukas Nöding[1], Helya Alaei[1], Ahmed Hassanien[1], Mashood Tariq Mir[1], Zdeněk Sofer[2], Jochen Mikosch[1], Thomas Baumert[1], and Arne Senftleben[1] — [1]Institute of Physics,University of Kassel, 34132 Kassel, Germany — [2]UCT Prague

It has been proposed that circularly polarised phonons can induce transient magnetisation in materials when driven by ultrafast laser pulses via the atomistic scale Barnett effect. In this ongoing study, we want to directly link the observation of circular atomic motion with magnetisation in 2D Van der Waals room temperature ferromagnetic materials. We have recently induced circularly polarised coherent phonons by a pair of femto-second laser pulses in a non-magnetic material namely graphite and detected the resulting lattice dynamics using Ultrafast Electron Diffraction (UED). In this contribution, we will review the results on graphite and show our recent progress in exfoliating ferromagnetic 2D materials. Furthermore, we will explore magnetisation measurements of our microscopic samples using Kerr microscopy and vibrating sample magnetometry.

MA 39.23 Wed 18:00 P2

D-wave Chiral Phonons from Electron-Phonon Coupling — •Dimos Chatzichrysafis[1] and Alexander Mook[1,2] — [1]Johannes Gutenberg Universität, Mainz — [2]University of Münster

Chiral phononics, the field of study of phonons carrying finite orbital angular momentum has recently attracted wide interest due to its rich, versatile physics and potential applications.

In search of mechanisms to generate unconventional phonon orbital angular momentum textures, we demonstrate theoretically that d-wave chiral phonons can emerge even in the absence of electronic spin order. We show that by considering an electronic system hosting a d-wave orbital angular momentum texture, non-relativistic electron-phonon coupling leads to the formation of d-wave chiral phonons.

In this way we expand the potential platforms of chiral phononics and offer application routes unique to d-wave textures, such as orbital phonon splitters.

MA 39.24 Wed 18:00 P2

Phonon Pumping Experiments — •Jeremias Mütschele, Luise Holder, Michaela Lammel, Richard Schlitz, and Sebastian T. B. Goennenwein — Department of Physics, University of Konstanz, Konstanz, Germany

Phonons carrying angular momentum have recently attracted significant attention in the field of spintronics, as they are considered promising candidates for information carriers that do not require electrical currents. The coupling of phonons to spin-wave excitations (magnons) opens up opportunities to manipulate them, and consequently the transmitted information, via magnon-phonon interactions. However, engineering such hybrid quasiparticles, known as magnon-phonon-polaritons, remains a major experimental challenge. To gain deeper insight into the properties of magnon-phonon-polaritons, we investigate phonon pumping from a ferromagnetic thin film into a paramagnetic bulk crystal under various geometrical configurations. We find that our approach enables the selective excitation and analysis of distinct magnon-phonon-polariton modes. This could open a pathway to tailor phonon-based information transport.

MA 39.25 Wed 18:00 P2

Thorium-229 as a Chiral Phonon Detector — •Martin Pimon[1], Kjeld Beeks[2], Thorsten Schumm[2], and Andreas Grüneis[1] — [1]Institute of Theoretical Physics, TU Wien, Vienna, Austria — [2]Institute of Atomic and Subatomic Physics, TU Wien, Vienna, Austria

The thorium-229 isotope features an exceptionally low-energy nuclear metastable excited state 8.4 eV above the ground state. This property makes it a viable candidate for probing level splitting in nuclear sub-levels using modern high-precision laser spectroscopy methods.

Magnetic interactions play a significant role in this level splitting, highlighting the potential of thorium-229 as a novel atomic-sized detector for the magnetic moment of chiral phonons. Moreover, the electric field gradient from the surrounding crystal lattice introduces additional level splitting, providing insights into structural properties.

By incorporating thorium atoms into an ionic crystal, our proposed technique enables the direct observation of both magnetic and electric interactions from within the crystal itself. This approach leverages high sensitivity to phonon-related phenomena, presenting a promising avenue for detecting chiral phonons.

In this poster, we will review the contributions to nuclear level splitting and explore the challenges and benefits of utilizing the thorium-229 nucleus as a detector for chiral phonons.

MA 40: Focus Session: Chiral phonons and crystals coupled to magnetic order II

Conventional magnetism arises from electron spin and orbital angular momentum, forming the basis of spintronics and orbitronics. Recent advances, however, have revealed that magnetism is also intimately linked to the chirality and angular momentum of the crystal lattice itself, often mediated by circular lattice vibrations known as chiral or axial phonons. These discoveries have uncovered novel mechanisms of spin and phonon transport and enabled direct access to phonon chirality and angular momentum as fundamental physical quantities. These developments prompt a re-examination of angular momentum coupling in solids, including well-established phenomena such as the Einstein-de Haas and Barnett effects, as well as the role of phonon angular momentum in the equilibrium state of magnetic materials. Chiral and axial phonons emerge as a powerful new platform for controlling magnetic order and dynamics, bridging lattice, spin, and angular momentum physics. This focus session aims to highlight recent breakthroughs in phonon angular momentum and magnetism and to connect the rapidly expanding field of chiral phononics with the broader magnetism community, spanning both experimental and theoretical perspectives.

As part of this focus session, we offer an excursion to the high-field THz user facilities at HZDR with an introduction to the planned Dresden Advanced Light Infrastructure (DALI). See MA 32 for details.

Organizers: Dominik Juraschek, d.m.juraschek@tue.nl; Michael Fechner, michael.fechner@mpsd.mpg.de; Sebastian Maehrlein, s.maehrlein@hzdr.de

Time: Thursday 9:30–12:45 Location: HSZ/0002

Invited Talk MA 40.1 Thu 9:30 HSZ/0002

Magnetic order induced chiral phonons in a ferromagnetic Weyl semimetal — •Luyi Yang — Tsinghua University, Beijing, China

Chiral phonons are vibrational modes in a crystal that possess a well-defined handedness or chirality, typically found in materials that lack inversion symmetry. Here we report the discovery of chiral phonon modes in the kagome ferromagnetic Weyl semimetal $Co_3Sn_2S_2$, a material that preserves inversion symmetry but breaks time-reversal symmetry. Using helicity-resolved magneto-Raman spectroscopy, we observe the spontaneous splitting of the doubly degenerate in-plane E_g modes into two distinct chiral phonon modes of opposite helicity when the sample is zero-field cooled below the Curie temperature, in the absence of an external magnetic field. As we sweep the out-of-plane magnetic field, this E_g phonon splitting exhibits a well-defined hysteresis loop directly correlated with the material's magnetization. The observed spontaneous splitting reaches up to 1.27 cm^{-1} at low temperatures, progressively diminishes with increasing temperature, and completely vanishes near the Curie temperature. Our findings highlight the role of the magnetic order in inducing chiral phonons, paving the way for novel methods to manipulate chiral phonons through magnetization and vice versa. Additionally, our work introduces new possibilities for controlling chiral Weyl fermions using chiral phonons.

Ref: [1] M. Che et al., Magnetic order induced chiral phonons in a ferromagnetic Weyl semimetal, Physical Review Letters 134, 196906 (2025).

MA 40.2 Thu 10:00 HSZ/0002

The effect of lattice vibrations on the Curie temperature — •Thorben Pürling[1,2,3] and Stefan Blügel[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institute for Theoretical Physics, RWTH Aachen University, 52074 Aachen, Germany — [3]Science Institute and Faculty of Physical Sciences, University of Iceland, 107 Reykjavík, Iceland

Lattice vibrations, or phonons, are important degrees of freedom that are excited in every magnet operating at finite temperatures. This is particularly true for magnets used in practical applications, which typically operate above room temperature. When predicting critical temperatures – a key property of magnets – from *ab initio* calculations lattice vibrations are typically neglected in favor of fluctuations only in the magnetic degrees of freedom. Conversely, in experiments at room temperature the lattice does contribute to the thermal properties of the system. We aim to close the gap between theory and experiment at room temperature by taking lattice vibrations into account explicitly. We present a numerical method based on the atomistic spin model and showcase how the lattice vibrations can be integrated out to an effective spin Hamiltonian that inherently depends on lattice fluctuations.

We acknowledge funding from the ERC grant 856538 (project "3D MAGIC") and DFG through SFB-1238 (project C1).

MA 40.3 Thu 10:15 HSZ/0002

Universal phonon angular momentum Hall effect — •Daniel Bustamante Lopez[1,2], Verena Brehm[2], and Dominik Juraschek[2] — [1]Boston University, Boston, MA, USA — [2]Eindhoven University of Technology, Eindhoven, Netherlands

The phonon angular momentum Hall effect was recently proposed as a phononic analogue of the spin and orbital Hall effects. Here, we demonstrate that a temperature gradient universally drives a transverse flow of phonon angular momentum in harmonic lattices. Using an exact Green's function method together with nonequilibrium molecular dynamics, we obtain closed-form expressions for the local phonon angular momentum density, bond-resolved current, and a corresponding conductivity kernel that ties them to spatial temperature variations. The Hall response originates from bath-induced mode mixing encoded in off-diagonal phonon correlations and does not require lattice chirality, Berry curvature, or inversion-symmetry breaking. It persists in the most simple centrosymmetric geometries, including square and honeycomb lattices. We predict robust edge accumulation and a tunable Hall angle for phonon angular momentum in various materials with quantitative agreement between analytic theory and simulations. Our results establish the phonon angular momentum Hall effect as a universal channel for transverse angular-momentum transport in crystalline solids.

MA 40.4 Thu 10:30 HSZ/0002

Phonon Angular Momentum Transfer Torque — •Verena Brehm[1], Daniel Bustamante Lopez[2], Shu Zhang[3], and Dominik Juraschek[1] — [1]Department of Applied Physics and Science Education, Eindhoven University of Technology, Eindhoven, Netherlands — [2]Department of Physics, Boston University, Boston, USA — [3]Okinawa Institute of Science and Technology, Okinawa, Japan

Angular momentum can be carried by a variety of (quasi)particles, including magnons, photons, and phonons, whose interplay has recently opened new directions in spintronics and optoelectronics. In this talk, we demonstrate the transfer of angular momentum from a phononic system to a magnetic system via an interfacial transfer torque, which we call the Phonon Angular Momentum Transfer Torque (PAMTT). We estimate the magnitude of phonon angular momentum originating from different mechanisms, among them the recently discovered phonon angular momentum Hall effect, and explore the possible magnetization dynamics that can be induced by the resulting PAMTT. Our analysis shows that both the precessional and relaxation components of the PAMTT can be detected as shifts in frequency and broadening of the linewidth in ferromagnetic resonance (FMR) experiments.

MA 40.5 Thu 10:45 HSZ/0002

The phonomagnet: Spontaneous order of phonon angular momentum — •Maike Fahrensohn and Matthias Geilhufe — Condensed Matter and Materials Theory Division, Department of Physics, Chalmers University of Technology, 41258 Göteborg, Sweden

Magnetism arises from the collective order of electron spin and orbital angular momentum. Here, we introduce a new type of magnetism, which appears due to spontaneous order of the phonon angular momentum. We consider a Hamiltonian containing an interaction term that couples the phonon angular momentum to the electronic spin density. Using an imaginary-time Dyson expansion, we evaluate the spin partition function and obtain an effective phonon Hamiltonian.

To first order in the coupling strength, this approach yields a Zeeman-like term, which couples the electronic magnetization to the phonon angular momentum and leads to a spin-induced bias of phonon chirality.

To second order, we obtain a bilinear interaction between ionic angular momentum modes on different sites, mediated by the Matsubara spin susceptibility. Decomposing the tensor into isotropic and anisotropic parts, we identify emergent phononic analogues of the Heisenberg (isotropic), Γ-model (symmetric, anisotropic), and Dzyaloshinskii-Moriya (antisymmetric, anisotropic) interactions.

Similarly to the conventional Heisenberg model for electronic spins, our model exhibits a phase transition in which ions spontaneously develop angular momentum at elevated temperatures.

15 min break

Invited Talk MA 40.6 Thu 11:15 HSZ/0002

Thermal Hall Effects of Magnons and Phonons — •Alexander Mook — Universität Münster

Thermal Hall transport in insulating magnets provides a powerful probe of topology, interactions, and spin-lattice coupling in charge-neutral quantum matter. I will discuss the magnon thermal Hall effect arising from Berry curvature in altermagnets, and show how symmetry and band geometry control transverse heat currents carried by spin waves [1]. Going beyond single-particle pictures, I highlight recent theoretical results demonstrating that magnon-magnon interactions can generate intrinsic thermal Hall responses even in topologically trivial magnon bands [2]. I then turn to magnetoelastic systems, where magnon-phonon coupling produces hybrid excitations whose combined Berry curvature and scattering processes can strongly enhance or even invert the thermal Hall signal [3,4]. Together, these results establish thermal Hall transport as a genuinely many-body phenomenon governed by topology, interactions, and spin-lattice hybridisation.

[1] Hoyer et al., PRB 111 (2), L020412 (2025) [2] Chatzichrysafis, Mook, PRB 111 (13), 134405 (2025) [3] Li et al., PRB 108 (14), L140402 (2023) [4] Nawwar et al., Reports on Progress in Physics 88 (8), 080503 (2025)

MA 40.7 Thu 11:45 HSZ/0002

Electrical conductivity from the axial phono-magnetic effect — •Natalia Shabala and Matthias Geilhufe — Department of Physics, Chalmers University of Technology, 412 96 Gothenburg, Sweden

Axial, or circularly polarized phonons, are characterized by the collective vibrations of atoms in circular patterns. These phonons have been shown to induce large magnetization in a phenomenon referred to as the phono-magnetic effect [1,2]. The mechanism behind this effect is believed to be the electron-phonon interaction. In combination with circular polarization of phonons this interaction leads to the time-reversal symmetry breaking and causes splitting of electronic energy levels. In this work, we aim to study the effect of this splitting on other physical phenomena. In particular, we are interested in the electrical conductivity, which can be studied through the Hubbard model. Additionally, we investigate whether the time-reversal symmetry breaking leads to the emergence of the anomalous Hall effect, as can be expected in 2D materials.

[1] N. Shabala, and R. M. Geilhufe, Phys. Rev. Lett. 133.26 (2024): 266702
[2] N. Shabala, F. Tietjen, R. M. Geilhufe, arXiv:2511.03329 (2025)

MA 40.8 Thu 12:00 HSZ/0002

Magnetic field induced pseudo angular momenta, chiral phonons, and anomalous EP interactions in some Weyl semimetals — Vladimir Gnezdilov[1], Florian Büscher[2], •Peter Lemmens[2], Angela Möller[3], Dirk Wulferding[4], Claudia Felser[5], and Chandra Shekar[5] — [1]ILTPE, Kharkiv, Ukraine — [2]IPKM, TU-BS, Braunschweig — [3]Dept. Chemistry, JGU, Mainz — [4]Dept. Physics and Astr., Sejong Univ., Korea — [5]MPI-CPfS, Dresden

Applying magnetic fields excite phonon chirality and induce angular momenta due to the time-reversal breaking [1]. This allows to study effects usually restricted to the boundary of the Brillouin zone. We show such results for several Weyl semimetals [2] with uncommon spin-phonon interactions and discuss novel possibilities for the transfer and interaction between the angular momenta of photons and phonons [3].

[1] T. Wang, H. Sun, X. Li, L. Zhang, Chiral Phonons: Prediction, Verification, and Application, Nano Lett. 24, 15, 4311 (2024).
[2] P. Sessi, et al., Handedness-dependent quasiparticle interference in the two enantiomers of the topological chiral semimetal $PdGa$, Nature Comm. 11, 3507 (2020).
[3] R. Rao, et al., Anomalous Raman scattering in layered $AgCrP_2Se_6$: Helical modes and excitation energy-dependent intensities, https://arxiv.org/abs/2501.17565 (2025).

MA 40.9 Thu 12:15 HSZ/0002

Phonon Polariton Hall Effect — •Omer Yaniv[1] and Dominik Juarschek[1,2] — [1]Tel Aviv University, Tel Aviv, Israel — [2]Eindhoven University of Technology, Eindhoven, Netherlands

The phonon Hall effect conventionally describes the generation of a transverse heat current in an applied magnetic field. In this work, we extend the effect to hybrid light matter excitations and demonstrate theoretically that phonon polaritons, formed by coupling optical phonons with terahertz radiation, support transverse energy flow when coherently driven in an applied magnetic field. Using the example of PbTe, which exhibits strongly coupled phonon polaritons, we show that the magnetic field splits the phonon-polariton branches into left and right-handed circular polarization, obtaining unequal group velocities. We derive the energy current operators for propagating phonon polaritons and show how their mixed phononic-photonic nature enables controllable transverse phonon-polariton transport in the terahertz regime. Our results demonstrate bending of light through a phonon polariton Hall effect, which provides a route towards terahertz polaritonic devices.

MA 40.10 Thu 12:30 HSZ/0002

Phonon angular momentum in ultrafast demagnetization and hybrid quasiparticles — •Markus Weissenhofer[1], MS Mrudul[1], Philipp Rieger[1], Luca Mikadze[1], Ulrich Nowak[2], and Peter M. Oppeneer[1] — [1]Uppsala University, Uppsala, Sweden — [2]Universität Konstanz, Konstanz, Germany

Transfer and manipulation of angular momentum is a key aspect in spintronics. Recently, it has been shown that angular momentum transfer between spins and phonons is possible even on ultrashort timescales [1]. To contribute to the understanding of this transfer, we investigate spin-phonon coupling using two different fully ab-initio based methods [2,4]. Using Ehrenfest nuclear dynamics simulations combined with time-dependent density functional theory, we demonstrate that after ultrafast demagnetization of FePt optical phonons carrying finite angular momentum are created [2]. In addition, we show how a novel framework [3] can be used to calculate magnon-phonon coupling parameters and hybridization from first principles, revealing the existence of chiral phonons in Fe arising from a chirality-selective magnon-phonon coupling [4].

[1] Tauchert al., Nature 602, 73 (2022); Luo et al., Science 382, 698 (2023). [2] Mrudul et al., PRB 112, L180407 (2025). [3] Mankovsky et al., PRL 129, 067202 (2022). [4] Weißenhofer et al., PRL 135, 216701 (2025).

MA 41: Focus Session: Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects II (joint session TT/DS/MA)

Time: Thursday 9:30–12:30 Location: HSZ/0003

See TT 69 for details of this session.

MA 42: Molecular Magnetism and Magnetic Particles / Clusters II

Time: Thursday 9:30–12:30 Location: HSZ/0004

MA 42.1 Thu 9:30 HSZ/0004

Towards a Physics-Informed Deep Learning Model for Parameterizing the Magnetism in 4f based Single-Molecule Magnets — •Zayan Ahsan Ali and Oliver Waldmann — Physikalisches Institut, Universität Freiburg, Germany

Single-molecule magnets (SMMs) have attracted interest in recent decades for their intriguing magnetic behavior and potential applications in quantum computing and spintronics. 4f based SMMs stand out because lanthanide ions can provide large magnetic anisotropies. However, the ligand environments that govern their magnetic properties involve up to 27 ligand-field parameters, while common experimental data such as temperature dependent magnetic susceptibility measured on powdered samples are comparatively featureless. Inferring ligand field parameters from such data is therefore a highly over-parameterized inverse problem. Machine learning approaches have shown promise in addressing this challenge [1]. Two central difficulties are identification of physically relevant regions of the ligand field parameter space and learning of a highly complex one-to-many mapping. This work presents a machine learning framework tailored to overcome both obstacles. It is shown that an informative training data set can be constructed via active learning with uncertainty sampling, and that incorporating the energy spectrum as an intermediate representation significantly improves the learnability of the high dimensional inverse mapping. The resulting architecture is found to be capable of predicting multiple possible ligand field parameter sets.

[1] Z. A. Ali *et al.*, PRB 112, 064403 (2025).

MA 42.2 Thu 9:45 HSZ/0004

Graphene-based quantum heterospin graphs — Gabriel Martínez-Carracedo[1], Amador García-Fuente[1], László Oroszlány[2], •László Szunyogh[3], and Jaime Ferrer[1] — [1]Universidad Oviedo, Spain — [2]Eötvös Loránd University, Budapest, Hungary — [3]Budapest University of Technology and Economics, Hungary

Harnessing quantum-regime functionalities without relying on rare-earth elements represents an important step toward developing globally accessible quantum technologies. In this contribution, we investigate a range of low-dimensional open quantum spin systems constructed from magnetic nanographene structures containing spin-1/2 and spin-1 triangulenes and/or olympicenes. These graphene nanostructures act as localized spins and can be effectively modeled using a quantum bilinear*biquadratic Heisenberg Hamiltonian. We compute the energy spectrum and the quantum numbers associated with the low-energy eigenstates. We identify a double degeneracy in the total spin quantum number S of the first excited state in three-leg spin graphs (3-LSGs) and in other heterospin nanostructures. This degeneracy depends on both the number of sites and the spin species, and arises from a swapping-transformation symmetry of the Hamiltonian. Numerical simulations further show that this degeneracy remains largely robust in $N = 7$ spin-1 3-LSGs under realistic perturbations relevant to experimental conditions. [1]

[1] G. Martínez-Carracedo *et al.*, DOI: 10.1103/v3fm-lvsh (2025)

MA 42.3 Thu 10:00 HSZ/0004

Femtosecond spin-state switching dynamics of Fe(II) complexes condensed in thin films — •Manuel Gruber[1], Lea Kämmerer[1], Gérald Kämmerer[1], Laurent Mercadier[2], Andreas Scherz[2], Felix Tuczek[3], Peter Kratzer[1], Uwe Bovensiepen[1], and Heiko Wende[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]European XFEL, Schenefeld, Germany — [3]Institute for Inorganic Chemistry, Kiel University, Germany

Significant progress has been made in tailoring spin-crossover films, driven by their potential for technological applications. However, studies of ultrafast switching in such films remain limited compared to their solution-phase counterparts. Here, we investigated photoinduced spin-state switching in a molecular film at room temperature, using the new capabilities offered by X-ray free-electron lasers. The sub-picosecond transition from the $S = 0$ low-spin state to the $S = 2$ high-spin state is tracked via transient changes in the Fe L_3 X-ray absorption edge. Our results reveal the involvement of an intermediate state in the switching dynamics [Kämmerer et al., ACS Nano 18, 34596 (2024)].

Financial support from CRC 1242 is gratefully acknowledged.

MA 42.4 Thu 10:15 HSZ/0004

Chirality-induced spin selectivity without intrinsic spin-orbit coupling: Role of non-equilibrium molecular orbital moment — •Sumit Ghosh[1] and Daniel E. Bürgler[2] — [1]The Institute of Physics of the Czech Academy of Sciences, 16200 Prague, Czech Republic — [2]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich GmbH, 52428 Jülich, Germany

We present an alternative theory of chirality induced spin selectivity (CISS) that does not require any intrinsic spin orbit coupling (SOC). The proposed mechanism is based on the formation of circulating currents in the molecular rings. In each ring, this current generates a non-equilibrium molecular orbital moment (MOM) which interacts with the spin of an injected electron, giving rise to CISS. The direction of the MOM is governed by the gauge field that arises from the chirality-induced structural distortion of the molecule. Being non-relativistic in nature, the gauge field induced MOM can be stronger than the effect generated by SOC. The presence of such a gauge field also overcomes the hurdle posed by Onsager's reciprocity. Finally we demonstrate that a non-equilibrium MOM can also form in the absence of the gauge field. However only the presence of the gauge field can produce the experimentally observed crossing I-V curve which is a characteristics of the CISS effect.

MA 42.5 Thu 10:30 HSZ/0004

Magnetocaloric effect of the centered-square, centered-hexagon, and double-pyramidal spin models — •Hamza Meel and Jürgen Schnack — Bielefeld University, Faculty of Physics, Bielefeld, Germany

Molecular magnetocalorics have been proposed as a replacement to ^{3}He for cryogenic applications, however the search for the best compound for such an application is still ongoing. Specifically, magnetic molecules exhibiting a high adiabatic entropy change in the kelvin and sub-kelvin range are sought after. Such an entropy change could for instance be achieved by a molecule whose ground state is highly degenerate. We investigate three frustrated systems, the centered square, the centered-hexagon, and the double-pyramidal spin models. Their figures of merits and their magnetocaloric effect are discussed.

MA 42.6 Thu 10:45 HSZ/0004

Exchange-biased toroidal moments in a family of homochiral Cu_6Ln_3 complexes studied by high-field EPR — •Jan Arneth[1], Deepanshu Chauhan[2], Sagar Paul[3], Bapan Jana[2], Wolfgang Wernsdorfer[3], Maheswaran Shanmugam[2], Gopalan Rajaraman[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]Department of Chemistry, Indian Institute of Technology Bombay, India — [3]Physikalisches Institut, Karlsruhe Institute of Technology, Germany

The vortex-like arrangement of the individual magnetic moments renders single-molecule toroics (SMT) promising candidates for application in quantum computing, molecular spintronics and the development of magneto-electric coupling in multiferroic devices. Here, we report the magnetic investigation of a family of heterobimetallic nonanuclear Cu_6Ln_3 (Ln = Y,Gd,Dy) clusters, featuring a homochiral Cu_3-Ln_3-Cu_3 triangular core, using combined theoretical *ab-initio*, ac and dc susceptibility, μ-SQUID and high-field EPR studies. Numerical analysis of our experimental data allow for the determination of the microscopic spin Hamiltonian parameters, which reveal an antiferromagnetic inter-triangular coupling between the two spin-frustrated Cu_3 units. In particular, Cu_6Dy_3 exhibits both single-molecule magnet (SMM) and SMT behaviour with a non-magnetic ground state persisting up to magnetic fields as high as $B \simeq 1.3$ T. The large excitation gap is found to result from the ferromagnetic Cu-Dy exchange interaction coupling the toroidal Dy_3 unit with the adjacent Cu_3 triangles.

15 min break

MA 42.7 Thu 11:15 HSZ/0004

Fully Quantum-Mechanical Simulations of Spin Crossover Behaviour in an Iron(II) Complex — •Ethan Crawford, Solveig Felton, and David Wilkins — Queen's University Belfast, Belfast, Northern Ireland

Spin-crossover (SCO) complexes change spin state when exposed to external stimuli such as light, temperature or pressure, allowing them to be used as sensors or magnetic memory devices. Predicting with precision when a crossover occurs would bring the technology closer to fruition, but it remains a significant challenge. Single-point energy calculations using Density Functional Theory (DFT) have been employed with limited accuracy, because they neglect the vibrational and other entropic contributions present at finite temperatures. Furthermore, a given calculation setup is not necessarily transferable to another complex. We trained a committee neural network potential (c-NNP) using data generated via Ab Initio Molecular Dynamics for an Iron (II) SCO complex. Two c-NNPs were trained, to model both the highest and lowest spin states respectively, encompassing all intramolecular interactions. The models were systematically improved using the query by committee approach. These systems were extended from a single complex to a bulk system combining the c-NNPs with a classical forcefield to account for the intermolecular interactions. The spin state for each complex is individually assigned to simulate experimental transitions. During the transition window, neither model can accurately predict the behaviour of the complex, but combining the three forcefields should replicate experimental behaviour.

MA 42.8 Thu 11:30 HSZ/0004

Symmetric finite-temperature Lanczos method for anisotropic magnetic molecules — •Jürgen Schnack — Bielefeld University, Faculty of Physics, Bielefeld, Germany

The finite-temperature Lanczos method (FTLM) constitutes a valuable approximation scheme for Hilbert space problems that exceed the dimension tractable by complete numerical diagonalization [1,2]. Several large magnetic molecules have been successfully modeled using FTLM [3]. It has been noted earlier that the method converges best for problems where the z-component of total spin commutes with the Hamiltonian. For anisotropic Hamiltonians the convergence is much poorer [4]. Here, we discuss conceptional improvements [5] as well as realizations on nowadays supercomputing architectures that employ CPUs as well as GPUs.

[1] J. Jaklic, P. Prelovsek, Phys. Rev. B 49, 5065 (1994). [2] J. Schnack, J. Richter, R. Steinigeweg, Phys. Rev. Research 2, 013186 (2020). [3] T. Tziotzi, D. Gracia, S. Dalgarno, J. Schnack, M. Evangelisti, E. Brechin, C.J. Milios, JACS 145, 7743 (2023). [4] O. Hanebaum, J. Schnack, Eur. Phys. J. B 87, 194 (2014). [5] M. Aichhorn, M. Daghofer, H. G. Evertz, W. von der Linden, Phys. Rev. B 67, 161103(R) (2003).

MA 42.9 Thu 11:45 HSZ/0004

Investigation of Magnetic Properties of Ce-Doped Ni-Based Composites as Near Infrared Absorbers Based on Soft-XAS and XMCD Measurements — •Timuçin Emre Tabaru[1], Ali Karatutlu[2], Iremnur Duru[1], and M. Fatih Kilicaslan[3] — [1]Department of Electrical Electronics Engineering, Sivas University of Science and Technology, 58000 Sivas, Turkey — [2]National Nanotechnology Research Center (UNAM), Bilkent University, Ankara 06800, Türkiye — [3]Department of Engineering Fundamental Sciences, Sivas University of Science and Technology, 58000 Sivas, Turkey

In this study, the X-ray Magnetism Circular Dichroism (XMCD) spectra of Ni-based composites produced by melt spinning and rapid solidification with ~75% Ni, ~10% Cr, ~8% Si, ~5% Fe, ~2% B, and 1% Ce doping were determined according to different Fe and Cerium (Ce) contents using soft X-ray absorption spectroscopy (XAS) at the HESEB beamline at the Synchrotron-Light For Experimental Science And Applications In The Middle East (SESAME). The L2 and L3 edges of Ni, Fe, and Ce were investigated for both Ce-doped and undoped samples. The areas under the XAS and XMCD spectra obtained from these measurements were determined, and the spin and orbital magnetic momenta of each sample were calculated. The results confirmed that the materials mentioned exhibit paramagnetic properties, in agreement with the literature. Ni-based composite doped with Ce demonstrated enhanced broadband infrared (IR) absorption, reaching a maximum efficiency of 93% in the 3-5 μm mid-IR window and maintaining over 80% absorption across the entire 3-15 μm spectral range.

MA 42.10 Thu 12:00 HSZ/0004

Magnetic Hexagonal Nanoferrite-Based Electrode: Structural Characterization and Electrochemical Detection of Caffeine in Drinks — •Sajjad Hussain — The Begum Nusrat Bhutto Women University, Sukkur, Sindh, Pakistan

Caffeine is a pharmacologically active alkaloid that is frequently incorporated into a wide range of food and beverage formulations. V-type hexagonal ferrite nanoparticles (SrSnFe*O**-NPs) were prepared through a sol*gel-based green auto-combustion route and analyzed using a range of advanced characterization techniques, including X-ray diffraction (XRD), X-ray absorption fine structure (XAFS), scanning electron microscopy (SEM), atomic force microscopy (AFM), Brunauer*Emmett*Teller (BET) surface area analysis, and vibrating sample magnetometry (VSM). The V-type hexaferrite exhibits a single-phase crystalline structure with an average crystallite size exceeding 30 nm. The local atomic structure was confirmed using XAFS analysis, while the surface morphology and particle size were examined through SEM and AFM. BET was used to confirm the surface area 209.6 m*/g. The magnetic studies revealed soft magnetic behavior. Furthermore, the synthesized V-type hexagonal ferrites were employed to modify a glassy carbon electrode (GCE), developing SrSnFe*O**-NPs/GCE for the electrochemical sensing of caffeine. Cyclic voltammetry studies revealed conductive and diffusion-controlled behavior, with the SrSnFe*O**-NPs/GCE demonstrating high sensitivity and selectivity for caffeine detection (linear ranges: 0.5 to 80 *M; detection limits: 0.025 *M, while the LOQ was 0.078 *M.

MA 42.11 Thu 12:15 HSZ/0004

Strain control of three-dimensional magnetic nanostructures — •José Claudio Corsaletti Filho, Mohammad Sedghi, Elina Zhakina, Markus König, Elena Gati, and Claire Donnelly — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

The study of nanoscale objects in three-dimensions has led to new discoveries and opportunities for technological development. Recent studies have shown that the magnetic landscape of 3D nanostructures can be controlled by geometrical effects, enabling innovations in design and magneto-mechanical devices. Consequently, a method to reversibly tune the properties of a three-dimensional nanostructure is highly desirable. Strain represents a particularly promising approach, as it directly influences the geometry. Indeed, while strain has been extensively applied to magnetic thin films for the tuning of global material properties, there the substrate restricts global strains to 0.7-1%. In this work, we describe how we strained 3D magnetic nanostructures and map out their geometrical changes through in situ electron microscopy. We are able to achieve ultimate strains of up to 20%, but we also identify regimes associated with the elastic and plastic deformations of 3D nanostructures with different geometries. By determining the mechanical properties of the nanowires, we obtain the fundamental insight to achieving reversible tuning of the geometry - and therefore the magnetic properties - of 3D nanostructures. Such reversible tuning will be of key interest for future technological applications.

MA 43: Spin-Dependent Phenomena in 2D

Time: Thursday 9:30–11:15 Location: POT/0112

Invited Talk MA 43.1 Thu 9:30 POT/0112

Defect-Induced Phase Transitions in the 2D Magnetic Semiconductor CrSBr — •Shengqiang Zhou — Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

As an air-stable van der Waals magnetic semiconductor, CrSBr has attracted great research interest due to its exceptional optical, electronic, and magnetic properties [1]. Below its Néel temperature of 132 K, CrSBr exhibits a typical A-type antiferromagnetic order consisting of antiferromagnetically coupled ferromagnetic monolayers [1, 2]. In this talk, I will present the magnetic phase transition from antiferromagnetic to ferromagnetic order in CrSBr induced by ion irradiation [3, 4]. We observe the emergence and subsequent suppression of the ferromagnetic phase in CrSBr as the irradiation fluence increases. Structural analysis combined with first-principles calculations suggests that the formation of interstitials promotes ferromagnetic coupling between the layers. At moderate irradiation fluences, the Curie temperature gradually decreases, reflecting the impact of crystalline degradation. Surprisingly, at even higher irradiation fluences, CrSBr does not amorphize but instead transforms into a new crystalline phase. These findings indicate that, by precisely tuning irradiation parameters and employing lithography techniques, one can selectively modulate the induced ferromagnetism in CrSBr in terms of magnetization strength, critical temperature, and spatial distribution. [1] E.J. Telford, et al. Adv. Mater., 32, 2003240 (2020). [2] F. Long, et al. Appl. Phys. Lett. 123, 222401 (2023). [3] F. Long, et al. Nano Lett. 23, 8468 (2023). [4] F. Long, et al. Adv. Phys. Res., 3, 2400053 (2024)

MA 43.2 Thu 10:00 POT/0112

Electric-field tunable valley excitons in proximity coupled WSe_2/CrI_3 heterostructures — Felix Hellenkamp[1], •Yiheng Li[1], Marc Schütte[1], Kenji Watanabe[2], Takashi Taniguchi[3], Lutz Waldecker[1], Christoph Stampfer[1,4], and Bernd Beschoten[1] — [1]2nd Institute of Physics and JARA-FIT, RWTH Aachen University, Germany — [2]National Institute for Materials Science, Tsukuba, Japan — [3]International Center for Materials Nanoarchitectonics, NIMS — [4]PGI-9, Forschungszentrum Jülich, Jülich, Germany

Two-dimensional (2D) transition metal dichalcogenides have attracted significant interest due to their unique optical properties. The possibility to address the K and K' valley selectively via σ^+ and σ^- polarized light enables optical initialization and readout of the valley degree of freedom. The valley degeneracy can be lifted via magnetic proximity coupling to a 2D magnet such as CrI_3. However, in the heterostructures the resulting exciton splitting lacks tunability, limiting its applicability in device architectures that demand adjustable valley splitting. Our work shows a large tunability of the exciton splitting in a WSe_2/CrI_3 heterostructure via external displacement fields. Reflection contrast measurements show a displacement field induced change in the exciton resonance energy which is asymmetric with respect to the excitons at the K and K' valleys, leading to a 35% increase in exciton splitting at a displacement field of -0.4V/nm. We attribute the change in resonance energy to a reduction in the optical bandgap, caused by a displacement-field-induced modification in the band alignment.

MA 43.3 Thu 10:15 POT/0112

Atomic-scale visualization of quasi-one-dimensional structure and magnetic-field-tunable electronic statesin CrSBr — •Keda Jin[1,2], Tobias Wichmann[1,3], F. Stefan Tautz[1,3], Felix Lüpke[1,4], Jose Martinez-Castro[1,2], and Markus Ternes[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich — [2]Institut für Experimentalphysik II B, RWTH Aachen, 52074 Aachen — [3]Institut für Experimentalphysik IV A, RWTH Aachen, 52074 Aachen — [4]Institute of Physics II, Universität zu Köln, 50937 Köln

The anisotropic two-dimensional (2D) van der Waals magnet CrSBr is famous for hosting a quasi-one-dimensional (1D) electronic structure, but its direct visualisation has remained elusive.

Using low-temperature scanning tunnelling microscopy and spectroscopy, we present the atomic-scale characterisation of this quasi- 1D conduction bands in monolayer CrSBr on $NbSe_2$. Our measurements reveal a spatial anisotropy in the local density of states, confirming the existence of conduction bands that are flat along one crystallographic direction but dispersive along the perpendicular direction. Moreover, we demonstrate that an applied magnetic field reconstructs its electronic structure, showcasing strong magneto-electronic coupling. Our work provides the real-space visualisation of the long-predicted electronic anisotropy and establishes its potential for developing magnetically-tunable low-dimensional electronic devices.

MA 43.4 Thu 10:30 POT/0112

Origin of Exchange Bias in Compensated and Orthogonal Spin Interfaces in vdW Heterostructures — •Aditya Kumar[1], Aravind Balan[1], Patrick Reiser[2], Sadeed Hameed[1], Thibaud Denneulin[3], Rafal E. Dunin-Borkowski[3], Patrick Maletinsky[2], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Staudinger Weg 7, 55128 Mainz, Germany — [2]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [3]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons and Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany

Van der Waals heterostructures formed by mechanical stacking can create atomically flat, defect-free interfaces, yet exhibit exchange bias in expected compen-

sated and orthogonal spin configurations. This work investigates the underlying spin-pinning mechanisms in heterostructures of out-of-plane ferromagnet Fe_3GeTe_2 interfaced with c-type out-of-plane antiferromagnet $MnPS_3$ and in-plane a-type antiferromagnet CrSBr. Using NV magnetometry and STEM holography imaging, we reveal distinct exchange bias origins: the spin reorientation transition in $MnPS_3$ induces large, robust exchange bias, while orthogonal coupling at the Fe_3GeTe_2/CrSBr interface generates circular flux closure domains that produce switchable exchange bias. [1] A. P. Balan et al., Advanced Materials 36, 2403685 (2024). [2] A. Kumar et al., Small 21, e06284 (2025).

MA 43.5 Thu 10:45 POT/0112

Spin-polarized scanning tunneling microscopy of antiferromagnetic spin ordering in a topological Hall material — Alexina Ollier[1,2], Valeria Sheina[1,2], Seik Pak[4], Corina Urdaniz[1,2], Muskan Sande[1,3], Soonhyung Lee[1,2], Lei Fang[1,2], Christoph Wolf[1,2], Woonghee Cho[6], Pyeongjae Park[7], Andreas Heinrich[1,3], Je-Geun Park[6], Moon jip Park[4,5], and •Won-Jun Jang[1,2] — [1]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS), Seoul, Korea — [2]Ewha Womans University, Seoul, Korea — [3]Department of Physics, Ewha Womans University, Seoul, Korea — [4]Department of Physics, Hanyang University, Seoul, Korea — [5]Research Institute for Natural Science and High Pressure, Hanyang University, Seoul, Korea — [6]Department of Physics and Astronomy, Seoul National University, Seoul, Korea — [7]Materials Science and Technology Division, Oak Ridge National Laboratory, Tennessee, USA

We report spin-polarized scanning tunneling microscopy measurements on Co1/3TaS2. STM images acquired with a conventional tip reveal the triangular atomic lattice of the surface, whereas SP-STM uncovers additional symmetry features directly linked to the spin-polarized electronic structure of TaS2 arising from the triple-Q magnetic order. The spin-dependent contrast observed with the SP tip confirms the presence of spin-polarized van Hove singularities, a hallmark of the non-coplanar magnetic state. These results demonstrate that SP-STM can directly probe the modified electronic structure arising from chiral magnetic textures in non-coplanar magnets.

MA 43.6 Thu 11:00 POT/0112

Super-Moiré Spin Textures in Twisted 2D Antiferromagnets — •King Cho Wong[1], Ruoming Peng[1], Eric Anderson[2], Jackson Ross[3], Adam Wei Tsen[4], Elton Santos[3], Xiaodong Xu[2], and Joerg Wrachtrup[1] — [1]3rd Physics Institute, University of Stuttgart, Stuttgart, Germany — [2]University of Washington, Seattle, USA — [3]University of Edinburgh, Edinburgh, UK — [4]University of Waterloo, Canada

Stacking two-dimensional (2D) layered materials offers a platform to engineer electronic and magnetic states. In general, the resulting states - such as Moiré magnetism - have a periodicity at the length scale of the Moiré unit cell. Here, we study magnetic order in twisted double bilayer chromium triiodide (tDB CrI3) by means of scanning nitrogen-vacancy microscopy. We observe long-range magnetic textures extending beyond the single Moiré unit cell, which we dub a super-Moiré magnetic state. At small twist angles, the size of the spontaneous magnetic texture increases with twist angle, opposite to the underlying Moiré wavelength. The spin-texture size reaches a maximum of about 300 nm in 1.1° twisted devices, an order of magnitude larger than the underlying Moiré wavelength. The vector field maps suggest the formation of antiferromagnetic Neel-type skyrmions spanning multiple Moiré cells. The twist angle dependent study combined with atomistic simulations suggests that magnetic competition between the Dzyaloshinskii-Moriya interaction, magnetic anisotropy, and exchange interactions produces the super-Moiré spin orders.

MA 44: Focus Session: Curvilinear magnetism: Magnetics with nanoscale curved geometries (joint session MA/TT)

The behaviour of any physical system is determined by the order parameter whose distribution is governed by the geometry and topology of the physical space of the object, in particular its dimensionality and curvature. Specifically, spin textures, static and dynamic magnetic responses become sensitive to bends and twists in physical space. In this respect, curvature effects emerged as a novel tool to tailor magnetic properties and responses relying on geometric deformations. In magnetism, coupling between geometry of a magnet and magnetic order parameter brings about novel responses of curved thin films, nanowires and nanoparticles and enforces topological constraints on the number and type of magnetic solitons living in a curved space. Curvatures can force a geometry-driven local interactions like Dzyaloshinskii-Moriya interaction (DMI) and anisotropy as well as novel non-local chiral symmetry breaking effects, which were confirmed experimentally using electron holography studies of magnetic cap-shaped structures. Advances in experimental techniques (fabrication and tomographic characterization) allow validating theoretically predicted effects and apply them for functional devices as was demonstrated with geometrically twisted 3D racetracks. Recent highlights of the community include experimental proof of curvature stabilised skyrmions, explorations of curvilinear altermagnets, tailoring magnetic solitons in curvilinear 2D magnets, curvilinear magnetoelectrics, use of curvilinear magnetic architectures to tune superconducting transport, and magnetoionic manipulation of magnetic states in nanostructures to name just a few representative topics, which will be covered at the focused symposium.

Organizers: Denys Makarov, d.makarov@hzdr.de; Paola Gentile, paola.gentile@spin.cnr.it

Time: Thursday 9:30–13:00 Location: POT/0151

Invited Talk MA 44.1 Thu 9:30 POT/0151

2D and 3D racetracks: Interplay of geometric and magnetic chiralities — •Stuart Parkin — Max Planck Institute for Microstructure Physics, Halle (Saale), Germany — Martin Luther University Halle-Wittenberg

Magnetic Racetrack Memory (RTM) is a unique memory-storage device that relies on the current driven motion of multiple domain walls along magnetic conduits that can be arranged either horizontally (2D) or vertically (3D). It has great potential as a high performance, non-volatile memory that has enormous data storage capacity compared to today*s memory technologies. Atomically engineered 2D magnetic racetracks in the form of synthetic antiferromagnets allow for very high current induced motion of nanoscopic chiral domain walls[1]. Recently we have shown that 2D RTM can be scaled to dimensions that are technologically relevant with widths of just ~50 nm[2]. 3D racetracks would allow for the highest density memories. Using a state-of-the-art multi-photon super-resolution lithography system we form 3D scaffolds of arbitrary shapes on which the racetracks can be subsequently deposited. We discuss 3D racetracks that are formed with clockwise and anticlockwise chiral twists and curved cross-sections. The interplay between the geometrical chirality and the spin chirality of the individual domain walls allows for domain wall diode devices [3]. [1] S. S. P. Parkin, S.-H. Yang, Nat. Nanotechnol. 2015, 10, 195. [2] J.-C. Jeon, A. Migliorini, J. Yoon, J. Jeong, S. S. P. Parkin, Science 2024, 386, 315. [3] A. M. A. Farinha, S.-H. Yang, J. Yoon, B. Pal, S. S. P. Parkin, Nature 2025, 639, 67.

Invited Talk MA 44.2 Thu 10:00 POT/0151

Combined MFM/KPFM at the Ultimate Sensitivity Limit for Probing Curvature-Engineered Micromagnetic States — •Emily Darwin[1], Reshma Peremadathil Pradeep[1,2], Luca Berchialla[3], Daniel Rotthardt[1,2], Ales Hrabec[3], and Hans Hug[1,2] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland — [2]Department of Physics, University of Basel, 4056 Basel, Switzerland — [3]aul Scherrer Institut PSI, 5232 Villigen, Switzerland

Curved substrates offer a promising route for tailoring the magnetic properties of multilayer systems, potentially stabilizing topologically non-trivial spin textures such as skyrmions. However, local variations in surface inclination can significantly affect growth conditions, altering crystallographic orientation or even disrupting the multilayer architecture.

In this study, we investigate a Pt/Co/Ru multilayer deposited on a polymer substrate patterned with nanoscale semispherical bumps using a combined single-pass Magnetic Force Microscopy (MFM) and Frequency-Modulated Kelvin Probe Force Microscopy (FM-KPFM) technique. Our system achieves

unprecedented sensitivity to both magnetic and electrostatic interactions. We find that steep, near-vertical walls at the perimeter of hemispherical features locally disorder the multilayer stack, resulting in distinct changes in the contact potential difference. This disruption facilitates magnetic flux return and enables the formation of circular magnetic domains aligned with the external magnetic field on the dome tops.

Invited Talk MA 44.3 Thu 10:30 POT/0151

Curvilinear magnetism in superconducting spintronics — •Sol Jacobsen — Center for Quantum Spintronics, Norwegian University of Science and Technology NTNU, Trondheim, Norway

Replacing semiconductor-based computational components with superconducting elements can give an energy saving of two orders of magnitude. To harness this, we need precise control of the interaction between superconducting and magnetic components. Geometric curvature controls the superconducting transition by affecting spin relaxation and precession in superconductor-magnet heterostructures [1]. To functionalize this in devices, we can dynamically alter the curvature by inducing bending-strain. This can for example lead to electrically controlled superconducting spin-valves, current-reversal, and chirality-dependent ground states in triplet-SQUIDs [1-3]. In this presentation, I will discuss how real-space geometric curvature provides new pathways for manufacturing and controlling the interaction between superconductivity and magnetism in wires and thin films, and anticipate future developments in the field.

[1] Salamone et al, Phys. Rev. B 104 (2021) L060505; 105, (2022) 134511. [2] Salamone et al, Appl. Phys. Lett. 125 (2024) 062602. [3] Skarpeid et al, J.Phys.:Condens.Matter, 36 (2024) 235302.

15 min break

Invited Talk MA 44.4 Thu 11:15 POT/0151

Advanced Control of Magnetic Nanostructures via Metasurface Engineering and Voltage-Driven Functionalities — •Anna Palau — Institut de Ciència de Materials de Barcelona (ICMAB-CSIC)

Understanding and manipulating magnetic micro- and nanostructures are fundamental to advancing technologies in data storage, spintronics, and magnetic sensing. Magnetic metasurfaces have recently attracted significant interest for their ability to locally configure magnetic field distributions and overcome limitations of traditional magnetic imaging techniques. In this work, we demonstrate how metasurfaces enable precise control of vortex motion, coercive fields, and saturation behaviour in magnetic nanostructures without altering their intrinsic anisotropy [1]. We show that metasurfaces can overcome magnetic field constraints in X-ray Photoemission Electron Microscopy (XPEEM), enabling high-resolution imaging of magnetisation states under conditions previously inaccessible. Additionally, we explore electric-field-driven ionic migration as a complementary route for voltage-controlled, non-volatile modulation of magnetic and superconducting properties [2], highlighting new opportunities for energy-efficient control and advanced characterisation. [1] Barrera et al. ACS Nano 19, 10461 (2025), [2] Günkel et al. Small 2411908 (2025), Spasojević et al. Nat. Commun. 16, 1990 (2025)

Invited Talk MA 44.5 Thu 11:45 POT/0151

Magnetic tomography of noncollinear spin textures in curvilinear geometries — •Sandra Ruiz-Gomez — ALBA Synchrotron, Barcelona, Spain

Three-dimensional nanomagnetic systems offer a unique platform for discovering and controlling complex spin textures. Recent advances in 3D nanofabrication, magnetic characterization techniques, and micromagnetic modeling are now enabling precise control of curvature, torsion, and geometry at the nanoscale, opening new routes for engineering spin textures in three-dimensional architectures.

In this talk, I will present our latest results on how geometrical design and 3D architecture can be exploited to tailor the energy landscape of domain walls, manipulate their topological properties, and guide their motion from straight nanowires to more complex curved cylindrical and tubular geometries. By combining state-of-the-art fabrication techniques with high-resolution imaging and theoretical analysis, we identify how curvature can be harnessed to stabilize complex spin textures, enabling deterministic control over their dynamics.

Overall, this work highlights how 3D nanomagnetism can be leveraged to access new regimes of topological control, with implications for next-generation spintronic devices, robust information carriers, and reconfigurable magnetic architectures.

MA 44.6 Thu 12:15 POT/0151

Transferred magnetic nanomembranes for curvilinear magnetism and spintronics — •Olha Bezsmertna[1], Oleksandr Pylypovskyi[1], Rui Xu[1], Mykola Vinnichenko[2], Andrea Sorrentino[3], Daniel Wolf[4], Axel Lubk[4], Peter Fischer[5,6], and Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Institute for Ceramic Technologies and Systems IKTS, 01277 Dresden, Germany — [3]Alba Light Source, MISTRAL beamline, Cerdanyola del Vallès 08290, Spain — [4]Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany — [5]University of California, Santa Cruz, United States — [6]Lawrence Berkeley National Laboratory, Berkeley, United States

The functionality of the magnetic nanomembranes can be extended through controlled transfer processes and geometric design. We show that advanced giant magnetoresistive thin films can be reliably transferred onto various substrates using green chemistry, preserving their structural integrity and magnetic performance, thus enabling mechanically conformal devices for applications where low weight, flexibility, and durability are essential [1]. With the developed technique, we demonstrate fabrication of curvilinear hierarchical magnetic nanotemplates and their subsequent transfer to an appropriate handling support enabling high-resolution transmission microscopy investigations (electron- and x-ray-based) of the impact of geometric curvature on complex magnetic states [2].

References: [1] Bezsmertna et al. Adv. Funct. Mater. 35, 2502947 (2025). [2] Bezsmertna et al. Nano Lett. 24, 15774 (2024).

MA 44.7 Thu 12:30 POT/0151

Magnetic solitons in spherical maghemite nanoshells — •Oleksandr V. Pylypovskyi[1], Gaspare Varvaro[2], Davide Peddis[2,3], Priyanka Mishra[4], Carmine Autieri[4], Filipp N. Rybakov[5], Denis D. Sheka[6], and Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., 01328 Dresden, Germany — [2]CNR-Istituto di Struttura della Materia, 00015 Roma, Italy — [3]Universitá degli Studi di Genova, 1-16146 Genova, Italy — [4]International Research Centre Magtop, Institute of Physics, Polish Academy of Sciences, 02668 Warsaw, Poland — [5]Uppsala University, Uppsala SE-751 20, Sweden — [6]Taras Shevchenko National University of Kyiv, 01601 Kyiv, Ukraine

Topology of the shape of magnetic nanoarchitecture makes a major impact on global properties of its magnetic textures [1,2]. Here, we present a fabrication of maghemite spherical shells and a theoretical analysis of magnetic solitons they host in equilibrium. The ferrimagnetic shells with a radius and shell thickness of about 4 nm and 1.4 nm have a radial easy axis that favors skyrmionic textures. Their ground state corresponds to a 3D onion state with the change of the radial component of magnetization at the equator. In this presentation, we will also report on the localization of magnetic solitons on spherical shells.

[1] V. P. Kravchuk et al., PRB **94**, 144402 (2016); [2] O. M. Volkov, O. V. Pylypovskyi et al., Nat. Commun., **15**, 2193 (2024).

MA 44.8 Thu 12:45 POT/0151

Coherent Spin Waves in Curved Ferromagnetic Nanocaps of a 3D-printed Magnonic Crystal — •Kilian Lenz[1], Huixin Guo[2], Mateusz Golebiewski[3], Ryszard Narkowicz[1], Jürgen Lindner[1], Maciej Krawczyk[3], and Dirk Grundler[2] — [1]Inst. of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]School of Engineering, Institute of Materials,Laboratory of Nanoscale Magnetic Materials and Magnonics, École Polytechnique Fédérale de Lausanne, Switzerland — [3]Institute of Spintronics and Quantum Information, Adam Mickiewicz University, Poznań, Poland

In this work we present ferromagnetic resonance measurements and simulations of a 3D magnonic crystals embedded in an on-chip microresonator. It was realized by two-photon lithography of a 3D woodpile structure and atomic layer deposition of a 30-nm-thin Ni film. Operated near 14 and 24 GHz, the microresonator output revealed numerous coherent magnons with distinct angular dependencies reflecting the underlying face-centered cubic lattice. The micromagnetic simulations show that some of the edge modes are localized at the curved nanocaps and that they remain robust against changes of the field orientation. These cap modes exhibit an unexpected phase evolution. The findings advance the development of functional microwave circuits with 3D magnonic crystals and strengthen their visionary prospects for edge-dominated magnon modes.

MA 45: Magnetic Relaxation and Gilbert Damping

Time: Thursday 9:30–11:00 Location: POT/0351

MA 45.1 Thu 9:30 POT/0351

Nonlinear magnon-magnon coupling in a ferrimagetic YIG sphere at cryogenic temperatures — •Johannes Weber[1,2], Richard Schlitz[3], Sebastian T. B. Goennenwein[3], Matthias Althammer[1,2], and Hans Huebl[1,2,4] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]TUM School of Natural Sciences, Technische Universität München, Garching, Germany — [3]Department of Physics, University of Konstanz, Konstanz, Germany — [4]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany

Yttrium ion garnet (YIG) is known for its low magnetic damping properties, which are optimized in single crystalline YIG spheres, making it a potent candidate for nonlinear magnonics. The magnetic spectrum shows numerous so called Walker modes. Here, we present two-tone pump and probe microwave spectroscopy measurements of the magnetization dynamics of a 250 μm YIG sphere. The data shows signatures of three-magnon scattering, when the drive exceeds the first order Suhl instability threshold. We quantitatively analyze the underlying non-linearity for different Walker modes. These experiments enable a pathway for probing quantum signatures in magnetic systems.

MA 45.2 Thu 9:45 POT/0351

Evidence of relativistic field-derivative torque in nonlinear THz response of magnetization dynamics — •Arpita Dutta[1], Pratyay Mukherjee[6], Swosti P. Sarangi[1], Somasree Bhattacharjee[6], Christian Tzschaschel[2,3], Debankit Priyadarshi[3], Kouki Mikuni[4], Takuya Satoh[4,5], and Ritwik Mondal[6] — [1]NISER Bhubaneswar, HBNI, Jatni, India — [2]Max-Born Institute, Berlin, Germany — [3]ETH Zurich, Switzerland — [4]Institute of Science Tokyo, Japan — [5]Quantum Research Center for Chirality, Okazaki, Japan — [6]IIT (ISM) Dhanbad, India

The selective addressing of spins by THz electromagnetic fields via Zeeman torque is one of the most successful means of controlling magnetic excitations. Here, we show that the conventional Zeeman torque on the spin is not sufficient, rather an additional relativistic field derivative torque is essential to realize the observed magnetization dynamics. We accomplish this by exploring the ultrafast nonlinear magnetization dynamics of a ferrimagnetic garnet when excited by two co-propagating THz pulses. Having identified the Kaplan-Kittel mode at 0.48 THz, resulting from the exchange interaction, we drive this to a nonlinear regime. We find that the observed nonlinear trace of the magnetic response cannot be mapped to the magnetization precession induced by the Zeeman torque, while the Zeeman torque supplemented by an additional FDT follows the experimental evidences.

MA 45.3 Thu 10:00 POT/0351

Quantum Landau-Lifshitz-Gilbert equation — •Yuefei Liu — Nordita, Stockholm University and KTH Royal Institute of Technology, SE-10691 Stockholm, Sweden — Center for Quantum Spintronics, Department of Physics, NTNU, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

The classical Landau-Lifshitz-Gilbert (LLG) equations describe magnetization dynamics. Extending them to quantum systems is difficult, but we introduce an effective equation that is considered as a quantum analog of LLG equation [PRL 133, 266704 (2024)]. It reproduces classical features for ferromagnetically coupled spin-1/2 dimers, yet deviates strongly in antiferromagnetic and entangled cases, suggesting a new paradigm beyond Lindblad-type master equations.

MA 45.4 Thu 10:15 POT/0351

Temperature dependence of volume and interface contributions to the magnetic damping of Permalloy thin films — Verena Ney[1], Kilian Lenz[2], Fabian Ganss[2], René Hübner[2], Jürgen Lindner[2], and •Andreas Ney[1] — [1]Johannes Kepler Universität, Linz, Österreich — [2]Helmholtz-Zentrum Dresden-Rossendorf, Deutschland

The magnetic damping of $Ni_{80}Fe_{20}$ (Permalloy, Py) thin films has been reported to be lowest when sandwiched in Al cap and spacer layers [1]. Here we study the Gilbert damping parameter α as a function of Py layer thickness via temperature- and frequency-dependent ferromagnetic resonance (FMR) experiments. The full FMR dataset allows to separate the Gilbert-like contributions to the FMR linewidth from non-Gilbert-like ones like two magnon scattering processes. In addition, the Py thickness series allows to deconvolute α into its respective bulk and interfacial contributions and their respective temperature dependencies. While the bulk contribution monotonously decreases with temperature from 0.0061(1) down to 0.0054(1), the interfacial contribution shows a subsequent increase at low temperature. The remaining bulk contribution, which is only of resistivity-like character, can be considered to reflect the intrinsic magnetic damping properties of Py thin films, while the interface contribution contains both resistivity- and conductivity-like contributions [2].

[1] V. Ney et al. Phys. Rev. Materials **8**, 124410 (2024)
[2] V. Ney et al. Phys. Rev. Materials (submitted, 2025)

MA 45.5 Thu 10:30 POT/0351

Thickness-dependent modulation of magnetization dynamics in ultralow-damping Co_2MnSi Heusler alloys measured by ultrafast TR-MOKE — •Levi Geier[1], Anulekha De[1], Anna Maria Friedel[1,2], Philipp Pirro[1], Martin Aeschlimann[1], and Georg von Freymann[1,3] — [1]RPTU University Kaiserslautern-Landau — [2]Institut Jean Lamour, UMR CNRS 7198, Université de Lorraine, 54000 Nancy, France — [3]Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern

We measure the laser-induced ultrafast demagnetization and subsequent damped precession of the magnetization dynamics in Co_2MnSi Heusler alloys of varying thicknesses (4 nm - 18 nm). The study is performed by a time-resolved magneto-optical Kerr effect (TR-MOKE) setup based on an all-optical pump-probe approach. An ultralow effective damping down to an effective Gilbert damping constant $\alpha = 0.004$ is measured for the 18-nm-thick sample, which increases with decreasing applied magnetic field and increasing pump fluence. We attribute this trend to the generation of incoherent magnons in addition to the coherent magnons after excitation by the laser pulse. Moreover, we observe a strong dependence of the effective damping parameter on the film thickness. The effective damping decreases significantly with increasing film thickness, presumably due to two-magnon scattering. Interestingly the quenching of the magnetization during the demagnetization does not change significantly with pump fluence.

MA 45.6 Thu 10:45 POT/0351

Systematic Theory of Real-Time Atomistic Spin Dynamics — •Sarah Damerow and Michael Potthoff — I. Institute of Theoretical Physics, University of Hamburg

We present a systematic response-theoretical approach for deriving indirect interactions and novel couplings in the effective dynamics of classical spins coupled to generic lattice-fermion models. Via a systematic twofold expansion of the exact time evolution operator, namely in the coupling strength and in the retardation time, one identifies a rich variety of spin-, orbital-, and site-dependent contributions to the equations of motion. These include the familiar Ruderman–Kittel–Kasuya–Yosida and the Dzyaloshinskii–Moriya interactions. Additional anisotropic terms, different types of Gilbert damping and of geometrical spin torques, as well as various spin-inertia terms emerge. While the order of expansion suggests the order of magnitude of the effects, symmetry analysis allows for their classification. The practical feasibility of the approach is demonstrated with numerical results obtained for a Chern insulator.

MA 46: Magnetic Imaging Techniques II

Time: Thursday 9:30–10:45 Location: POT/0361

MA 46.1 Thu 9:30 POT/0361

Spin-Disorder-Induced Angular Anisotropy in Polarized Magnetic Neutron Scattering — Ivan Titov, •Venus Rai, and Andreas Michels — Department of Physics and Materials Science, University of Luxembourg, 162A Avenue de la Faiencerie, 1511 Luxembourg

We experimentally report a hitherto unseen angular anisotropy in the polarized small-angle neutron scattering (SANS) cross section of a magnetically strongly inhomogeneous material [1]. Based on an analytical prediction using micromagnetic theory, the difference between the spin-up and spin-down SANS cross sections is expected to show a spin-disorder-induced anisotropy. The effect is particularly pronounced in inhomogeneous magnetic materials, such as nanoporous ferromagnets, magnetic nanocomposites, or steels, which exhibit large nanoscale jumps in the saturation magnetization at internal pore-matrix or particle-matrix interfaces. Analysis of the experimental neutron data constitutes a method for determining the exchange-stiffness constant. Our results for the nuclear-magnetic interference terms contained in the polarized magnetic neutron scattering cross section might also be of relevance to other neutron techniques.

[1] I. Titov, M. Bersweiler, M. P. Adams, E. P. Sinaga, V. Rai, Š. Liščák, M. Lahr, T. L. Schmidt, V. M. Kuchkin, A. Haller, K. Suzuki, N.-J. Steinke, D. A. Venero, D. Honecker, J. Kohlbrecher, L. F. Barquín, and A. Michels, Phys. Rev. Lett. **135**, 196706 (2025)

MA 46.2 Thu 9:45 POT/0361

Beam focusing with nested mirror optics(NMO) at RESEDA — •Florian Schönleitner[1,2], Denis Mettus[2], Johanna Jochum[2], and Christian Pfleiderer[1,2] — [1]Physik-Department, Technische Universität München, Germany — [2]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching, Germany

The RESEDA(REsonance Spin Echo for Diverse Applications) instrument is a spectrometer that can use the MIEZE(Modulated IntEnsity with Zero Effort) method, a variant of neutron spin echo(NSE) that uses radio frequency(RF) spin flippers instead of static magnetic fields and that can measure samples that depolarise the beam. As a next step for improving the experimental setup it was proposed that nested mirror optics should be integrated to focus the beam at varios components of the instrument. Focusing the beam at the sample might allow measurements of samples with smaller sizes, such as samples in a diamond anvil cell. It also might allow for measurements at higher scattering angles, as it could reduce phase aberrations for the MIEZE method. Focusing the beam at the RF-flippers allows to build smaller AC-coils, leading to higher accessible frequencies, and consequently might lead to a better energy resolution of the spectrometer. In order to create an efficient setup that does not introduce additional artifacts, careful consideration of all effects caused by inserting NMO is necessary. Here we will present preliminary results of the simulations of NMO integration and discuss their potential.

MA 46.3 Thu 10:00 POT/0361

Towards Halbach spheres - Icosahedral symmetry is not just cool anymore — •Ingo Rehberg[1] and Peter Blümler[2] — [1]Experimental Physics, University of Bayreuth, Germany — [2]Institute of Physics, University of Mainz, Germany

Halbach spheres [e.g.1] are an ideal theoretical solution for generating homogeneous magnetic fields. Experimentally, a continuous magnetisation profile is difficult to realise, and the inaccessibility of the sphere's interior favours the use of Halbach rings [2,3]. An alternative is to arrange discrete magnets on the surface of a sphere. Regular polyhedra with a high degree of symmetry are well suited to approximate spherical Halbach configurations [3,4]. Icosahedral symmetry is especially effective at producing uniform magnetic fields (4th order saddle points).

[1] Peter Blümler and Helmut Soltner, Practical Concepts for Design, Construction and Application of Halbach Magnets in Magnetic Resonance. Appl. Magn. Reson. 54, 1701 (2023).

[2] Ingo Rehberg and Peter Blümler, Analytic approach to creating homogeneous fields with finite-size magnets, Phys. Rev. Appl. 23, 064029 (2025).

[3] Ingo Rehberg and Peter Blümler, Halbach two point oh: Optimize uniform fields with clusters and rings of permanent magnets. https://doi.org/10.5281/zenodo. 15006677 (2025).

[4] Ingo Rehberg, Dipole Cluster Inspector - A Duty-Free Python GUI for Exploring 569 Magnetic Configurations. https://doi.org/10.5281/zenodo. 10084573 (2025).

MA 46.4 Thu 10:15 POT/0361

Shaken, not stirred: Using vibrations for sub-10nm resolution scanning X-ray microscopy imaging — •Simone Finizio, Benjamin Watts, Benedikt Rösner, and Jörg Raabe — Paul Scherrer Institut, Villigen PSI, Switzerland

In order to fully exploit the significantly higher coherent photon flux offered by the novel diffraction-limited light sources for high-resolution imaging, scanning microscopy techniques need to tackle imaging overheads and the unavoidable vibrations at the nanometric scales, both hindering the achievement of sub-10nm resolutions in routine conditions.

In most scanning microscopy endstations, significant effort and expense is dedicated to fight these unavoidable vibrations. In this work, we propose to stop fighting vibrations, and instead harness their potential to provide a uniform sampling at the nanoscale. This is achieved by relaxing the positioning precision requirements and sampling the position of the sample with a fast (10 kHz) clock, significantly above the mechanical eigenfrequencies of the sample assembly. An image is then created by binning the recorded positions and photon counts according to a user-defined pixel size. With this method, the routine imaging of sub-10nm features could be demonstrated.

MA 46.5 Thu 10:30 POT/0361

Magnetic interactions and magnetic field distributions in van der Waals heterostructures with Fe_3GeTe_2 — •Joachim Dahl Thomsen[1], Qianqian Lan[1], Eva Duft[1], Zdeněk Sofer[2], Nikolai Kiselev[3], and Rafal Dunin-Borkowski[1] — [1]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons, Forschungszentrum Jülich, Jülich, Germany — [2]Department of Inorganic Chemistry, University of Chemistry and Technology Prague, Prague, Czech Republic — [3]Peter Grünberg Institute and Institute for Advanced Simulations, Forschungszentrum Jülich, Jülich, Germany

Magnetic van der Waals (vdW) materials are promising for memory and logic applications because their properties are highly tunable and they integrate readily into heterostructures that exploit proximity and interlayer effects. However, depth-resolved imaging of interlayer coupling is challenging in plan-view, where contrast is integrated through the sample. Here we use cross-sectional Fe_3GeTe_2 (FGT)/graphite/FGT heterostructures to probe coupling between vertically stacked FGT layers across separations of 0-110 nm. We use Lorentz TEM and off-axis electron holography to visualize the domain structure and map the magnetic field inside and outside the vdW heterostructures, resolving how the interaction evolves with spacer (graphite) thickness. We find that domain alignment between FGT flakes is set by their separation, and that a weak interaction persists even at a separation of 110 nm. These measurements provide design guidance for vdW heterostructure devices that rely on controlled interlayer interactions between magnetic textures.

MA 47: Altermagnets V

Time: Thursday 15:00–18:00 Location: HSZ/0002

MA 47.1 Thu 15:00 HSZ/0002

Electronic correlations and non-colinear spins driving chirality-induced spin selectivity — Jacek Herbrych[1], Nicole Naber[2], and •Maria Daghofer[2] — [1]Wroclaw University of Science and Technology, Wroclaw, Poland — [2]FMQ, Universität Stuttgart, Stuttgart, Germany

Starting from a non-interacting p-orbital model for helical organic molecules, we look at the impact of onsite Hubbard and Hund's-rule interactions. We find that they can induce an orbital-selective Mott transition as well as a block spiral with non-colinear helical magnetic order. We then investigate the resulting chiral bands and find them to be partially spin polarized, a manifestation of p-wave magnetism. Using density-matrix renormalization group, cluster perturbation theory and Monte-Carlo methods, we find that small spin-orbit coupling together with strong correlations robustly leads to spin-polarized bands, even at moderately high temperature and for short correlation lengths. We thus propose this combination as an explanation of chirality-induces spin selectivity and also discuss the interplay of such non-colinear spin patterns with magnetised leads.

MA 47.2 Thu 15:15 HSZ/0002

Chiral phonon-electron interaction in altermagnets — •Armando Consiglio[1], Giancarlo Panaccione[1], and Domenico Di Sante[1,2] — [1]CNR-Istituto Officina dei Materiali (IOM), Unità di Trieste, Strada Statale 14, km 163.5, 34149 Basovizza (TS), Italy — [2]Department of Physics and Astronomy, University of Bologna, 40127 Bologna, Italy

The recent discovery of altermagnetism has opened new frontiers in condensed matter physics, bridging the behaviour of collinear antiferromagnets and ferromagnets. Altermagnetic materials exhibit zero net magnetization while hosting spin-split electronic bands, suggesting novel couplings between lattice and electronic degrees of freedom with potential implications for chiral phonon formation and magneto-phononic effects. In this study, we focus on MnTe and CrSb and present two main results. First, we identify signatures of chiral phonons in the presence of altermagnetic order. Second, we analyze the coupling between these chiral phonon modes and the low-energy electronic states of the compounds, revealing new magneto-phononic interactions. The work provides insight into the interplay between spin order and lattice dynamics in altermagnetic materials, highlighting their potential for novel spintronic and phononic functionalities.

MA 47.3 Thu 15:30 HSZ/0002

Spin polarized optical excitation in altermagnetic RuO_2 — •Paul Herrgen[1], Luca Haag[1], Stephan Wust[1], Marius Weber[1], Akashdeep Akashdeep[2], Mathias Kläui[2], Gerhard Jakob[2], Hans Christian Schneider[1], Benjamin Stadtmüller[3], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany — [3]Institute of Physics, University of Augsburg, 86159 Augsburg, Germany

Altermagnetic materials open new avenues for spintronic applications in compensated magnets due to the spin-split band structure. This unconventional electronic configuration enables access to spin-polarized, all-optical excitation despite the absence of a net magnetization.

In this work, we experimentally probe optically induced spin polarization in the altermagnetic material candidate RuO_2 [1]. The out-of-plane Néel vector of the system allows for the detection of the induced spin polarization via polar magneto-optical Kerr effect (MOKE) measurements. In light of the ongoing debate surrounding the altermagnetic nature of RuO_2, we conducted a systematic study across a range of film thicknesses. Our results show that altermagnetic behavior is observable only in the thinnest films, while increasing thickness leads to a progressive suppression of the characteristic altermagnetic response.

[1]: Weber et al., arXiv:2408.05187 (2024)

MA 47.4 Thu 15:45 HSZ/0002

Non-collinear achiral altermagnetic semiconductor — •Mengli Hu[1], Mikel Iraola[1], Paul McClarty[2], Jeroen van den Brink[1,3], and Maia G. Vergniory[4,5] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, Helmholtzstraße 20, 01069 Dresden, Germany — [2]Laboratoire Léon Brillouin, CEA, CNRS, Université Paris-Saclay, CEA-Saclay, 91191 Gif-sur-Yvette, France — [3]Würzburg-Dresden Cluster of Excellence Ct.qmat, Technische Universitat Dresden, 01062, Dresden, Germany — [4]Département de Physique et Institut Quantique, Université de Sherbrooke, Sherbrooke, J1K 2R1 Québec, Canada. — [5]Donostia International Physics Center, 20018 Donostia-San Sebastian, Spain

Altermangnets (AMs) constitute a novel family of magnetic materials characterized by the absence of net magnetization and the presence of spin-polarized band structures. Whereas AM phases were initially proposed in collinear structures, the recently discovered noncollinear chiral AMs stand out for their distinct hedgehog spin texture and multifunctionality in spintronics. In this work, we deepen the characterization of these systems by constructing a Landau theory for noncollinear achiral AMs. Furthermore, we demonstrate that the achiral symmetry of the crystal is reflected in the spin texture in reciprocal space, which presents only spatial-even multipoles. These multipoles, distinguished from those in collinear AMs via the high-order secondary order parameters, can couple to many phenomena. Our results suggest non-collinear achiral AMs as a promising platform for spintronics applications due to the potential to achieve various spin textures.

MA 47.5 Thu 16:00 HSZ/0002

Circular Dichroism in Resonant Photoelectron Diffraction on Altermagnetic MnTe Films — •Lena Hirnet, Marco Dittmar, Maximilian Ünzelmann, and Friedrich Reinert — Exp. Physik VII and Würzburg-Dresden Cluster of Excellence ctd.qmat, Universität Würzburg, Germany

Altermagnets have lately attracted great attention combining antiferromagnetic spin alignment in real space with a momentum-dependent spin polarization of the electronic states in the band structure. One of the proposed altermagnet work horse materials is MnTe [1,2]. Recently, it has been theoretical predicted that the circular dichroism observed in resonant photoelectron diffraction patterns serves as a direct probe of the altermagnetic sublattice texture [3]. Here, we present resonant photoemission experiments conducted at soft x-ray photon energies corresponding to the Mn $L_{2,3}$ absorption edge. In the corresponding photoelectron diffraction pattern, we can identify the scattering processes of electrons — photoexcited from the Mn-3d states — with the surrounding sublattice atoms. In particular, we find Mn-Mn and Mn-Te forward-scattering peaks and will discuss their dichroic texture which compares very well with the theoretical calculations [3].

[1] L. Šmejkal *et al.*, Phys. Rev. X **12**, 031042 (2022)
[2] J. Krempaský *et al.*, *Nature* **626**, 517-522 (2024)
[3] P. Krüger, Phys. Rev. Let **135**, 196703 (2025)

MA 47.6 Thu 16:15 HSZ/0002

Atomic altermagnetism — •Rodrigo Jaeschke-Uiergo[1], Venkata K. Bharadwaj[1], Warlley Campos[2], Ricardo Zarzuela[1], Nikolaos Biniskos[3], Rafael M. Fernandes[4], Tomáš Jungwirt[5], Jairo Sinova[1], and Libor Šmejkal[2,6,1,5] — [1]Johannes Gutenberg Universität, Mainz, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]Charles University, Prague, Czech Republic — [4]University of Illinois Urbana-Champaign, Urbana, USA — [5]Czech Academy of Sciences, Prague, Czech Republic — [6]Max Planck Institute for Chemical Physics of Solids, Dresden Germany

Altermagnetism has recently been verified experimentally in MnTe and CrSb, which feature two sublattices with antiparallel magnetic dipole moments. In this talk, I will introduce the concept of atomic altermagnetism, a form of ferroic higher-order partial waves of the atomic spin density. Using spin-symmetry analysis and a partial-wave decomposition of first-principles spin densities, we demonstrate such non-dipolar spin order in MnTe, CrSb and KV_2Se_2O, where it coexists with the Néel order. In the Mott insulator Ba_2CaOsO_6, we uncover a striking case of pure atomic altermagnetism, which is entirely absent of dipolar sublattice order. These results show that altermagnetism can occur without Néel order. Finally, I will show that KV_2Se_2O and Ba_2CaOsO_6 are predicted to host giant spin-splitter angles of up to 42° and 26°, respectively demonstrating that strong altermagnetic responses can emerge without requiring the staggered Néel order of local dipole moments.

15 min break

MA 47.7 Thu 16:45 HSZ/0002

High-field magnetotransport and quantum oscillations in altermagnetic CrSb — •Sajal Naduvile Thadathil[1,2], B. V. Schwarze[1], T. Kotte[1], M. Uhlarz[1], C. Muller[3,4], P. Ritzinger[3,4], K. Vyborny[3], T. Speliotis[5], J. Pospisil[4], R. G. Hernandez[6], H. Reichlova[3], D. Kriegner[3], J. Wosnitza[1,2], and T. Helm[1] — [1]Dresden High Magnetic Field Laboratory (HLD-EMFL), HZDR, Germany — [2]Institute of Solid-State and Materials Physics, TU Dresden, Germany — [3]Institute of Physics ASCR, Czech Republic — [4]Charles University, Czech Republic — [5]Institute of Nanoscience and Nanotechnology, Greece — [6]Universidad del Norte, Colombia

Within the family of altermagnets, CrSb is a metallic, collinearly ordered material that exhibits particularly strong symmetry-induced spin splitting in its band structure. In this study, we combine electrical magnetotransport measurements up to 70 T on microfabricated single-crystalline CrSb with first-principles calculations to investigate its Fermi surface. Our experiments reveal a non-saturating magnetoresistance and nonlinear Hall resistivity consistent with multiband charge transport. Notably, we report the observation of Shubnikov-de Haas quantum oscillations in CrSb. Band-structure calculations, when compared with our measurements, accurately reproduce the expected Fermi-surface geometry. These results confirm the predicted electronic band structure of CrSb, establish robust multi-charge-carrier transport at high fields, and highlight the importance of high-field experiments for mapping electronic band structures of altermagnets.

MA 47.8 Thu 17:00 HSZ/0002

Altermagnetism in RuO_2? An experimental study on strain and stoichiometry in heterostructures — •Maik Gaerner[1], Niklas Schmolka[1], Alexander Weissbach[2], Joachim Wollschläger[2], Karsten Rott[1], Jan Schmalhorst[1], Martin Wortmann[3], and Günter Reiss[1] — [1]Bielefeld University, Germany — [2]Osnabrück University, Germany — [3]Bielefeld University of Applied Sciences and Arts, Germany

RuO_2 is a widely studied altermagnetic candidate material, but its magnetic ground state remains actively debated. While some studies find little to no evidence of altermagnetic order in RuO_2 thin films [1,2], others report on clear signatures of altermagnetism [3]. Strain and stoichiometry are widely regarded as key parameters for electronic and magnetic properties of RuO_2 [4,5].

Here, we analyze the impact of strain as well as stoichiometry on the appearance of altermagnetic order in RuO_2. Therefore, we investigate RuO_2 heterostructures, probing e.g. spin-torques and tunnel magneto-resistance. Through an accompanying, systematic X-ray photoelectron spectroscopy study, we analyze the thermal instability of oxidation states in the near surface region to elucidate the role of process temperature in the production of heterostructures.

[1] Akashdeep et al., arXiV:2510.08064 (2025)
[2] Jechumtál et al., arXiV:2508.11481 (2025)
[3] Noh et al. Phys., Rev. Lett. 134, 246703 (2025)
[4] Brahimi et al., J. Phys. Condens. Matter 37 395801(2025)
[5] Smolyanyuk et al., Phys. Rev. B 109, 134424 (2024)

MA 47.9 Thu 17:15 HSZ/0002

Altermagnetic non-reciprocal magnon transport in insulating d-wave orthoferrites — •Jonas Köhler[1], Edgar Galindez-Ruales[1], Shixun Cao[2], Ulrich Nowak[3], Gerhard Jakob[1], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany. — [2]Materials Genome Institute, Institute of Quantum Science and Technology, International Center for Quantum and Molecular Structures, Shanghai University, 99 Shangda Road, Shanghai, 200444, China. — [3]Fachbereich Physik, Universität Konstanz, Universitätsstr. 10, Konstanz, 78457, Germany.

Altermagnetic materials have recently been predicted to host unique magnonic phenomena, including chiral magnon modes, anisotropic magnon lifetimes, and spin transport without additional symmetry breaking by magnetic fields [1].

We present non-local transport in the insulating rare-earth orthoferrites $LuFeO_3$ and $YFeO_3$. We observe a non-zero magnon spin-transport signal for the Spin-Hall-injected magnons, indicating a field-free spin-biased magnon transport. Using thermal excitation via the Spin-Seebeck effect, we observe a strong directional dependence. The signal in the $\Gamma - U$ direction has the opposite sign from the one in the $\Gamma - U'$ direction, while it vanishes along and perpendicular to the easy axis, suggesting a suppression along those crystallographic directions. This shows the altermagnetic spin split magnons, and we can reproduce the observation with an atomistic spin dynamics model.

[1] L. Šmejkal, Phys. Rev. Lett., 2023, 131, 256703.

MA 47.10 Thu 17:30 HSZ/0002

Magnetic structure and the detwinning effect under applied magnetic field in the altermagnet α-MnTe — •Feihao Pan[1], Yishui Zhou[1], Sabreen Hammouda[1], Yinghao Zhu[1], Soohyeon Shin[1], Karin Schmalzl[2], Wolfgang Schmidt[2], Eric Ressouche[3], Oscar Ramon Fabelo Rosa[4], and Yixi Su[1] — [1]Jülich Centre for Neutron Science (JCNS) at the Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich, Lichtenbergstrasse 1, D-85747 Garching, Germany — [2]Jülich Centre for Neutron Science (JCNS) at ILL, Forschungszentrum Jülich, F-38000 Grenoble, France — [3]IRIG, CEA and Université Grenoble Alpes, CEA Grenoble, F-38054 Grenoble, France — [4]Institut Laue-Langevin, 71 avenue des Martyrs, 38042 Grenoble Cedex 9, France

Altermagnetism has garnered significant interest due to spin splitting without relativistic spin-orbit coupling and its promising applications in spintronics. We have recently carried out a detailed single-crystal neutron diffraction study of α-MnTe under applied in-plane magnetic field. We found that a moderate field can generate a strong detwinning effect of magnetic domains. The determination of the magnetic structure of α-MnTe, carried out under both the twined and detwinned conditions, allows us to conclude that the magnetic moment of Mn is indeed colinearly ordered and is uniquely aligned along the crystallographic [1,1,0] direction. This important finding can pave the way for future investigations of altermagnetic phenomena, such as chiral magnon splitting and unconventional spin transport, in α-MnTe under almost detwinned conditions via a wide range of experimental probes.

MA 47.11 Thu 17:45 HSZ/0002

Altermagnetism from the point of view of Mössbauer spectroscopy and other local probes — •Felix Seewald[1], Tillmann Weinhold[1], Cornelius Herrmann[1], Jan Friedrichsen[1], Domenic Nowak[2], Rowena Wachtel[2], Rajib Sarkar[1], Sabine Wurmehl[2], and Hans-Henning Klauss[1] — [1]IFMP, TUD Dresden University of Technology — [2]Leibniz Institute for Solid State and Materials Research, IFW, Dresden

Altermagnetism has emerged as a hot topic of interest in solid state magnetism during recent years. Altermagnets combine a compensated antiferromagnetic structure with spin-split electronic bands. [1, 2]

We want to discuss what one can learn about altermagnetism from (nuclear) local probe spectroscopy, focusing mainly on Mössbauer spectroscopy (MBS) and NMR/NQR.

Depending on the type of altermagnet and the easy axis of the antiferrromagnetic order, local probes can prove or disprove the altermagnetic order. For d-wave altermagnets in Mössbauer spectroscopy and NMR/NQR studies the interplay between the local electric field gradient and the local magnetic hyperfine field may directly differentiate the altermagnetic sites.

We wull discuss Mössbauer spectroscpy as well as NMR/NQR studies on candidates FeF_2, FeF_3, $La_2O_2FeMnOSe_2$ and furthermore highlight the challenges and restrictions they are connected with.

[1] L. Smejkal et al., Phys. Rev. X 12, 031042 (2022)
[2] Fender et al., J. Am. Chem. Soc., 147, 2257-2274 (2025)

MA 48: Magnonics II

Time: Thursday 15:00–18:00 Location: HSZ/0004

MA 48.1 Thu 15:00 HSZ/0004

Linear and nonlinear zero-field spin waves in transversally magnetised low-damping, half-metallic Co_2MnSi waveguides — •Anna Maria Friedel[1,2], Moritz Bechberger[1], Björn Heinz[1], Sébastien Petit-Watelot[2], Stéphane Andrieu[2], and Philipp Pirro[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]Institut Jean Lamour, UMR CNRS 7198, Université de Lorraine, 54000 Nancy, France

We report on zero-field spin waves in the linear and nonlinear regime propagating over tens of micrometers in transversally magnetised Co_2MnSi waveguides. The remanent configuration is stabilised by the intrinsic cubic magnetocrystalline anisotropy of the $L2_1$-ordered Heusler compound, which enables an operation in the favourable Damon-Eshbach geometry, yielding large spin wave group velocities and propagation lengths associated with the large saturation magnetisation $M_s \approx 1000\,\mathrm{kA/m}$ and the low Gilbert damping $\alpha \leq 10^{-3}$ in the half-metallic, $L2_1$-ordered Co_2MnSi. The cubic anisotropy not only allows for a reconfigurable remanent geometry and stable remanent operation, but also impacts the nonlinear magnetisation dynamics, yielding for instance a first order instability suppression range over several GHz. Investigating the linear and nonlinear dynamics in microstructured waveguides in remanence by Brillouin light scattering, this study consolidates the great interest in the half-metallic Co_2MnSi particularly for hybrid magnonic-spintronic applications at zero external bias fields.

MA 48.2 Thu 15:15 HSZ/0004

Long-range propagating paramagnon-polaritons in organic free radicals — •Sebastian Knauer[1], Roman Verba[2], Rostyslav O. Serha[1,3], Denys Slobodianiuk[2], David Schmoll[1,3], Andreas Ney[4], Sergej O. Demokritov[5], and Andrii V. Chumak[1] — [1]Faculty of Physics, University of Vienna, 1090 Vienna, Austria. — [2]V. G. Baryakhtar Institute of Magnetism of the NAS of Ukraine, 03142 Kyiv, Ukraine. — [3]Vienna Doctoral School in Physics, University of Vienna, 1090 Vienna, Austria. — [4]Institut für Halbleiter- und Festkörperphysik, Johannes Kepler Universität, 4040, Linz, Austria. — [5]Institute for Applied Physics, University of Münster, 48149 Münster, Germany.

Magnetic materials can host magnons below their Curie or Néel temperature, whereas in their paramagnetic phase, only short-range paramagnons are observed. We show that the organic free radical TEMPO supports long-range coherent spin dynamics well above its Néel temperature. Using all-electrical propagating spin-wave spectroscopy with on-chip microwave lines and external fields, we observe coherent excitations up to 23 GHz with group velocities above 100 $\mathrm{km\,s^{-1}}$ over 8 mm, exceeding calculated paramagnon velocities. Dispersion and pulse-propagation modelling identify these modes as paramagnon-polaritons, hybrid spin-photon excitations guided by the TEMPO column. This establishes organic free radicals as tunable paramagnetic magnonic media for microwave circuitry, spintronics, and high-frequency classical and quantum information processing [1].

[1] S. Knauer et al., RS, 2025 DOI: 10.21203/rs.3.rs-7990671/v1

MA 48.3 Thu 15:30 HSZ/0004

Nonlinear frequency mixing in spin-wave transducers — •Matthias Wagner, Felix Kohl, Björn Heinz, and Philipp Pirro — Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU Kaiserslautern- Landau, D-67663 Kaiserslautern, Germany

The demand for higher data transmission rates and high level of miniaturization has drawn attention to spin waves as a potential platform for building future radio frequency devices. So far, a lot of research has been carried out in optimizing prototype devices solely relying on continuous single-frequency operation. Nevertheless, the question how spin-wave transducers perform when real, multi-frequency signals are applied still is an open research subject that is especially relevant in the high-power regime where nonlinear spin-wave scattering leads to intermixing of frequency components within the passband. In this study, we quantify the nonlinear distortions caused by two-tone signals in spin-wave transducers by measuring relevant parameters, such as the 1-dB compression point and the third-order intercept point. Our results enable direct comparison between spin-wave based devices and conventional RF technology at the application level.

MA 48.4 Thu 15:45 HSZ/0004

Temperature-dependent characterization of spin-wave transducers — •Julien Schäfer, Björn Heinz, and Philipp Pirro — Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU Kaiserslautern- Landau, D-67663 Kaiserslautern, Germany

In radiofrequency technology, spin-wave-based (SW) communication building blocks, such as limiters and isolators, offer a low-energy alternative to traditional electronic devices. These magnonic communication devices consist of micrometer-sized antenna pairs that allow for tuning of the bandwidth and the frequency range through antenna shaping and adjustment of the applied magnetic field. Especially their compact size makes magnonic circuits attractive for on-chip integration, aiming to replace bulky electronic counterparts in crowded surroundings, such as cryostats and satellites. Following the objective to expand the SW transducer applicability to low-temperature environments, we study the propagation of SWs at various temperatures ranging from room temperature to 2 K. Understanding the impact of temperature-dependent variations in magnetic material parameters, including saturation magnetization and SW lifetime, on dispersive propagation characteristics is essential for engineering suitable devices. Our research provides insight into temperature-dependent insertion loss and isolation, consequently validating the applicability of SW transducers beyond room temperature conditions.

MA 48.5 Thu 16:00 HSZ/0004

Uniaxial strain response of antiferromagnetic magnons — •Manuel Knauft, Arthur von U.-S. Schwark, Matteo Minola, and Bernhard Keimer — Max Planck Institute for Solid State Research, Stuttgart, Germany

With the suggested paradigm shift away from conventional transistors towards lower loss devices, magnonics has attracted considerable attention in recent years. Generation, manipulation and detection of magnons are prerequisites for successful integration into microstructured chips. One potential phase space pa-

rameter to control magnon behavior is strain. In particular, in antiferromagnetic iridates with perovskite structure, it has recently been shown that the magnon energy can be varied by as much as 40% with small uniaxial strain of about 0.1% [1]. These ideas can also be extended to spatially inhomogeneous strain environments. We will demonstrate ideas of guiding magnons through bending single crystals and show results of finite element simulations and confocal Raman scattering.

[1] Kim *et al.*, Nat. Commun. **13**, 6674 (2022)

MA 48.6 Thu 16:15 HSZ/0004

Antiferromagnetic magnon condensation — •David Angster[1], Tobias Dannegger[1], Ulrich Nowak[1], and Verena Brehm[2] — [1]University of Konstanz, Germany — [2]Eindhoven University of Technology, Netherlands

The Bose-Einstein condensation (BEC) is a phase transition of a boson gas in which the ground state becomes macroscopically occupied below a critical temperature. BEC of bosonic quasiparticles, such as magnons, has been realised experimentally through active pumping of their density above a threshold value, since their number is not conserved in thermal equilibrium. This non-equilibrium magnon BEC was first demonstrated by Demokritov et al. [1]. Here, we present atomistic spin dynamics (ASD) simulations of antiferromagnetic hematite. The pumping of high-energy magnon modes triggers magnon redistribution via scattering processes that ultimately lead to condensation in the ground state, visible as an overproportional and non-thermal occupation of the low-frequency modes. Exploiting the non-linearity of ASD, we explore the key characteristics of BEC formation [2]: 1. a pumping threshold, 2. the spontaneous emergence of coherence, and 3. the shift of the magnon chemical potential.

[1] Demokritov et al., Nature 443, 430-433 (2006)

[2] Schneider et al., Nat. Nanotechnol. 15, 457-461 (2020)

MA 48.7 Thu 16:30 HSZ/0004

High-Resolution Field Mapping of Parametric-Instability Thresholds in YIG Films: Fine Structure and Magnon-Phonon Hybridization — •Tamara Azevedo[1], Rostyslav O. Serha[2], Yannik Kunz[1], Matthias R. Schweizer[1], Vitaliy I. Vasyuchka[1], Mikhail Kostylev[3], Burkard Hillebrands[1], and Alexander A. Serga[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]Faculty of Physics, University of Vienna, 1090 Vienna, Austria — [3]Faculty of Physics, University of Western Australia, 6009 Perth, Australia

Parametric electromagnetic pumping of magnons is a central technique for exciting and amplifying spin waves. Determining the parametric-instability threshold where the supplied energy compensates intrinsic magnon damping is essential for understanding and controlling this process. Using a highly sensitive automated measurement scheme based on quasi-continuous-wave excitation from a vector network analyzer and a microstrip resonator, we determined the instability threshold in tangentially magnetized yttrium-iron-garnet (YIG) films as a function of the external field $\mathbf{H}_0$ with unprecedented magnetic-field resolution. For parallel pumping, the threshold power exhibits distinct features originating from magnon hybridization with transverse and longitudinal phonons, as well as fine structure caused by the competitive excitation of thickness modes. These results highlight the dynamics specific to parallel parametric pumping that govern the onset of instability and provide crucial insight for efficient magnonic devices.

15 min break

MA 48.8 Thu 17:00 HSZ/0004

Stability of a magnon Bose-Einstein condensate under two-tone pumping — •Franziska Kühn[1], Lars Schiesser[1], Matthias R. Schweizer[1], Vitaliy I. Vasyuchka[1], Georg von Freymann[1,2], Mathias Weiler[1], Burkard Hillebrands[1], and Alexander A. Serga[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]Fraunhofer Institute for Industrial Mathematics ITWM, Fraunhofer Platz 1, 67663 Kaiserslautern, Germany

In our work we investigate the stability of magnon Bose-Einstein condensates (BEC) in yttrium-iron-garnet films under two-tone pumping. First, to create a magnon BEC, the magnon gas is populated above the thermal level by external injection of magnons through parametric pumping. For flexible control of the excitation conditions, we employ a broadband microstrip antenna, allowing continuous tuning of the pumping frequencies. Second, after the magnon BEC is formed, its stability is tested by disturbing it with a second pumping pulse at a lower frequency. By shaking the magnon system without generating additional magnons, we aim to properly identify stability conditions of the magnon BEC in a time-varying environment. The measurements are performed using wave vector resolved Brillouin light scattering spectroscopy as an optical detection method for magnons. This research was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation)-TRR 173/3-268565370 Spin+X (Project B04 and B13).

MA 48.9 Thu 17:15 HSZ/0004

Modelling spin-wave interference with electromagnetic leakage in micron-scaled spin-wave transducers — •Felix Kohl[1], Björn Heinz[1], Matthias Wagner[1], Christoph Adelmann[2], Florin Ciubotaru[2], and Philipp Pirro[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU Kaiserslautern- Landau, D-67663 Kaiserslautern, Germany — [2]imec, Kapeldreef 75, 3001 Heverlee, Belgium

Utilization of spin-wave transducers for radio-frequency signal processing provides significant potential due to intrinsic tunability, scalability and nonlinearity. However, such components can exhibit passband ripples, distortions in their transmission band, diminishing their operation and functionality. In this work, we experimentally identify the interference with the electromagnetic crosstalk (EM) as a major source of passband ripples and provide a simple analytic model to predict its impact on device operation. The results are in good agreement with the experimental observation. In addition, we test multiple transducer geometries to identify operational regimes and minimize the EM impact. Finally, the effect of nonlinear device operation on the interference with the EM is addressed, which is of relevance for the exploitation of the spin-waves intrinsic nonlinear traits.

MA 48.10 Thu 17:30 HSZ/0004

Avoided Crossings of Magnon Modes and Superconducting Lumped Element Resonator in YIG Microplatelet — •Seth W. Kurfman[1], Anoop Kamalasanan[1], Karl Heimrich[1], Philipp Geyer[1], Frank Heyroth[2], Kwangyul Hu[3], Tharnier Puel[3], Michael Flatté[3,4], and Georg Schmidt[1,2] — [1]Martin Luther Universität Halle-Wittenberg Institut für Physik, Halle, Germany — [2]Interdisziplinäres Zentrum für Materialwissenschaften, Halle, Germany — [3]University of Iowa Department of Physics and Astronomy, Iowa City, Iowa (USA) — [4]Eindhoven University of Technology Department of Applied Physics, Eindhoven, The Netherlands

Yttrium iron garnet (YIG) has been considered for decades as a gold standard material for magnonics due to its low-loss magnonic properties, and has successfully been used to demonstrate strong-coupling in macroscopic device geometries [1-4]. However, strong coupling of magnons in truly sub-10 micron YIG structures to date has not yet been realized. Here, we demonstrate the use of a YIG microplatelet placed on superconducting lumped element LC resonator to achieve strong coupling between numerous magnon modes and the LC resonator photons. These experimental findings are qualitatively backed by micromagnetic simulations and analytical calculations to identify the magnon modes corresponding to the experimentally observed anti-crossings in the microwave transmission signal.

[1] Lachance-Quirion, et al., Appl. Phys. Express 12, 070101 (2019). [2] Zhang, et al. Phys. Rev. Lett. 113, 156401 (2014). [3] Tabuchi et al. PRL 113, 083602 (2014). [4] Huebl, et al., PRL 111, 127003 (2013).

MA 48.11 Thu 17:45 HSZ/0004

Auto-oscillations and directional magnonemission induced by spin current injection into large magnetic volumes — •R. Schlitz[1,2], V. E. Demidov[3], M. Lammel[1], S. O. Demokritov[3], and P. Gambardella[2] — [1]Department of Physics, University of Konstanz, Konstanz, Germany — [2]Department of Materials, ETH Zurich, Zurich, Switzerland — [3]Institute of Applied Physics, University of Muenster, Muenster, Germany

Magnons are quantized excitations of the magnetization texture in ordered magnets, which can be used to transport spin information. In magnetic insulator/heavy metal bilayers angular momentum conversion from the electrical to the magnonic domain allows to electrically generate and detect magnon spin currents in the magnetic layer [1]. Recent studies showed, that in the nonlinear regime the changes of the nonlocal transport allow to also obtain information on the transported magnon manifold [2,3]. We show that local modifications of the magnon dispersion in the nonlinear regime can sensitively affect nonlocal magnon transport, giving rise to a strong enhancement of the number of specific low energy magnons. Considering the role of nonlinear relaxation processes, the nonlocal transport can be understood in terms of the nonequilibrium modification of the magnon dispersion. Our results showcase that nonlocal transport measurements are a sensitive probe to unravel changes to the magnon manifold [4].

[1] L. J. Cornelssien et al., Nature Physics **11**, 1022-1026 (2015)

[2, 3] R. Kohno et al., Physical Review B **108**, 14410 and 14411 (2023)

[4] R. Schlitz et al., Nature Communications **16**, 8472 (2025)

MA 49: Magnetic Imaging, Information Technology, and Sensors

Time: Thursday 15:00–17:15 Location: POT/0112

MA 49.1 Thu 15:00 POT/0112

Scalable magnetoreceptive e-skin for high-resolution interaction towards undisturbed extended reality — •Pavlo Makushko[1], Jin Ge[1], Gilbert Santiago Cañón Bermúdez[1], Oleksii Volkov[1,5], Yevhen Zabila[1], Stanislav Avdoshenko[2], Rico Illing[1], Leonid Ionov[3], Martin Kaltenbrunner[4], Jürgen Fassbender[1], Rui Xu[1], and Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., Dresden, Germany — [2]Leibniz Institute for Solid State and Materials Research Dresden, Dresden,Germany — [3]University of Bayreuth, Bayreuth, Germany — [4]Johannes Kepler University, Linz, Austria — [5]Goethe-Universität Frankfurt, Frankfurt am Main, Germany

Electronic skins seek to go beyond the natural human perception, e.g., by providing magnetoperception to detect magnetic fields. However, realizing magnetoreceptive e-skin with spatially continuous sensing over extended areas is challenging due to escalating circuit complexity and power consumption with increasing sensing resolution or interactive area. Here, by incorporating the GMR effect and electrical resistance tomography, we achieve continuous sensing of magnetic trigger across an area up to $120 \times 120\,mm^2$ with a sensing resolution of better than 1 mm [1]. A simplified circuit design enables optically transparent, mechanically compliant, and vapor/liquid permeable devices, that can be conveniently applied onto any surface including human skin. These achievements pave the way to numerous applications, including undisturbed recognition of fine-grained gesture touchless interaction. [1] P. Makushko et al., Nat Commun 16, 1647 (2025).

MA 49.2 Thu 15:15 POT/0112

Probing the magnetic order in a ferromagnetic monolayer — •Paritosh Karnatak[1], Andriani Vervelaki[1], Katharina Kress[1], Boris Gross[1], Daniel Jetter[1], Menghan Liao[2,3], Ritadip Bharati[2,3], Fengrui Yao[2,3], Ignacio Gutierrez[2,3], Kenji Watanabe[4], Takashi Taniguchi[5], Alberto Morpurgo[2,3], and Martino Poggio[1,6] — [1]Department of Physics, University of Basel, Basel, Switzerland — [2]Department of Quantum Matter Physics, University of Geneva, Geneva, Switzerland — [3]Group of Applied Physics, University of Geneva, Geneva, Switzerland — [4]Research Center for Functional Materials, National Institute for Material Science, 1-1 Namiki, Tsukuba 305-0044, Japan — [5]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan — [6]Swiss Nanoscience Institute, University of Basel, Basel, Switzerland

Understanding magnetism in two-dimensional (2D) van der Waals (vdW) magnets requires nanoscale local probes. Scanning SQUID microscopy (SSM), with ~100 nm resolution, enables direct imaging of magnetic structures in mono- and few-layer materials. Using SSM, we investigate the magnetic behavior of $CrPS_4$, a weakly anisotropic vdW interlayer antiferromagnet. Monolayer $CrPS_4$ shows no remanence and a zero coercive field, unlike thicker odd layers that exhibit 20-50 mT coercivity and nearly 100% remanence.

These layer-dependent studies reveal the role of interlayer coupling and dimensionality on magnetic responses. Our findings provide insights into mechanisms driving long-range magnetic order in 2D.

MA 49.3 Thu 15:30 POT/0112

SQUID-on-lever scanning probe for magnetic imaging with sub-100-nm spatial resolution — Timur Weber[2], •Daniel Jetter[1], Martino Pogio[1], and Dieter Kölle[2] — [1]Department of Physics, University of Basel, 4056 Basel, CH — [2]Physikalisches Institut, University of Tübingen, 72076 Tübingen, Germany

Scanning superconducting quantum interference device (SQUID) microscopy is a magnetic imaging technique combining high field sensitivity with nanometer-scale spatial resolution. We demonstrate a scanning probe that combines the magnetic and thermal imaging with the tip-sample distance control and topographic contrast of a non-contact atomic force microscope. We pattern the nanometer-scale SQUID, including its weak-link Josephson junctions, via neon or helium focused ion beam milling on a niobium coated cantilever. These SQUID-on-lever probes overcome many of the limitations of existing devices, achieving spatial resolution better than 100 nm, magnetic flux sensitivity of $0.3\ \mu\Phi_0/\sqrt{\mathrm{Hz}}$, operation in magnetic fields up to about 0.5 T and the incorporation of a third Josephson junction for shifting its phase. Its advanced functionality, high spatial resolution, and the ease of use of a cantilever-based scanning probe, extends the applicability of scanning SQUID microscopy to a wide range of magnetic, superconducting, and quantum Hall systems. We demonstrate magnetic imaging of skyrmions at the surface of bulk Cu2OSeO3. Analysis of the SQUID's point spread function yields a full-width-half-maximum of 71 nm that allows to image modulated magnetization patterns with a period of 65 nm.

MA 49.4 Thu 15:45 POT/0112

Magneto-Mechanical Resonator with Stimulus-Responsive Hydrogel for pH Sensing — •Nora Timm[1], Jonas Faltinath[2,3], Bruno Kluwe[1], Jonas Schumacher[1], Pascal Stagge[1], and Tobias Knopp[1,2,3] — [1]Fraunhofer Research Institution for Individualized and Cell-based Medical Engineering IMTE, Lübeck, Germany — [2]Section for Biomedical Imaging, University Medical Center Hamburg-Eppendorf, Hamburg, Germany — [3]Institute for Biomedical Imaging, Hamburg University of Technology, Hamburg, Germany

Magneto-mechanical resonators (MMRs) offer a promising platform for passive and wireless sensing. We present a novel chemical sensor by integrating a miniaturized MMR (2 mm×2 mm×7 mm) with a pH-responsive poly(2-hydroxyethyl methacrylate) (pHEMA) hydrogel functionalized with acrylic acid. In our implementation, the stimulus-responsive hydrogel modulates the distance between two permanent magnets through reversible volumetric changes in response to pH variations. One magnet serves as the stator and the other as the rotor of the MMR that is excited into torsional oscillations by external magnetic fields. Since the resonance frequency depends on magnet separation, frequency analysis of the inductively detected signal enables pH sensing. We demonstrate the sensor's response to pH variations in the range of pH 5-7 with observable shifts in resonance frequency of more than 40 Hz, which corresponds to a relative shift of more than 12 %. This proof-of-concept establishes hydrogel-integrated MMR sensors as a viable approach for wireless chemical sensing.

MA 49.5 Thu 16:00 POT/0112

Deep learning enabled wearable magnetoelectronics — •Guannan Mu, Rui Xu, Proloy T. Das, Jan Schmidtpeter, Lin Guo, Oleksandr Pylypovskyi, Andreas Knüpfer, Rico Illing, Olha Bezsmertna, and Denys Makarov — Helmholtz-Zentrum Dresden-Rossendorf e.V., 01328 Dresden, Germany

A wide variety of magnetic field sensors is already integrated into human-machine interfaces in wearable electronics [1,2]. However, the currently available interfaces are limited in the number of recognizable gestures and operation distance. To overcome these limitations, we integrate deep learning into two magnetic interaction platforms. First, we employ a flexible magnetoresistive sensor for user-definable temporal multipattern classification. Furthermore, we realize a compact LSTM-enabled wearable magnetic-interaction system integrated into a wrist-worn platform that incorporates a planar Hall magnetoresistive sensor, enabling a single sensor to recognize multiple predefined gestures and achieving a high classification accuracy of 99.4 % at a long range interaction distance of 12 cm, highlighting the potential of deep learning-enhanced magnetic sensing to expand functionality and enable long-range magnetic interaction recognition in smart wearable interfaces.

[1] R. Xu et al., ACS Nano 19, 21891 (2025)
[2] O. Bezsmertna et al., Adv. Funct. Mater. 2502947 (2025)

MA 49.6 Thu 16:15 POT/0112

Eco-sustainable printed magnetoresistive sensors — •Lin Guo, Xiaotao Wang, Proloy Taran Das, Yevhen Zabila, Ihor Veremchuk, Rui Xu, and Denys Makarov — Helmholtz-Zentrum Dresden-Rossendorf e.V., 01328 Dresden, Germany

Magnetoresistive sensors (MR), capable of non-contact detection of magnetic fields and consequently relative motion, have been extensively used across a broad spectrum of applications[1].Meanwhile, the massive deployment of magnetoresistive sensor arise the sustainability concerns from two aspects: 1. Carbon footprint in fabrication. 2. Electronics waste issue at the end of their lifetime.

Here, we propose the printed eco-sustainable magnetoresistance sensors. First, the recyclable printed MR sensors is developed based on a polyepichlorohydrin binder[2]. The hazardous MR ([Co/Cu]50) fillers are realized a close loop recycle once after the sensor lifetime. Further, we develop a healable and recyclable printed MR sensor via a full biomaterial gelatin-choline-citric acid ionogel. The additional healable capability extends the service time of the printed MR sensors and the full biomaterial binder decreased the carbon footprint. Finally, we developed a fully green printed magnetoresistance with Fe@Fe3O4 core-shell particles as functional filler, carboxymethyl cellulose as matrix binder, and water as solvents. Given that the skill-fully engineered magnetic structure and spin dependent transport, the printed sensors exhibit the remarkable low field magnetoresistance and sensitivity.

[1]Guo, L. et al., Chin. J. Struct. Chem. 44, 100428 (2025).
[2]Wang, X., Guo L. et al., J. Mater. Chem. A. 12, 24906 (2024).

MA 49.7 Thu 16:30 POT/0112

Mechanically Flexible High-Resolution Planar-Hall Effect Sensors — •Proloy Taran Das, Jan Schmidtpeter, Pavlo Makushko, Yevhen Zabila, Conrad Schubert, and Denys Makarov — Helmholtz-Zentrum Dresden-Rossendorf e.V., Institute of Ion Beam Physics and Materials Research, Bautzner Landstrasse 400, 01328 Dresden, Germany

Planar Hall effect (PHE) magnetic field sensors are attractive for applications requiring sub-nanoTesla resolution and vector field sensing [1,2]. In this presentation, we will discuss a comparative investigation of rigid and flexible PHE devices, linking their thin-film design and substrate mechanics to performance in sensitivity, linearity, and low-frequency noise. We show that flexible PHE sensors [3], fabricated as bi- and tri-layer elements on polymer substrates, maintain linear response under bending and achieve a magnetic field resolution to a few nT/*Hz at 10 Hz. The performance, rivalling that of rigid silicon-based references, is attained through careful tuning of unidirectional and uniaxial anisotropy through exchange bias, shape and growth effects and a synchronous demodulation readout. The results underscore the potential of PHE sensors for high-resolution biomagnetic sensing and robotics.

References: 1.Proloy T. Das et al. IEEE Trans. Magn. 60(9), 1-4 (2024) 2.*J. Schmidtpeter, Proloy T. Das et al. IEEE Magn. Lett. 15, 4100205 (2024) 3.*H. Nhalil et al. Appl. Phys. Lett. 123, 024102(2023)

MA 49.8 Thu 16:45 POT/0112

Probing nuclear spin dynamics in a single-atom magnet using Landau-Zener transitions — •Seunghyeok Jang[1,4], Valeria Sheina[1,3], Luciano Collazo[1,3], Georg A. Traeger[5], Denis Jankovic[1,3], Alexina Ollier[1,3], Muskan Sande[2,3], Sejong Kahng[4], Andreas Heinrich[2,3], and Won-jun Jang[1,3] — [1]Center for Quantum Nanoscience, Institute for Basic Science (IBS) — [2]Departure of Physics, Ewha Woman University — [3]Ewha Woman University — [4]Departure of Physics, Korea University — [5]Physik, Georg-August-Universitat Gottingen

Single-atom magnets provide a unique platform to probe quantum dynamics driven by hyperfine interactions. Holmium atoms on MgO thin films constitute a model system with exceptionally long-lived electronic states and well-resolved avoided level crossings, enabling electron-spin inversion via Landau-Zener (LZ) tunneling. Here, using spin-polarized scanning tunneling microscopy, we perform single-shot measurements of LZ tunneling events on 2-monolayer (ML) MgO at millikelvin temperatures, observing nuclear-spin polarization and resolving a ~10 peV gap at the avoided level crossing. We further measure the nuclear-spin lifetimes on both 2 ML and 3 ML MgO by applying LZ transitions twice in a pump-probe scheme. On 3 ML MgO, the lifetime reaches several hundred seconds, representing an enhancement of roughly two orders of magnitude compared with 2 ML. The exceptionally long nuclear-spin lifetime highlights single Ho atoms on MgO as a promising platform for quantum information processing based on coupled electron-nuclear spin states.

MA 49.9 Thu 17:00 POT/0112

Sensing Electric Currents in an a-IGZO TFT-Based Circuit Using a Quantum Diamond Microscope — •Pralekh Dubey[1], Mayana Yousuf Ali Khan[2], Lakshmi Madhuri P[3], Ashutosh Kumar Tripathi[3], Phani Kumar Peddibhotla[1], and Pydi Ganga Bahubalindruni[2] — [1]Department of Physics, Indian Institute of Science Education and Research, Bhopal — [2]Department of Electrical Engineering and Computer Science, Indian Institute of Science Education and Research, Bhopal — [3]National Centre for Flexible Electronics, Indian Institute of Technology, Kanpur

Quantum diamond microscopy (QDM), based on nitrogen-vacancy centers in diamond, provides a new approach for non-invasive magnetic imaging and diagnostics of electronic circuits under ambient conditions. By detecting magnetic fields generated by on-chip currents, QDM can probe device regions inaccessible to conventional electrical methods. It enables reconstruction of current density maps with sub-micron spatial resolution and sensitivity down to sub-microampere currents. Here, we employ a home-built QDM to map current flow in amorphous indium-gallium-zinc oxide (a-IGZO) thin-film transistor (TFT) circuits, a key technology for flexible and transparent electronics. As a demonstration, we map magnetic fields produced by current flowing through an a-IGZO TFT-based current mirror circuit. The corresponding current density was reconstructed, enabling direct visualization of current pathways. This study establishes QDM as a novel and powerful diagnostic tool for evaluating oxide-semiconductor circuits and emerging technologies.

MA 50: Bulk Materials: Soft and Hard Permanent Magnets

Time: Thursday 15:00–17:15 Location: POT/0151

MA 50.1 Thu 15:00 POT/0151

Ag-induced hardening and enhanced magnetic performance in SPS-consolidated CoCrFeMnNi high-entropy alloys — •Emmanouil Kasotakis[1], Ivan Tarasov[1], Tatiana Smoliarova[1], Hamed Shokri[2], Bilal Gökce[2], Michael Farle[1], and Natalia Shkodich[1] — [1]Faculty of Physics and Center of Nanointegration (CENIDE), University of Duisburg-Essen, Duisburg, 47057 Germany — [2]Chair of Materials Science and Additive Manufacturing, School of Mechanical Engineering and Safety Engineering, University of Wuppertal, Wuppertal, 42119 Germany

Nanocrystalline CoCrFeMnNi-Agx (x = 0; 1; 2.5; 5.5 at. %) high-entropy alloy (HEA) powders, produced via rapid two-step high-energy ball milling (HEBM) in Ar [1], were consolidated into ferromagnetic (Tc ~ 80 K) bulk samples by spark plasma sintering (SPS) at 700 K and 1000 K. Ag-free CoCrFeMnNi sintered at 1000 K formed a single-phase fcc alloy with uniform elemental distribution and a Vickers microhardness (HV0.2) of 2.4 GPa. Ag addition created distinct powder microstructures, from Ag-segregated regions (1 and 2.5 at. %) to uniform Ag distribution (5.5 at. %), increasing HV0.2 by 12% (to 2.7 GPa) in SPS-consolidated HEAs. In-field annealing (up to 700 K, 9 T) enhanced magnetization (M), coercivity (Hc), and remanence (Mr). CoCrFeMnNi-Agx (x = 5.5 at. %, 700 K) showed a tenfold rise in M (9 T, 310 K) to 40.2 Am2/kg, Hc = 46 kA/m, and Mr = 12.1 Am2/kg. We acknowledge DFG support (project ID: FA209/27-1).

[1] E. Kasotakis, et al. Acta Mater. 303, 121717 (2026).

MA 50.2 Thu 15:15 POT/0151

Transition-Metal-Induced Uniaxial Anisotropy in Fe_3Y — •M. Nur Hasan[1], Santa Pile[2], Rafael M. Vieira[1,3], Alexander Kovacs[2], Samuel RJ Holt[4], Martin Lang[4], Swapneel Pathak[4], Andrea Petrocchi[4], Hans Fangohr[4], Thomas Schrefl[2], and Heike C. Herper[1] — [1]Uppsala University, Sweden — [2]University for Continuing Education Krems, Austria — [3]Luleå University of Technology, Sweden — [4]MPSD, Hamburg, Germany

The rising demand for sustainable energy increases the need for rare-earth-free high-performance permanent magnets. The intermetallic compound Fe_3Y is a promising candidate due to its high saturation magnetization and Curie temperature. However, its intrinsic easy-plane magnetocrystalline anisotropy (MCA) hinders its use as a permanent-magnet material. Here, we combine first-principles density functional theory, spin-dynamics and micromagnetic simulations to explore mechanisms for reorienting the MCA toward a desired uniaxial direction through selective transition-metal doping. Our results show that Fe-site substitution, particularly with V, Zn, Nb, and Ta reverses the MCA to a uniaxial, reaching values up to 2 MJ/m^3, while the Curie temperature remains unaffected by these dopants. Micromagnetic simulations reveal dopant-specific hysteresis trends and indicate that the systems maintain stability in low-temperature regimes.

Acknowledgment: This work is supported by the European Union's Horizon Europe research and innovation programme under grant agreement No. 101135546 (MaMMoS).

MA 50.3 Thu 15:30 POT/0151

Magnetic imaging of interaction domains in nanocrystalline Nd-Fe-B by X-rays — P. Klassen[1], D. Günzing[2], A. Aubert[3], B. Eggert[1], T. Feggeler[2,4], •L. Kämmerer[1], G. Kämmerer[1], F. Maccari[3], J. Neethijaran[5], A. Ditter[2], D. Shapiro[2], H. Wende[1], K. Skokov[3], O. Gutfleisch[3], C. Donnelly[5], and K. Ollefs[6] — [1]Uni. Duisburg-Essen and CENIDE, GER — [2]LBNL, ALS, CA US — [3]Mat. Sc., TU Darmstadt, GER — [4]BNL, NSLS-II, NY US — [5]MPI-CPfS, Dresden, GER — [6]KIP, Uni. Heidelberg, GER

Nd-Fe-B magnets play a key role in sustainable energy conversion due to their high energy density. We provide insights into the magnetic domain structure of nanocrystalline Nd-Fe-B magnets obtained by X-ray ptychographic coherent diffractive imaging. The magnetic interaction domains of nanocrystalline Nd-Fe-B magnets with different compositions and grain structures ($Nd_2Fe_{14}B$ and $Nd_{15}Fe_{78}B_7$ melt spun ribbons and hot-deformed Nd-Fe-B from MQU-F) are shown and correlated to its microstructure. The soft X-ray imaging at the Fe L_3 edge provides detailed insights into the complex magnetic structure within the magnets, down to individual grains in the nanometer regime (10 nm). With 3D X-ray ptycho-tomography imaging we investigate the nature and local character of the domain wall in the hot-deformed Nd-Fe-B and correlate it to the microstructure in the material. Misalignment in magnetization of individueal grains from the interaction domain direction can be seen. We gratefully acknowledge funding from the DFG via the CRC/TRR 270 and used resources of the Advanced Light Source (contract no. DE-AC02-05CH11231).

MA 50.4 Thu 15:45 POT/0151

Nanoscale origins of coercivity in Cu-modified Sm(Co,Zr)6.7 alloys with globular 1:5/2:17 nanostructure — •Burcak Ekitli[1], Alex Aubert[1], Xinren Chen[2], Konstantin Skokov[1], Fernando Maccari[1], Esmaeil Adabifiroozjaei[3], Leopoldo Molina-Luna[3], Baptiste Gault[2], and Oliver Gutfleisch[1] — [1]Functional Materials, TU Darmstadt, 64287 Darmstadt, Germany — [2]Max-Planck-Institut for Sustainable Materials, 40237 Düsseldorf, Germany — [3]Advanced Electron Microscopy, TU Darmstadt, 64287 Darmstat, Germany

Sm-Co permanent magnets are commercially available in two main forms: the SmCo5 nucleation type and the more complex Sm(Co,Fe,Cu,Zr)7-7.5 (2:17-type), where coercivity is controlled by domain-wall pinning linked to a Cu concentration gradient within a cellular nanostructure. In this work, we investigate the Sm(CobalCuyZr0.023)6.7 composition to examine how Cu content affects microstructure and magnetic performance. HRSEM, TEM, and atom probe tomography reveal a previously unreported globular nanostructure, consisting of nanoscale 2:17 regions embedded in a continuous 1:5 matrix. Coercivity increases with Cu concentration and reaches up to 2 T when the Cu gradient is sufficiently strong. This underscores the superior efficiency of the cellular structure, which achieves comparable coercivity with less Cu. However the globular structure provides more stable coercivity at elevated temperatures (>700 K). These results connect microstructure and thermal stability, guiding new designs for high-temperature Sm-Co magnets.

MA 50.5 Thu 16:00 POT/0151

Unraveling the Magnetic Interactions of Nanocrystalline Rare-Earth-Lean Nd-Fe-B Powder and the Influence of Additive Manufacturing on the Magnetic Properties — •Priyatosh Sahoo[1], Lukas Schäfer[1], Kilian Schäfer[1], Franziska Scheibel[1], Esmaeil Adabifiroozjaei[1], Rebekka Hlawaty[1], Enrico Bruder[1], Philipp Gabriel[2], Anna Ziefuss[2], Stephan Barcikowski[2], Leopoldo Molina-Luna[1], Karsten Durst[1], Oliver Gutfleisch[1], and Konstantin Skokov[1] — [1]TU Darmstadt, Germany — [2]Universität Duisburg-Essen, Germany

MQP-S powder is a promising material for Laser Powder Bed Fusion (PBF-LB/M) thanks to its excellent flowability and hard magnetic properties. It shows enhanced remanence despite an isotropic microstructure, indicating exchange-spring-like behavior. However, PBF-LB/M processing fully melts the powder, erasing its initial microstructure and possibly affecting magnetic interactions. This study explores how PBF-LB/M parameters influence both density and magnetic performance in MQP-S magnets. Selected samples were characterized using Henkel and Thamm-Hesse plots, First-Order Reversal Curves (FORC) and magnetic domain imaging give insides about the global and local magnetic properties and interaction. A comparative analysis between the initial powder and the additively manufactured samples shows distinct magnetic coupling behaviors linked to the changing microstructure, providing new insights into the relationships among processing, microstructure, and properties in these magnets.

MA 50.6 Thu 16:15 POT/0151

Accelerating Sm-Fe-V Phase-Diagram Mapping via an Active-Learning Pipeline — •Aaron Dextre, Alex Aubert, Konstantin Skokov, Oliver Gutfleisch, and Pelin Tozman — Technische Universität Darmstadt

Sm1Fe12-based compounds are promising candidates to replace Nd-Fe-B, yet realizing their potential requires specific microstructures where grains are isolated by a low-melting-point phase. To locate the specific phase equilibria required for this coexistence, we developed an active-learning framework to accelerate the mapping of the Sm-Fe-V phase diagram. Integrating Neural Networks and Random Forests, our ensemble model iteratively directed the synthesis and annealing of target alloys to refine phase boundaries efficiently. After six cycles, we determined that the 1:12 phase is stable over a broader V range, while the target two-phase field is more confined than previously reported. These findings revise the Sm-Fe-V equilibria and demonstrate active learning*s utility in magnetic materials discovery.

MA 50.7 Thu 16:30 POT/0151

A new look at the magnetic properties of $DyCo_5$ — Alena Vishina[1], Konstantin Skokov[2], Hiroki Tsuchiura[3], Patrik Thunström[1], Alex Aubert[2], Oliver Gutfleisch[2], Olle Eriksson[1,4], and •Heike C. Herper[1] — [1]Uppsala University, Uppsala, Sweden — [2]Technische Universität Darmstadt, Germany — [3]Tohoku University, Sendai, Japan — [4]WISE-Wallenberg Initiative Materials Science, Uppsala University

Rare earth (RE) intermetallics such as $RECo_5$ impress with a huge variety of magnetic properties arising from the interplay of RE 4f and transition metal 3d orbitals. Our recent study provides new insights in $DyCo_5$.[1] Measurements were carried our on single crystals in applied fields up to 14T. We employed a multiscale modelling theory combining dynamical mean field theory (as implemented in the LMTO code RSPt) and atomistic spin-dynamics (UppASD) simulations with the effective spin model for RE compounds to understand the origin of the experimental findings.

Our multiscale method allows to explain the experimentally observed magnetisation anisotropy as well as the behaviour around the magnetic compensation point. For $DyCo_5$, both experiment and theory, show that the compensation is incomplete and field dependent. Furthermore, key experimental features - such as the saturation behaviour at high fields and the evolution of the magnetic moment at different temperatures - are successfully reproduced.

[1] http://arxiv.org/abs/2511.17087

MA 50.8 Thu 16:45 POT/0151

Orbital magnetic moment and magnetocrystalline anisotropy of Fe_2AlB_2 — •Nicolas Josten[1], Benedikt Eggert[1], Benedikt Beckmann[2], Anna Semisalova[1], Ralf Meckenstock[1], Konstantin Skokov[2], Hanna Pazniak[3], Thierry Ouisse[3], Katharina Ollefs[1], Heiko Wende[1], Oliver Gutfleisch[2], Michael Farle[1], and Ulf Wiedwald[1] — [1]Faculty of Physics and Center for Nanointegration (CENIDE), University Duisburg Essen, Germany — [2]Functional Materials, Institute of Materials Science, Technical University of Darmstadt, Germany — [3]LMGP, Grenoble INP, CNRS, Université Grenoble Alpes, France

Fe_2AlB_2 is a ferromagnet known for its considerably high magnetocrystalline anisotropy (1 MJ·m^{-3} at 10 K [1]), tunable Curie-temperature around ambient temperature (stoichiometric T_C = 291 K [1]) and magnetocaloric effect of moderate size (ΔT_{ad}(2 T) = 2.2 K [2]). It can be easily synthesized out of earth-abundant and low-cost elements. Here we combine X-ray magnetic circular dichroism (XMCD) and ferromagnetic resonance (FMR) measurements on single crystals to determine the orbital moment and correlate it with the high magnetocrystalline anisotropy. Additional magnetometry measurements along the principal crystallographic directions show the development of anisotropy across the ferromagnetic to paramagnetic phase transition.

Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 405553726 – SFB/TRR 270.

[1] N. Josten et al. Phys. Rev. Materials 9, 054405 (2025)
[2] B. Beckmann et al. J. Appl. Phys. 133, 173903 (2023)

MA 50.9 Thu 17:00 POT/0151

Enabling Ce Substitution in Nd-Fe-B Magnets for Wind Turbines via the 2-Powder Method — •Chi-Chia Lin[1,2], Konrad Opelt[1], Abdullatif Durgun[2], Imants Dirba[2], and Oliver Gutfleisch[2] — [1]Fraunhofer IWKS, Hanau, Germany — [2]TU Darmstadt, Darmstadt, Germany

Wind turbines contain Nd-Fe-B magnets weighing up to several tonnes. As deployment accelerates, demand for Nd rises, increasing supply risk and cost. Ce substitution can reduce critical-RE usage but degrades performance due to inferior intrinsic properties of $Ce_2Fe_{14}B$, formation of detrimental phases, and microstructural degradation.

We present a 2-powder method (2PM) enabling substantial Ce substitution without geometry constraints. A coarser (Ce,Nd)-Fe-B main powder is blended with a finer Nd-Fe-B powder and conventionally sintered, producing a uniform core-shell structure in which Nd-enriched shells magnetically harden $RE_2Fe_{14}B$ grain surfaces. Relative to single-powder processing at identical overall composition, 2PM boosts coercivity, remanence, and energy product by increasing local anisotropy fields at grain surfaces and optimizing grain-boundary chemistry. In addition, we introduce a hybrid segmented magnet that positions the 2PM Ce-substituted segment between Nd-Fe-B segments, extending local magnetic hardening to a bulk macroscopic effect and enhancing demagnetization resistance while concentrating Nd only where peak coercivity is required.

Together, 2PM and hybrid segmentation offer a scalable route to thrift Nd with abundant Ce toward wind-turbine performance targets.

MA 51: Spin Transport and Orbitronics, Spin-Hall Effects II (joint session MA/TT)

Time: Thursday 15:00–17:00 Location: POT/0361

MA 51.1 Thu 15:00 POT/0361

Spin-pumping and induced magnetic polarization in permalloy/platinum heterostructures — •Verena Ney[1], Kilian Lenz[2], Fabrice Wilhelm[3], René Hübner[2], Fabian Ganss[2], Andrei Rogalev[3], Jürgen Lindner[2], and Andreas Ney[1] — [1]Johannes Kepler Universität Linz, Österreich — [2]Helmholtz Zentrum Dresden-Rossendorf, Deutschland — [3]ESRF, Grenoble, Frankreich

Spin pumping is the transfer of angular momentum across interfaces into a non-ferromagnetic material driven by the precessing magnetization of an adjacent ferromagnet. Using ferromagnetic resonance (FMR) the presence of spin pumping can be evidenced by an increase of the Gilbert damping parameter α [1]. Here we study platinum-permalloy (Pt/Py) heterostructures using temperature-dependent broadband FMR. A clear increase of α is seen in a temperature range from 10 to 300 K when Pt and Py are in direct contact. The temperature dependence of the spin-pumping contribution can be derived by comparing with an Al-sandwiched Py reference film from [2]. Surprisingly, upon insertion of a thin Al spacer layer between Pt and Py the increase in α is suppressed. X-ray magnetic circular dichroism at the Pt L_3-edge reveals a clear magnetic polarization in Pt/Py whereas it is absent when a spacer layer of only 2 nm of Al is inserted.

The induced polarization of Pt can thus be associated with spin pumping, while non-polarized Pt in proximity to Py shows an almost identical $\alpha(T)$ behavior as the Py reference sample in [2].

[1] Y. Tserkovnyak Phys. Rev. Lett. **88**, 117601 (2002)
[2] V. Ney et al. Phys. Rev. Materials **7**, 124403 (2023)

MA 51.2 Thu 15:15 POT/0361

Single and double spin Hall anomalous Hall and Hanle effects in Pt/YIG and Ta/YIG bilayers — •Akashdeep Akashdeep, Duc Minh Tran, Mathias Kläui, Gerhard Jakob, and Timo Kuschel — Johannes Gutenberg University Mainz, Germany

Anomalous Hall effect data of heavy metal / magnetic insulator bilayers, such as $Pt/Y_3Fe_5O_{12}$ (YIG), are commonly explained by magnetoresistance effects that are quadratically depending on the spin Hall angle (SHA) [1-4]. This is because they usually consist of two spin Hall processes as for example valid for spin Hall magnetoresistance [1,2]. In addition, S. Zhang et al. predicted theoretically a single spin Hall process combined with interfacial spin-dependent scattering which results in a linear SHA dependence [5] not reported experimentally so far.

In this contribution, we present anomalous Hall effect results for Pt/YIG and Ta/YIG with opposite sign in SHA of Pt and Ta. Thus, we can probe even and odd SHA dependencies. For thin Pt and Ta thicknesses, we observe results that are even in the SHA which is consistent with experimental literature. However, we found an odd SHA dependence for thicker heavy metal layers which is only partially mentioned in theory. We will present the separation of the effects and discuss the impact of the SHA on the individual effect contributions.

[1] H. Nakayama et al., Phys. Rev. Lett. 110, 206601 (2013)
[2] S. Meyer et al., Appl. Phys. Lett. 106, 132402 (2015)
[3] S. Vélez et al., Phys. Rev. Lett. 116, 016603 (2016)
[4] J. Li et al., Phys. Rev. B 106, 184420 (2022)
[5] S. S.-L. Zhang, G. Vignale, Phys. Rev. Lett. 116, 136601 (2016)

MA 51.3 Thu 15:30 POT/0361

Current-induced spin and orbital polarization in the ferroelectric Rashba semiconductor GeTe — •Sergio Leiva-Montecinos[1], Libor Vojáček[2], Jing Li[2], Mairbek Chshiev[2], Laurent Vila[2], Ingrid Mertig[1], and Annika Johansson[3] — [1]Martin-Luther-Universität Halle-Wittenberg, Germany — [2]Univ. Grenoble Alpes, CEA, CNRS, Grenoble, France — [3]Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

The Edelstein effect is a promising mechanism for generating spin and orbital polarization from charge currents in systems without inversion symmetry. In ferroelectric materials, such as Germanium Telluride (GeTe), the combination of bulk Rashba splitting and voltage-controlled ferroelectric polarization provides a pathway for electrical control of the sign of the charge-spin conversion [1, 2].

In this work [3], we investigate current-induced spin and orbital magnetization in bulk GeTe using Wannier-based tight-binding models derived from *ab initio* calculations and semiclassical Boltzmann theory. Employing the modern theory of orbital magnetization, we demonstrate that the orbital Edelstein effect surpases its spin counterpart by one order of magnitude. Moreover, the orbital Edelstein effect remains largely unaffected in the absence of spin-orbit coupling, highlighting its distinct physical origin compared to the spin Edelstein effect.

[1] D. Di Sante *et al.*, Adv. Mater. **25**, 509 (2012).
[2] C. Rinaldi *et al.*, Nano Lett. **18**, 2751 (2018).
[3] S. Leiva-Montecinos *et al.*, arXiv:2505.21340 (2025).

MA 51.4 Thu 15:45 POT/0361

Orbital contribution to g-tensor from first-principles modern theory — •Garima Ahuja[1], Mirco Sastges[2,3], Dongwook Go[4], Shobhana Narasimhan[1], Yuriy Mokrousov[2,3], and Stefan Blügel[2,5] — [1]Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru, India — [2]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, Jülich, Germany — [3]Institute of Physics, Johannes Gutenberg University Mainz, Mainz, Germany — [4]Department of Physics, Korea University, Seoul, South Korea — [5]Institute for Theoretical Physics, RWTH Aachen University, Aachen, Germany

The electronic g-factor, which measures how angular momentum couples to magnetic fields, is a key descriptor of magnetic behavior in solids. In crystalline materials, the orbital contribution to the g-factor can significantly modify its value. In this talk, we present a first-principles framework for computing g-factors, based on multiband perturbation theory with the DFT-Wannier approach, to reveal microscopic origins of the orbital contribution, highlighting the roles of local and non-local orbital currents. We resolve both orbital and spin responses, determine the full g-tensor, and show how interband couplings and band geometry shape the g-tensor across the Brillouin zone. g-tensor plays a key role in quantum technologies, where qubit coherence and control depend on accurate knowledge of magnetic response. We present our findings for some interesting bulk and 2D systems, offering a predictive route for engineering magnetic responses in materials relevant to quantum computing, spin-orbitronics, and spectroscopy.

MA 51.5 Thu 16:00 POT/0361

Inherent Electro-Optic Kerr Rotation — •Erlend Syljuåsen[1], Alireza Qaiumzadeh[1], Rembert Duine[2,3], and Arne Brataas[1] — [1]Center for Quantum Spintronics,Trondheim, Norway — [2]Institute for Theoretical Physics, Utrecht University, The Netherlands — [3]Department of Applied Physics, Eindhoven University of Technology, The Netherlands

Static electric-field–induced Kerr rotation of reflected light is used to probe symmetry breaking, electronic properties, and transport phenomena as the spin and orbital Hall effects. In this talk, we uncover a previously overlooked contribution to the electric-field–induced Kerr rotation, arising from the interplay of matter, the static electric field, and the magnetic component of light. This contribution remains nonzero even in isotropic nonmagnetic homogeneous materials, making this effect inherent to any such Kerr measurement. We present analytical expressions for both two-dimensional layers and semi-infinite bulk metals, and find within the relaxation-time approximation signal magnitudes directly relevant for experiments.

MA 51.6 Thu 16:15 POT/0361

Thermally Activated Spin Transport in a Multiferroic $LiCu_2O_2$/Pt Heterostructure — •Mathew James, Ankita Nayak, István Kézsmárki, and Aisha Aqeel — University of Augsburg, 86159 Augsburg, Germany

Multiferroics, in which electric and magnetic orders are coupled, are potential materials for low-power spintronic devices. $LiCu_2O_2$ is a Type II multiferroic material known to exhibit spiral (non-collinear) spin ordering below its antiferromagnetic transition temperature, $T_N \approx 23$ K [1]. In this material, the magnetic Cu^{2+} ions form double chains along the crystallographic b-axis, resulting in a double-leg spin-ladder configuration.

In this study, we use the Spin Seebeck Effect (SSE) as an electric probe to investigate the thermally activated magnetic response of $LiCu_2O_2$ across different magnetic configurations. In the SSE, a temperature gradient across a magnetic insulator generates non-equilibrium magnons that carry a spin current. This spin current is converted into a measurable voltage in a heavy-metal layer deposited on top of the insulator, via the Inverse Spin Hall Effect [2]. Our preliminary results indicate that the SSE voltage is sensitive to the spiral ordering in $LiCu_2O_2$. References: [1]S. Park, et al., Phys. Rev. Lett., 98, 5 (2007). [2]K. Uchida et al., Nature, vol. 455, no. 7214, (2008).

MA 51.7 Thu 16:30 POT/0361

Current-induced orbital dynamics in magnetic oxides — •Mahmoud Zeer[1], Marjana Ležaic[1], Dongwook Go[1,2], Leonid Pourovskii[3], Stefan Blügel[1,4], Mathias Kläui[2], Olena Gomonay[2], and Yuriy Mokrousov[1,2] — [1]Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institute of Physics, Johannes Gutenberg-University Mainz, 55099 Mainz, Germany — [3]CPHT, CNRS, École polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France — [4]Institute of Theoretical Physics, RWTH Aachen University, 52074 Aachen, Germany

Magnetic oxides provide an ideal platform for exploring orbital de- grees of freedom emerging from strong orbital angular momentum and spin-orbit coupling. The resulting unquenched orbital moments en- able rich orbital-transport phenomena, particularly in antiferromag- netic systems. In this work, we investigate current-induced orbital dy- namics in representative transition-metal oxides using first-principles calculations in both bulk and thin-film geometries. We identify siz- able orbital response and highly efficient orbital-to-spin conversion mechanisms, which give rise to substantial torque components on the magnetic sublattices [1]. In addition, we analyze the contributions of dipole, quadrupole, and octupole magnetic moments to the overall orbital response. Our findings establish magnetic oxides as a promis- ing and realistic platform for harnessing orbital degrees of freedom for next-generation spin-orbital technologies. [1] S. Krishnia, C. Schmitt, M. Zeer et al., under review.

MA 51.8 Thu 16:45 POT/0361

Disentangling angular momentum transport in ferromagnet-diamagnet structures via suspended systems — •Fiona Sosa Barth[1,2], Matthias Grammer[1,2], Richard Schlitz[3], Tobias Wimmer[1,2], Janine Gückelhorn[1,2], Luis Flacke[1,2], Sebastian T.B. Goennenwein[3], Rudolf Gross[1,2,4], Hans Huebl[1,2,4], Akashdeep Kamra[5], and Matthias Althammer[1,2] — [1]Walther-Meißner-Institut, BAdW, Garching, Germany — [2]School of Natural Sciences, TUM, Garching, Germany — [3]Department of Physics, University of Konstanz, Konstanz, Germany — [4]Munich Center for Quantum Science and Technology, München, Germany — [5]RPTU Kaiserslautern-Landau, Kaiserslautern, Germany

Spintronics relies on the transfer of angular momentum between electrons and solid state excitations such as magnons and phonons. In our recent work, we demonstrate angular momentum transfer between two ferromagnetic strips on diamagnetic substrates [1]. A DC current on one of the strips is converted into a non-equilibrium magnon accumulation, which transfers angular momentum to the magnonic system of the second FM strip, detected electrically by the inverse processes. In this work, we investigate how the nature of this angular momentum transport is affected by the substrate. We first examine how SiOx, SiN and

SiN/SiOx layers on Si substrates impact the transport response, and then study the effect in freestanding ferromagnetic strips fully decoupled from the substrate. This allows us to separate potential dipolar from phononic contributions to the coupling between the FM strips. [1] R. Schlitz et al., Phys. Rev. Lett. 132, 256701 (2024)

MA 52: Poster Magnetism III

Time: Thursday 15:00–17:00 Location: P4

MA 52.1 Thu 15:00 P4

Coupling between spin waves and excitons in CrSBr bilayers — •Luis Rolf Gieselmann, Thorsten Deilmann, and Michael Rohlfing — Institute of Solid State Theory, University of Münster, Germany

CrSBr is a layered van der Waals semiconductor characterized by its peculiar magnetic structure, possessing ferromagnetic ordering within and antiferromagnetic ordering between its layers.

The antiparallel alignment of spins in neighboring layers directly affects the excitonic properties of the material, as interlayer transitions of electrons and holes are thus optically forbidden in the magnetic ground state. External manipulation of the spins, however, produces partially parallel alignments between layers and thus enables excitations of interlayer excitons.

Such excitonic effects have previously been studied for canting by an external magnetic field. In our work, we have considered an alternative, namely canting of the spins induced by spin waves within CrSBr bilayers. The spin wave behavior of the material is studied using coherent states and then employed in a simple model Hamiltonian to calculate the change of excitonic energies.

MA 52.2 Thu 15:00 P4

Holstein-Primakoff Expansions and the Goldstone Theorem for Ferromagnetic Spin Chains — •Hendrik Wächter, Fred Hucht, and Jürgen König — University of Duisburg-Essen, Faculty of Physics, Duisburg, Germany

A common approach to investigate collective magnetic excitations is to represent spins as bosons. A popular representation that achieves this is the Holstein-Primakoff transformation, which comes at the cost of introducing square roots containing the occupation number operator to the spin ladder operators. For many applications, it is preferable to expand these square roots in power series. Typically, this is done by a Taylor series expansion in powers of $1/S$, sacrificing essential virtues of the Holstein-Primakoff transformation by coupling to an unphysical Hilbert space. We consider Newton series expansions as an alternative [1]. Ferromagnetic spin chains are used to compare the efficacy of both expansions, focusing on ground-state and low-energy excitation properties, notably including Goldstone modes. Matrix product states and the density-matrix renormalization group method are used to obtain highly accurate numerical results. We find that the Newton series expansion up to a finite order respects the existence of gapless spin excitations within the relevant Hilbert space.

[1] J. König and A. Hucht, SciPost Phys. **10**, 007 (2021)

MA 52.3 Thu 15:00 P4

Local Spin Seebeck Effect in Hematite — •Florian Kraft[1], Maximilian Thiel[1], Katharina Lasinger[1,2], Matthias R. Schweizer[1], and Mathias Weiler[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU Kaiserslautern-Landau, Germany — [2]Clarendon Laboratory, Department of Physics, University of Oxford, United Kingdom

Antiferromagnets such as hematite (α-Fe_2O_3) are key candidates for spintronic and magnonic devices due to their ultra-low magnetic damping and vanishing stray fields. However, the inherent compensation of magnetic moments makes probing the magnetic order challenging.

We employ the Local Spin Seebeck Effect (LSSE), generated by focused laser heating of an α-Fe_2O_3/Pt bilayer, to spatially resolve thermal spin currents. Our measurements are performed at room temperature, where hematite orders in a weak ferromagnetic state, characterized by an intrinsic net magnetization (**m**). In our r-cut single crystal, the crystallographic c-axis is obliquely aligned relative to the surface plane, thus enabling us to vary the in-plane and oblique components of **m** and the Néel vector **n** by rotating the external magnetic field.

The local heat-to-spin conversion mechanism is analyzed through the field and field-angle dependence of the LSSE signal. We place particular emphasis on alignments close to the in-plane projection of the c-axis, as this direction maximizes the competition between the magnetic field and intrinsic anisotropies. Resolving the contributions of the in-plane and oblique components of **m** and **n** is critical for understanding magnon transport in complex antiferromagnetic systems.

MA 52.4 Thu 15:00 P4

Entanglement and Dissipation in Quantum Spin Systems — •Jakob Wagner, Daniel K. J. Boness, and Wolfgang Belzig — Department of Physics, University of Konstanz, D-78457 Konstanz, Germany

Squeezing in quantum systems allows the reduction of quantum fluctuations in one observable of interest at the cost of enhanced uncertainty in its conjugate. Spin systems common in magnonics naturally exhibit squeezing [1, 2]. Generally, dissipation changes the amount of squeezing, possibly also amplifying it [3, 4]. Here, we relate the effects of dissipation in spin systems to linearized bosonic systems. We extend previous considerations by assuming a general linear system-bath coupling. Associating the position coordinate of the bosonic system with spin fluctuations in one direction, as well as the momentum coordinate with the orthogonal direction we demonstrate the equivalence of the Landau-Lifschitz-Gilbert equation to an unconventionally damped harmonic oscillator. We demonstrate several coupling dependent effects like control of the squeezing direction and modified entanglement properties. Our results thus give new controls over decoherence in magnonic systems via engineered dissipation.

[1] A. Kamra et al, Phys. Rev. B 100, 174407 (2019)
[2] D. Wuhrer et al, Appl. Phys. Lett. 125, 022404 (2024)
[3] G. Rastelli, New. J. Phys. 18, 053033 (2016)
[4] H. Y. Yuan et al, Phys. Rev. B 106, 224422 (2022)

MA 52.5 Thu 15:00 P4

Silicon ion implantation of YIG thin films for magnonics — •Richa Bhardwaj[1], Jannis Bensmann[1], Robert Schmidt[1], Kirill O. Nikolaev[2], Dimitri Raskhodchikov[1], Shraddha Choudhary[1], Shabnam Taheriniya[3,4], Sven Niehues[1], Akhil Varri[1,3], Ahmad El Kadri[1], Johannes Kern[1], Wolfram H. P. Pernice[1,3,4], Sergej O. Demokritov[2], Vladislav E. Demidov[2], Steffen Michaelis de Vasconcellos[1], and Rudolf Bratschitsch[1] — [1]Institute of Physics and Center for Nanotechnology(CeNTech), UniversityofMünster — [2]InstituteofAp- plied Physics, University of Münster — [3]Center for Soft Nanoscience, University of Münster — [4]Kirchhoff-Institute for Physics, Heidelberg University

Magnons hold the promise for novel computing architectures due to their low power consumption. Recently, magnonic YG waveguides have been demonstrated using a maskless silicon ion-implantation technique [1]. Here, we examine how silicon ion implantation modifies the structural, optical, and magneto-optical properties of YIG thin films. Our findings establish design guidelines for YIG improved spin-wave manipulation for magnonic integrated circuits. Reference: [1] J. Bensmann, et al., Nat. Mater. 24, 1920-1926 (2025).

MA 52.6 Thu 15:00 P4

Linear Spin Wave Theory for Resonant Inelastic X-ray Scattering — •Paul Hille and Maurits W. Haverkort — Institute for Theoretical Physics, Heidelberg University, 69120 Heidelberg

Magnon excitations provide a key window into the collective magnetic behavior of correlated materials. While inelastic neutron scattering (INS) has long been the standard technique to map magnon dispersion relations and intensities, in recent years, resonant inelastic X-ray scattering (RIXS) has grown into a complementary technique to measure dispersing magnetic excitations. Within the RIXS process one can not only excite single magnons but also multiple magnetic excitations with a single photon.

The central goal of this work is to extend existing linear spin wave theory (LSWT) routines for INS to handle multi-magnon excitations characteristic of RIXS spectra. This is combined with an effective RIXS scattering operator incorporating the resonant energy and light polarisation dependence. We obtain a general and extensible computational framework that enables RIXS modeling for realistic magnetic materials within LSWT. Furthermore, quantitative comparison with experimental RIXS data enables assessment of the validity of treating magnons as non-interacting quasiparticles.

MA 52.7 Thu 15:00 P4

Electric Control of Magnon Phase via the Aharonov–Casher Effect — •Gabriel Schwöbel[1], Rostyslav O. Serha[2], Matthias R. Schweitzer[1], Vitaliy I. Vasyuchka[1], Mathias Weiler[1], Burkard Hillebrands[1], and Aleksander A. Serga[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU Kaiserslautern-Landau, Kaiserslautern, Germany — [2]Faculty of Physics, University of Vienna, Vienna, Austria

A promising approach toward nonreciprocal magnon phase manipulation is offered by the Aharonov–Casher effect—a mechanism whereby particles or quasiparticles with a magnetic moment acquire an additional phase when traveling through an electric field. While this effect has been theoretically predicted for magnons, direct experimental confirmation is still lacking. Additionally, electric fields also influence magnetic systems through the magnetoelectric effect by modifying the magnetization.

Our experiments demonstrate that the Aharonov–Casher effect and magnetoelectric contributions can be independently quantified and unambiguously distinguished. By applying an in-plane electric field to a perpendicularly magnetized YIG film, we achieve controlled manipulation of the phase of the forward-volume magnetostatic spin waves. The resulting phase shifts depend on both the propagation direction and the polarity of the applied electric field, demonstrating electric-field tunability of magnon transport and offering a pathway toward nonreciprocal phase control in magnonic systems.

MA 52.8 Thu 15:00 P4

Femtosecond noise correlation spectroscopy of magnon fluctuations in bismuth doped yttrium iron garnet — •C. Runge[1], F. S. Herbst[1], M. A. Weiss[1], N. Beaulieu[2], J. B. Youssef[2], A. Leitenstorfer[1], M. Lammel[1], R. Schlitz[1], and S. T. B. Goennenwein[1] — [1]Department of Physics, University of Konstanz, Germany — [2]LabSTICC, CNRS, Université de Bretagne Occidentale, France

Magnetic systems exhibit a rich variety of dynamic phenomena on ultrafast timescales, which are of both fundamental and technological interest. For example, magnons, the quanta of spin waves, are discussed as promising candidates for information carriers due to their ability to propagate without charge transport. Femtosecond noise correlation spectroscopy (FemNoC) has been established [1] as a time-resolved optical technique that directly probes the local magnetization correlation function of a spin system. Thus, FemNoC is sensitive to incoherent magnetization dynamics like thermal magnons or random telegraph switching in the anisotropy landscape and allows to distinguish them by their respective correlation characteristics [1]. Here, we apply FemNoC to bismuth doped yttrium iron garnet. We investigate the magnon population of the sample both in thermal equilibrium and excited by ferromagnetic resonance. Introducing a quantitative model we can fit both regimes and determine the number of magnons induced by the resonant drive.

[1] M. A. Weiss et al., Nat. Commun. **14**, 7651 (2023).

MA 52.9 Thu 15:00 P4

Active noise spectroscopy of magnon-photon polaritons — •Lars Nikolas Hess, Philipp Schwenke, Vitaliy Vasyuchka, Kevin Künstle, and Mathias Weiler — Fachbereich Physik and Landesforschungszentrum OPTIMAS, Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, 67663 Kaiserslautern, Germany

Microwave (MW) cavities offer a wide range of applications for exciting ferromagnetic resonance (FMR) in solid-state magnets [1]. Due to the interaction of resonant MW photons with the magnonic excitations of a magnetic sample, their coupling behaviour can be studied in detail [2]. In this study, we use a MW cavity designed to operate in the frequency range from 500 MHz to 600 MHz to investigate the thermally excited MW photons and their coupling to magnons in the ferrimagnetic insulator $Y_3Fe_5O_{12}$ (YIG). To this end, a 2 *m thick YIG film is positioned inside the cavity. The resonant coupling between the MW photons and the YIG FMR is realised. An active feedback loop inspired by a similar setup for surface acoustic wave resonators [3] is implemented to specifically amplify the thermal photons in the MW cavity, that couple to the magnetic excitations in YIG. The resonator used in combination with the active amplification process makes it possible to determine characteristic parameters of the coupled systems without the use of an external MW source.

[1] H.Huebl *et. al*, Phys. Rev. Lett. **111**, 127003 (2013)
[2] L.Liensberger *et. al*, Phys. Rev. B **104**, L100415 (2021)
[3] Z.Xi *et. al*, Phys. Rev. App. **23**, 024054 (2025)

MA 52.10 Thu 15:00 P4

Low-temperature-compatible iron garnet films grown by liquid phase epitaxy — Jamal Ben Youssef[1], Nathan Beaulieu[1], Richard Schlitz[2], Davit Petrosyan[3], •Michaela Lammel[2], and William Legrand[4] — [1]LabSTICC-CNRS, Université Bretagne Occidentale, Brest — [2]Department of Physics, University of Konstanz, Konstanz — [3]Department of Materials, ETH Zurich, Zurich — [4]CNRS, Institute Néel, Université Grenoble Alps, Grenoble

Integrating thin epitaxial yttrium iron garnet (YIG) - one of the prototypical material systems in the field of magnonics, owing to its record-low damping of the magnetization dynamics - into hybrid (quantum) systems promises a platform to study the interaction of magnons with other (quasi)particles. However, up to now the usability of YIG in such devices is limited due to the losses occurring at low temperatures due to the paramagnetic gadolinium gallium garnet (GGG) substrate, and eventually Gd intermixing in the first layers. To circumvent this problem, we use liquid phase epitaxy (LPE) to grow ultrathin films of strained YIG on a commercial diamagnetic substrate, yttrium scandium gallium garnet (YSGG) [arXiv:2509.06242]. We investigate their magnetization dynamics between 3 K and 300 K, and compare them to films grown on paramagnetic GGG. We demonstrate that our LPE YIG on YSGG substrates features a ferromagnetic resonance linewidth below 1 mT at 3 K, together with a very weak temperature and frequency dependence of the losses. Therewith, the growth of YIG/YSGG by LPE provides a straightforward approach for the fabrication of YIG thin films for low-temperature investigations.

MA 52.11 Thu 15:00 P4

Magnetoacoustic interaction in Yttrium-Iron-Garnet / Aluminium-Scandium-Nitride heterostructures — •Kaya Gauch[1], Kevin Künstle[1], Yannik Kunz[1], Agne Žukauskaite[2,3], Stephan Barth[2], and Mathias Weiler[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, Rheinland-Pfälzisch Tech nische Universität Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]Fraunhoferr Institute for Electron Beam und Plasma Technology FEP, 01277 Dresden, Germany — [3]Institute of Solid State Electronics, Technische Universität Dresden, 01062 Dresden, Germany

The magnetoelastic interaction between surface acoustic waves (SAWs) and spin waves (SWs) has attracted considerable attention in recent years. Magnetoelastic excitation of SWs is particularly promising in low-damping ferrimagnets such as yttrium iron garnet (YIG). Electri cal excitation of SAWs necessitates a piezoelectric layer, such as ZnO [1]. Here, we investigate magnetoelastic interactions in a heterostruc ture consisting of a YIG/GGG bilayer coated with a piezoelectric AlScN thin film. The coupling between SAWs and SWs is characterized using micro-focused Brillouin light scattering (BLS) spectroscopy and vector network analyzer (VNA) measurements. In addition, the ob served magnetoelastic interaction is benchmarked against the coupling in the more established ZnO/YIG/GGG heterostructure. [1] Ryburn et al., Phys. Rev. Appl. 23, 034062 (2025)

MA 52.12 Thu 15:00 P4

Distinctive Propagation of Phonon-mediated Magnons in YIG/GGG — •Youngseon Soon[1], Moojune Song[1], Phuoc Cao Van[2], Jinhyun Baek[1], Byong-Guk Park[3], Jong-Ryul Jeong[2], Albert Min Gyu Park[1], and Kab-Jin Kim[1] — [1]Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 34141, Republic of Korea — [2]Department of Materials Science and Engineering, Chungnam National University, Daejeon 34134, Republic of Korea — [3]Department of Materials Science and Engineering, Korea Advanced Institute of Science and Technology, Daejeon 34141, Republic of Korea

Magnonic systems enable information processing via collective spin excitations and couple efficiently to other quasiparticles. We study magnetostatic surface spin waves (MSSWs) coupled to standing acoustic waves in a 200-nm YIG film on GGG. Using two microwave antennas and VNA measurement, we observe 3.5 MHz periodic modulation in transmission spectra arising from magnetoelastic interaction. As the magnon wave vector k increases, these phononic signatures weaken and eventually vanish, reflecting both the k-dependence of the coupling and the momentum selectivity of antennas. Phonon-mediated magnon modes emerge at lower frequencies than directly excited MSSWs and propagate much farther, providing a low-k channel for long-distance spin-wave transport without acoustic resonators. These distinctive features highlight the wavevector-dependent magnon-phonon hybridization and demonstrate that both coupling strength and propagation behavior can be engineered through excitation geometry.

MA 52.13 Thu 15:00 P4

Broadband Floating-Electrode SAW Transducers for Magnetoelastic Spin-Wave Excitation in CoFeB thin films — •Kawa Noman[1], Ryusuke Hisatomi[2], Kotaro Taga[2], Teruo Ono[2], Vitaliy Vasyuchka[1], and Mathias Weiler[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]Kyoto University, Institute for Chemical Research,Kyoto,Japan

Microwave filters based on surface acoustic wave (SAW) devices exhibit low insertion loss and enable wideband operation in the GHz range. In this study, we microfabricate custom-designed floating-electrode in terdigital transducers (FE-IDTs) on piezoelectric LiNbO3 substrates, whose unique geometry with additional electrically floating metal fin gers enhances electromechanical coupling and broadband SAW exci tation [1]. We then deposit a 10 nm CoFeB thin film by DC mag netron sputtering within the SAW propagation path. We investigate the magnetic-field dependence of the SAW-driven magnetoelastic spin-wave resonance using vector network analysis. Systematic variation of the electrode material, aperture, and duty cycle reveals a rich spec trum of high-amplitude Rayleigh modes at odd and even harmonics of FE-IDT excitation. Moreover, we observe clear signatures of SAW-driven magnetoelastic excitation of spin-waves in CoFeB. High-amplitude SAWs enable non linear magnon generation [2].

[1] K. Yamanouchi et al., IEEE Ultrasonics Symposium (2013)
[2] M. Geilen et al., Applied Physics Letters 120, 242404 (2022)

MA 52.14 Thu 15:00 P4

Backward volume spin waves in ion-implanted magnonic YIG waveguides — •Sven Niehues[1], Jannis Bensmann[1], Robert Schmidt[1], Kirill O. Nikolaev[2], Dimitri Raskhodchikov[1], Shraddha Choudhary[1], Richa Bhardwaj[1], Shabnam Taheriniya[1,3,4], Akhil Varri[1,3], Ahmad El Kadri[1], Johannes Kern[1], Wolfram H. P. Pernice[1,3,4], Sergej O. Demokritov[2], Vladislav E. Demidov[2], Steffen Michaelis de Vasconcellos[1], and Rudolf Bratschitsch[1] — [1]Institute of Physics and Center for Nanotechnology (CeNTech), University of Münster — [2]Institute of Applied Physics, University of Münster — [3]Center for Soft Nanoscience, University of Münster — [4]Kirchhoff-Institute for Physics, Heidelberg University

Magnonics offers a promising alternative approach to conventional information processing due to the low-energy nature of spin waves and distinctive features such as nm-scale wavelengths. Recently, the fabrication of dispersion-tunable magnonic waveguides and a large-scale spin-wave network with 198 crossings have been demonstrated using a newly developed maskless silicon ion implantation technique [1]. Here, we show that backward volume spin waves (BVSW) propagate in silicon-ion implanted waveguides written into YIG thin films. Using time-resolved Faraday rotation spectroscopy, we extract the dispersion relation, the mode profile and damping of the BVSWs. Our results demonstrate the versatility of silicon-ion implanted magnonic waveguides, offering a promising route toward magnonic integrated circuits. Reference: [1] J. Bensmann, et al. Nat. Mat. 24, 1920-1926 (2025).

MA 52.15 Thu 15:00 P4

Quantum Geometry of Magnons — •Sidhartha Chatterjee[1], Andreas Haller[1], Peter P. Orth[2], and Thomas L. Schmidt[1] — [1]University of Luxembourg — [2]Saarland University

We develop a theoretical framework for magnon dynamics in a one-dimensional antiferromagnetic Heisenberg chain that includes next-nearest-neighbour Dzyaloshinskii-Moriya interaction (DMI) and a position-dependent magnetic field applied along the easy axis. This combination leads to a spin spiral ground state. The collective excitations above the ground state are magnons, spin-1 bosonic modes. We perform the Holstein-Primakoff transformation to obtain the magnon Hamiltonian, which is quadratic in nature. For the diagonalisation, we use the Bogoliubov transformation, and we show that the quantum geometric tensor of magnons naturally exhibits symplectic structure. This geometric structure yields corrections to the semiclassical equations of motion for magnon wave packets, resulting in anomalous velocity terms and metric-driven contributions. Overall, the framework provides a systematic route for incorporating geometric effects and symplectic structure into magnon dynamics, where no particle number conserving framework exists, and offers a pathway for engineering transport phenomena in magnetic materials through the direct manipulation of the quantum geometry of their collective excitations.

MA 52.16 Thu 15:00 P4

Impact of Magnetic Ground State on the Generation of an All-Magnonic Frequency Comb — •Alexandra Schrader, Chris Körner, Rouven Dreyer, and Georg Woltersdorf — Martin Luther University Halle-Wittenberg

We have observed the emergence of a magnonic frequency comb in extended Permalloy films as well as in microstructures of Permalloy and CoFeB. Since the frequency comb generation appears to be a unique feature of softmagnetic materials at very low bias fields (below 2 mT), we anticipate a strong correlation between the static ground state and the emerging dynamics. In the case of microstructures, the higher harmonic generation is indeed connected to the non-uniform domain structure at the edges.

However, the presence of these edge effects reduces the frequency multiplication efficiency. In this work, stripes of different aspect ratios are investigated to bridge the gap between extended layers and microstructures. This allows to explore the correlation between the static magnetization pattern obtained in Kerr microscopy and the generation of the frequency comb revealed via SNS-MOKE and NV-center microscopy. Both static and dynamic features are complemented by micromagnetic simulations.

MA 52.17 Thu 15:00 P4

Surface Acoustic Wave Generation and Detection in AlScN/GGG Heterostructures — •Karl Heimrich[1], Seth Kurfman[1], Frank Heyroth[2], Katrin Lehmann[2], Fabian Lofink[3], and Georg Schmidt[1,2] — [1]Martin Luther Universität Halle-Wittenberg Institut für Physik, Halle, Germany — [2]Interdisziplinäres Zentrum für Materialwissenschaften, Halle, Germany — [3]Frauenhofer ISIT, Itzehoe, Germany

Surface acoustic waves (SAWs) can be excited and detected in piezoelectric materials using interdigitated transducers (IDTs). In magnetostrictive materials, particularly with low-loss magnetic properties (e.g. Yttrium-Iron-Garnet, YIG), the coupling between SAWs and magnons provides unique opportunities for device applications. Different groups have already successfully demonstrated the coupling of ferromagnetic resonance with acoustic surface waves [1, 2, 3, 4]. Even the coupling to the low loss material YIG has been shown[3, 5]. Here we demonstrate the use of an Aluminium-Scandium-Nitride (AlScN)/Gallium-Gadolinium-Garnet (GGG) heterostructure to excite and detect SAWs that propagate in a pure GGG surface, offering the possibility to couple into micropatterned or even suspended YIG structures [6].

[1] Weiler et al., PRL: 106.11 (2011): 117601. [2] Dreher et al., PRB: 86.13 (2012): 134415. [3] Kunz et al., arXiv preprint: 2503.11203 (2025). [4] Rayburn et al., PRA: 23.3 (2025): 034062. [5] Wong et al., APL 349.6246 (2024): 125.5 [6] Heyroth, Schmidt et al., PRA: 12.5 (2019): 054031

MA 52.18 Thu 15:00 P4

Magnon-phonon coupling in suspended nanostructure — •Giovanni Del Bufalo[1,2], Matthias Grammer[1,2], Johannes Weber[1,2], and Hans Huebl[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]TUM School of Natural Sciences, Technische Universität München, Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany

High-overtone bulk acoustic wave resonators were among the first mechanical systems explored in the quantum regime, enabling studies of vacuum fluctuations and non-classical states. Integrating magnetic thin films with these resonators creates hybrid magneto-phononic excitations through magnetoelastic coupling, allowing energy exchange between phonons and magnons. Beyond energy transfer, these hybrid modes can inherit angular momentum from their constituent excitations, raising a fundamental question: how is angular momentum transferred and shared between phonons and magnons in such systems? We address this by implementing a suspended silicon membrane as a bulk acoustic wave resonator, coupled to a 40nm $Co_{25}Fe_{75}$ metallic film. Using broadband ferromagnetic resonance spectroscopy at cryogenic temperatures, we quantify the magnon-phonon coupling strength and assess its implications for angular momentum transfer and magnetization damping. Our results highlight the potential of this device architecture for probing spin-mechanical interactions and advancing hybrid quantum systems that combine magnetic and mechanical degrees of freedom.

MA 52.19 Thu 15:00 P4

Characterization of spin-Hall nano-oscillators — •Christine Strickler, Moritz Bechberger, Julien Schäfer, Björn Heinz, and Philipp Pirro — Fachbereich Physik and Landesforschungszentrum OPTIMAS, Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, D-67663 Kaiserslautern, Germany

Within the research field of spintronics, spin-Hall nano-oscillators (SHNOs) have emerged as promising candidates for building blocks in neuromorphic computing. These devices typically consist of a bi layer comprising a ferromagnetic (FM) and a heavy metal (HM) layer. Typically, a direct charge current is applied to the HM, which injects a spin current into the FM via the spin Hall effect, exerting spin orbit torques that can counteract the natural damping of the FM and thereby excite coherent auto-oscillations. We perform ferromagnetic resonance spectroscopy on fabricated full-film bilayer systems to opti mize the material stack in terms of FM-layer thickness and FM/HM interface quality. The materials selected for this study are CoFeB and NiFe as FM and Pt and W as HM, which leads to four potential ma terial stacks. The optimized stacks are fabricated in several SHNO geometries and sizes to investigate their properties concerning mode spectrum and threshold current for auto-oscillation via Brillouin light scattering spectroscopy. This study of SHNO fabrication paves the way for further investigation into such structures and their potential coupling phenomena.

MA 52.20 Thu 15:00 P4

Frequency-dependent parametric injection of magnons in yttrium iron garnet — •Lars Schiesser, Franziska Kühn, Matthias R. Schweizer, Vitaliy Vasyuchka, Alexander A. Serga, and Mathias Weiler — Fachbereich Physik and Landesforschungszentrum OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany

Parametric generation of magnons in low-damping yttrium iron garnet (YIG) films offers a flexible approach to excite magnons across a broad range of wavenumbers, enabling the creation of high magnon densities, which are essential for the preparation of magnon gases preceding condensation phenomena. Using parallel parametric pumping driven by a broadband stripline antenna, we investigate the frequency dependence of pumping thresholds and the ensuing nonlinear scattering processes. By tuning both the external magnetic field and the pumping frequency, we selectively control the initial position of parametrically injected magnons in momentum space and thus define the starting conditions for subsequent multi-magnon scattering dynamics. Time-resolved Brillouin light scattering (BLS) spectroscopy is employed for the direct observation of the temporal and spectral evolution of the magnon population.

These frequency characteristics provide the basis for the implementation of pumping schemes with arbitrary waveforms, which will enable the realization of complex, tailored excitation signals, opening new pathways for the precise control of nonlinear magnon dynamics.

MA 52.21 Thu 15:00 P4

Spatially-Localized Second Harmonic Generation via Spin Wave Concentration in Patterned YIG Structures — •Marc Eger[1], Stephanie Lake[1], Philipp Geyer[1], Seth Kurfman[1], Rouven Dreyer[1], and Georg Schmidt[1,2] — [1]Martin-Luther-Universität Halle-Wittenberg Insitut für Physik, Halle, Germany — [2]Interdisziplinäres Zentrum für Materialwissenschaften, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

The anisotropic dispersion and inherent non-linearity of (magnetostatic) spin waves in thin films and confined structures provide unique opportunities for

implementation in next-generation radio-frequency devices [1]. A particular challenge remains in establishing effective and useful means to locally generate and subsequently exploit higher harmonics without extraneous non-linear losses [2]. In order to compensate these losses, one method to achieve this is to focus low-intensity spin waves in a low-loss magnetic material to a localised region far from the exciting antenna. This can be done, for example, with deterministically tuning the dispersion relation by modifying film thickness along with a geometric confinement through standard patterning processes. Here we compare micromagnetic simulations and experimental results obtained by frequency- and spatially-resolved SNS MOKE [3] within passive, lithographically-patterned YIG funnel structures, wherein we demonstrate second harmonic generation of magnons.

[1] Ustinov et. al, IEEE Magnetics Letters 10, 1-4, 2019
[2] T. Hula et. al, Appl. Phys. Lett. 117, 042404, 2020
[3] Rouven Dreyer et. al., Phys. Rev. Materials 5, 064411, 2021

MA 52.22 Thu 15:00 P4

Enhancing Mechanical Stability of Heusler Alloys via the Powder-in-Tube Method — •T. Niehoff[1,2], L Beyer[3,4], J. Puy[5], J. Freudenberger[3,4], O. Gutfleisch[5], J. Wosnitza[1,2], F. Scheibel[5], and T. Gottschall[1] — [1]Dresden High Magnetic Field Laboratory (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Dresden, Germany — [3]Leibniz-Institut für Festkörper- und Werkstoffforschung IFW, Dresden, Germany — [4]TU Bergakademie Freiberg, Freiberg, Germany — [5]Institute of Materials Science, Technical University of Darmstadt Darmstadt, Germany

We address the long-standing problem of mechanical fatigue in Heusler-based elastocaloric and multicaloric materials by applying the Powder-in-Tube (PIT) method to stabilize the material inside a steel shell. This significantly enhances mechanical robustness. Under cyclic loading up to 100,000 cycles and high-load tests, PIT samples retain their structural integrity, showing only minor, non-critical end cracks while the core remains thermally connected to the shell. Even after plastic deformation, the Heusler core stays intact. Magnetization before and after cycling exhibits only minimal changes, confirming durability, and magnetocaloric measurements demonstrate excellent thermal coupling between core and metal shell. Overall, the PIT method extends the operational lifetime of Heusler alloys by orders of magnitude and allows independent optimization of mechanical stability and caloric performance.

MA 52.23 Thu 15:00 P4

Significant Enhancement of Magnetocaloric Performance of LaFe12B6 via Microstructure Optimization — •Protyasha Prachurja, Wei Liu, Alex Aubert, Benedikt Beckmann, Konstantin Skokov, and Oliver Gutfleisch — Institute of Materials Science, Technische Universität Darmstadt, Darmstadt, Germany

Light rare-earth magnetocaloric (MC) materials are appealing because of their abundance and reduced criticality risks [1]. Within this group of materials, LaFe12B6 - a first-order MC compound - undergoes a phase transition around 36 K, making it a potential candidate for hydrogen liquefaction applications [2]. However, its pronounced MC effect emerges only under relatively high magnetic fields (>5 T), which restricts its performance at lower fields [3]. This limitation is linked to its antiferromagnetic ground state and the presence of secondary phases in the microstructure. We carried out a systematic optimization of the synthesis conditions to improve phase purity and magnetocaloric properties. We found that annealing at 1383 K for 24 hours with a 3% La excess reduced the secondary phase content from 13.2 to 7.7 wt.% and sharpened the first-order transition. Consequently, the peak magnetic entropy change increased significantly from -1 to -10 J/kgK under a 5 T field. References: [1] Wei Liu et al. J. Phys. Energy, 2023, 5.3, 034001; [2] L.V.B. Diop; O. Isnard; J. Rodríguez-Carvajal Phys. Rev. B, 2016, 93.1, 80; [3] L.V.B. Diop; O. Isnard J. App. Phys., 2016, 119.21, 213904. Acknowledgement: We acknowledge financial support by the DFG within the CRC/TRR 270 (Project-ID 405553726).

MA 52.24 Thu 15:00 P4

Superconducting magnetic system for magnetocaloric hydrogen liquefaction — •C. Estillac Leal Silva[1,2], T. Platte[4], M. Strassheim[1,3], T. Niehoff[1,3], C. Salazar-Meija[1], J. Wosnitza[1,3], and T. Gottschall[1] — [1]Dresden High Magnetic Field Laboratory (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf Dresden, Germany — [2]TU Bergakademie Freiberg, Freiberg, Germany — [3]Institüt für Festkörper und Materialphysik, TU Dresden, Dresden, Germany — [4]Magnotherm Solutions GmbH, Darmstadt, Germany

As hydrogen's importance in the clean-energy sector continues to expand, improving its liquefaction efficiency becomes crucial, since the liquid form provides high volumetric energy density for storage and transport. Traditional compression systems, however, remain both costly and energy-intensive, prompting interest in magnetic refrigeration as an alternative process. This approach employs the adiabatic temperature variation of magnetocaloric materials in an Active Magnetocaloric Regenerator (AMR) to reach the final cooling stage required for hydrogen liquefaction. Achieving large temperature spans requires large variations in the magnetic field. In addition, higher operating frequencies are needed to reach greater cooling powers. Therefore, a magnetic system capable of sustaining high fields while supporting rapid cycling, whether through linear or rotary motion of the magnetocaloric material, is necessary. This presentation discusses the development of a superconducting magnetic system meeting these requirements, targeting a concentrated 5-7 T field which enables a sharp field change.

MA 52.25 Thu 15:00 P4

MnCrNiGeSi high-entropy alloy: structural, magnetic and magnetocaloric properties — •Atakan Tekgül[1] and Kağan Şarlar[2] — [1]Uludag University, Bursa, Turkey — [2]Karamanoglu Mehmetbey University, Bursa, Turkey

This study investigates the structural, magnetic, and magnetocaloric properties of two rare-earth-free high-entropy alloys, $Mn_{20}Cr_{14}Ni_{33}Ge_{25}Si_5$ and $Mn_{24}Cr_{10}Ni_{33}Ge_{25}Si_8$, produced by arc melting. Rietveld refinement of X-ray diffraction data confirms that both alloys crystallize in an orthorhombic Pnma structure. Increasing the Mn content from 20% to 24% strengthens the ferromagnetic exchange interactions, resulting in an enhancement of the saturation magnetization (43.8->56.7 $Am^{-1}kg^{-1}$) and an upward shift of the Curie temperature (361->387 K). Isothermal magnetization measurements and Arrott plot analyses reveal a second-order magnetic phase transition. The magnetocaloric effect, calculated via the Maxwell relation, yields a magnetic entropy change of 2.1 $Jkg^{-1}K^{-1}$ for the alloy with 20% Mn and 3.6 $Jkg^{-1}K^{-1}$ for the Mn-rich alloy under a magnetic field of 2 T. The combination of low hysteresis, high Curie temperature, and enhanced entropy change demonstrates that Mn-enriched Mn-Cr-Ni-Ge-Si HEAs offer promising performance for environmentally friendly, high-temperature magnetic refrigeration. These results confirm that compositional tuning, particularly Mn substitution, is an effective route for optimizing the magnetocaloric response in rare-earth-free HEAs.

MA 52.26 Thu 15:00 P4

Spin structure analysis on Fe_2AlB_2 powder and single-crystals — •Joachim Landers[1], Niels Kubitza[2], Soma Salamon[1], Ulf Wiedwald[1], Christina Birkel[2,3], and Heiko Wende[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen — [2]Department of Chemistry and Biochemistry, TU Darmstadt — [3]School of Molecular Sciences, Arizona State University

The MAB phase Fe_2AlB_2 exhibits ferromagnetic ordering below the Curie temperature $T_C \approx 290$ K, showing a strong magnetocaloric effect close to room temperature, which makes it a promising candidate for magnetic cooling applications. We utilize Mössbauer spectroscopy under high magnetic fields to analyze the spin structure and ferro- to paramagnetic phase transition of Fe_2AlB_2 microparticle powders. Field- and temperature-dependent measurements on an Fe_2AlB_2 single-crystal sanded down to appropriate thickness for transmission experiments are used as reference and allow for specific characterization along easy and hard magnetic directions with regards to magnetic alignment. Funding by the DFG via CRC/TRR 270 (project number 405553726, subprojects B02, B03, and B05) is gratefully acknowledged. We thank T. Ouisse and H. Pazniak (LMGP, Grenoble) for providing single crystals.

MA 52.27 Thu 15:00 P4

Combining X-ray absorption spectroscopy with a multifunctional probe to decipher first-order phase transitions — •Benedikt Eggert[1], Alex Aubert[2], Shingo Yamamoto[3], Ana Kurtanidze[3,4], Thomas Herrmannsdörfer[3], Oliver Gutfleisch[2], Kurt Kummer[5], Nick Brookes[5], Jochen Wosnitza[3,4], Katharina Ollefs[6], Konstantin Skokov[2], and Heiko Wende[1] — [1]University Duisburg-Essen — [2]TU Darmstadt — [3]HZDR, HLD-EMFL — [4]TU Dresden — [5]ESRF — [6]KIP, University Heidelberg

Here, we present a new instrumental setup designed for the investigation of magnetostructural phase transition, installed within the high field magnet at beamline ID32 of the European Synchrotron Radiation Facility in Grenoble, France. With these newly established setups, we can perform dichroic X-ray absorption spectroscopy, while accessing other subsystems via bulk probes (e.g., lattice expansion or change in electrical resistivity) within a temperature range from 4 K to 650 K in the soft X-ray regime.

Here, we will show first experimental results from La(Fe,Si)13 during the field and temperature-induced magnetostructural phase transition showcasing some of the possibilities.

Funding by the BMFTR under Grant BMBF-Projekt05K2022, and the Deutsche Forschungsgemeinschaft via CRC/TRR 270 HoMMage (Project-ID 405553726) is gratefully acknowledged. We thank the ESRF for the allocation of beamtime.

MA 52.28 Thu 15:00 P4

Magnetic and transport properties of compensated ferrimagnetic Heusler alloys at finite-temperature predicted by *ab inito* spin fluctuation theory — •Shogo Yamashita[1], Esita Pandey[1], Gerhard Fecher[1], Claudia Felser[1], and Atsufumi Hirohata[1,2] — [1]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany. — [2]Center for Science and Innovation in Spintronics, Tohoku University, Sendai, Japan

Fully compensated ferrimagnets have been attractive for spintronics because their net zero magnetization suppresses stray fields, enabling high-density memory integration. Among them, Heusler alloys which have 24 valence electrons are of particular interest since they can exhibit both half-metallicity with 100 % spin polarization at the Fermi level and fully compensated ferrimagnetism. However, a fully compensated half metallic Heusler alloy $Mn_{1.5}V_{0.5}FeAl$ reported previously has a Curie temperature below room temperature, limiting its device applications. To find alternatives, we investigated $Mn_2Co_{0.5}V_{0.5}Al(Ga)$, which is regarded as a mixture of half-metallic $Mn_2VAl(Ga)$ and $Mn_2CoAl(Ga)$ exhibiting high Curie temperature, with 24 valence electrons. Using an *ab inito* spin-fluctuation theory based on the coherent potential approximation and disordered local moments, we examined its electronic structure, magnetic properties, and spin conductivities at finite-temperature. In this presentation, we will also discuss possible future control in the properties.

MA 52.29 Thu 15:00 P4

Broadly tunable compensation in ferrimagnetic MnFeVAl Heusler alloy — •Esita Pandey[1], Shogo Yamashita[1], Edouard Lesne[1], Gerhard Fecher[1], Claudia Felser[1], and Atsufumi Hirohata[1,2] — [1]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany — [2]Tohoku University, Sendai, Japan

Zero-moment spintronic systems are highly desirable, as they minimize stray fields while maintaining stability against external magnetic perturbations. Unlike antiferromagnets, compensated ferrimagnets offer an ideal solution, combining a net-zero magnetic moment with spin-polarized conduction [1-3]. In this study, we demonstrate the realization of a near-zero-moment state in Mn1.5V0.5FeAl Heusler alloy thin films with a wide tunable compensation range. Films of varying thickness were fabricated on thermally oxidized Si substrates with a W buffer layer using simultaneous triple-target sputtering in an ultra-high-vacuum system. Structural analysis via X-ray diffraction shows that the W underlayer is stabilized in the body-centered cubic (bcc) α-phase with (110) orientation, while the Heusler films exhibit pronounced [110] texture and a lattice parameter close to bulk values. Magnetometry measurements reveal that the samples are magnetically isotropic and exhibit an exceptionally low saturation magnetization at RT. These results position MnFeVAl films as promising candidates for thermally stable, stray-field-free spintronic devices with robust spin-polarized transport. Reference: [1] V. Baltz et al., Rev. Mod. Phys. Vol. 90, No. 1 (2018); [2] A. Hirohata, Magnetochemistry 8, 37 (2022); [3] R. Stinshoff et al., Phys. Rev. B 95, 060410(R) (2017).

MA 52.30 Thu 15:00 P4

Halbach 2.0 - Creating homogenous fields with finite size magnets — •Peter Blümler[1] and Ingo Rehberg[2] — [1]Institute of Physics, University of Mainz, 55128 Mainz, Germany — [2]Institute of Physics, University of Bayreuth, 95440 Bayreuth, Germany

Homogeneous magnetic fields can be generated with permanent magnet arrangements, most notably Halbach rings made of idealized, infinitely long magnetic rods. However, this classical concept is limited when using real, finite magnets. To address this, three-dimensional configurations have been investigated. Optimal single and stacked rings of point dipoles are identified, offering greater field strength and homogeneity than traditional Halbach designs and earlier numerical estimates.

A central innovation is the "focused configuration" (I.R. & P.B., Phys. Rev. Appl. 23 (2025) 064029), where dipoles are tilted out of the ring plane, producing highly homogeneous fields shifted away from the magnet plane. Rotating multiple tilted rings relative to each other further improves homogeneity, though at the cost of a fixed field direction (still confined to the transverse plane).

Experiments with cuboid magnets confirm the theoretical predictions, showing that these configurations overcome finite-magnet limitations and provide enhanced field strength and homogeneity. All configurations can be explored and exported for 3D printing using a dedicated Python GUI (https://zenodo.org/records/15064360).

MA 52.31 Thu 15:00 P4

Towards Sustainable NdFeB Magnets Using Advanced Recycling — •Aybike Paksoy[1], Amrita Khan[1], Abdullatif Durgun[1], Mario Schönfeldt[2], Hasan Mahmudul[2], Iliya Radulov[2], Imants Dirba[1], and Oliver Gutfleisch[1] — [1]Functional Materials, Technical University of Darmstadt, Darmstadt, Germany — [2]Fraunhofer IWKS, Fraunhofer Research Institution for Materials Recycling and Resource Strategies, Hanau, Germany

NdFeB permanent magnets exhibit the highest maximum energy product (BH)max at room temperature, making them important for many technologies essential to the clean energy transition. However, their reliance on critical rare earth elements raises significant environmental, economic, and geopolitical challenges [1]. Consequently, increasing attention has been directed toward the recycling of end-of-life NdFeB permanent magnets. Enhancing the sustainability of rare earth permanent magnets and reducing their criticality are key requirements for environmentally responsible products. The magnetic properties of NdFeB magnets are strongly governed by their microstructure. Recycling routes can alter grain size, crystallographic texture, and defect density, which in turn influence magnetic performance. In this work, advanced recycling strategies are explored with the aim of producing sustainable NdFeB magnets while preserving their functional properties. [1] M. Schönfeldt et al., J. Alloys and Compounds (2023) https://doi.org/10.1016/j.jallcom.2023.168709

MA 52.32 Thu 15:00 P4

Resource efficient recycling and additive manufacturing of Nd-Fe-B magnets — •Amrita Khan[1], Lukas Schäfer[1], Priyatosh Sahoo[1], Iliya Radulov[2], Mahmudul Hasan[2], Konstantin Skokov[1], Igor Lubomirsky[3], and Oliver Gutfleisch[1] — [1]TU Darmstadt, Darmstadt, Germany — [2]Fraunhofer IWKS, Hanau, Germany — [3]Weizmann Institute of Science, Rehovot, Israel

Recycling Nd-Fe-B magnets is crucial for maintaining a sustainable supply of rare-earth elements for clean energy applications while significantly reducing the environmental impact and energy footprint. Additive manufacturing (AM) is a promising production route for functional magnetic materials, especially for achieving high geometric complexity, energy-efficient processing, and waste minimization. In this work, the PBF-LB/M process is used to directly produce permanent magnets, which are not yet optimized with regard to magnetic performance. The recycling of Nd-Fe-B scrap magnets and powder production is a critical step for successful processing via PBF-LB/M. In this study, different recycling processes are investigated: (i) hydrogen decrepitation, (ii) electrolytic decrepitation, and (iii) ultrasonic atomization, which are characterized regarding their particle size distribution, morphology, and flowability. The goal is to identify the influence of the powder properties on the PBF process and the resulting magnetic performance of additively manufactured magnets. This work was supported by the Volkswagen-Stiftung through the project MagCycleAM (9D878 Project No. 0071952-00).

MA 52.33 Thu 15:00 P4

Inverse garnet/Pt heterostructures by lateral crystallization — •Christian Holzmann[1], Stephan Glamsch[1], David Stein[1], Maximilian Mihm[1], Aladin Ullrich[1], Richard Schlitz[2], Michaela Lammel[2], Johannes Boneberg[2], and Manfred Albrecht[1] — [1]Institute of Physics, University of Augsburg, 86159 Augsburg, Germany — [2]Department of Physics, University of Konstanz, 78457 Konstanz, Germany

Rare-earth iron garnet thin films are known for their low Gilbert damping, insulating nature, and tunable magnetic properties. These favorable properties are mostly limited to single-crystalline films grown on specific substrates like GGG, which limits their applications [1]. To expand the functionallity of garnet thin films, we grow a thulium iron garnet film on a thin Pt layer by means of lateral crystallization. The Pt layer is sputter-deposited on a GSGG substrate, followed by garnet deposition by PLD. Hereby, a hole pattern in the Pt layer - either created naturally by thermal dewetting or artifically patterned - acts as crystallization seed. While the as-grown film is amorphous, post-deposition annealing at 700°C results in a lateral garnet crystallization rate of about 1 um/min and a single-crystalline garnet film on top of the Pt layer. This garnet film exhibits similar properties to an epitaxially grown film, including Gilbert damping as low as 0.008 [2]. Therefore, the lateral crystallization of garnet films opens up new possibilities to combine garnet and metal films for spintronic devices.

[1] Sailler, S. et al., Phys. Rev. Mater. 8, L020402 (2024).
[2] Holzmann, C. et al., Phys. Rev. Mater. 9, 114416 (2025).

MA 52.34 Thu 15:00 P4

FMR in chiral Mn_2TiO_4 — •Amruthavarshini Anand[1], Rajendra Loke[1], Ahmed Rasheed[1], Agustinus Agung Nugroho[2], and Joachim Hemberger[1] — [1]Institute of Physics II, University of Cologne, 50937 Cologne, Germany — [2]Institut Teknologi Bandung, Bandung 40116, Indonesia.

Ferromagnetic resonance (FMR) is a powerful technique for probing the dynamic magnetic properties of materials. In this study, we investigate FMR in Mn_2TiO_4, an inverse spinel tetragonal oxide. When Mn occupy full of tetrahedrally coordinated A site and half of B site, the space group $P4_322$, posses a chiral axis along c. Which via spin orbit coupling influences the magnetic resonance.

FMR measurements performed across different frequencies and magnetic field orientations allow us to extract resonance fields, linewidths, damping parameters, and magnetic anisotropy constants. Analysis of the FMR data using Kittel fitting enables determination of the frequency-field relationship, effective magnetization, and g-factors, while linewidth fitting provides quantitative values of the Gilbert damping parameter. And we also performed a FMR configuration with circularly polarized microwave excitation to enhance sensitivity to chiral magnetic effects and enable a more comprehensive investigation of the system's frequency- and field-dependent behaviour.

MA 52.35 Thu 15:00 P4

Magnetic interactions in compositionally complex and high entropy perovskites BaIn1-xMxO3-δ (M = Fe, Co, Sn, Ti) — •Auguste Stanionyte[1], Laura T. Corredor[2], Richard Matyšek[2,3], Anja U. B. Wolter[4], Giuditta Perversi[3], and Anna Isaeva[1,2] — [1]University of Amsterdam, The Netherlands — [2]TU Dortmund University and Research Center Future Energy Materials and

Systems, Germany — [3]Maastricht University, The Netherlands — [4]Leibniz IFW Dresden, Germany

High configurational entropy exerts unprecedented effects on a material's phase stability and functional properties and raises questions about possible interrelationships between the two.[1] In our recent work, the BaIn1-xMxO3-δ series were obtained as phase-pure cubic perovskites where Co, Fe, Sn, Ti and In share the B-site in increasing configurational entropy.[2] The present study investigates the magnetic behavior of these compounds. We observe antiferromagnetic-like behavior in the M(T) curves below 20 K, and varying levels of hysteresis in the M(H) experiments at 2K. Specific heat measurements show a field-dependent magnetic entropy release at low temperatures, but neutron diffraction rules out long-range order. With AC susceptibility measurements showing a shift in transition temperatures for higher frequencies, the study so far indicates a glassy magnetic structure with clusters. Altogether, our experimental results give an intriguing look into the emergent properties of such complex and disordered structures, but the exact microscopic mechanism remains to be uncovered. [1] Adv. Sci. (2022) 9, 2200391; [2] Solid State Ion. (2024) 427, 116901.

MA 52.36 Thu 15:00 P4

FMR in chiral Mn_2TiO_4 — •Amruthavsarshini Anand[1], Rajendra Loke[1], Ahmed Rasheed[1], Agustinus Agung Nugroho[2], and Joachim Hemberger[1] — [1]Institute of Physics II, University of Cologne, 50937 Cologne, Germany — [2]Institut Teknologi Bandung, Bandung 40116, Indonesia.

Ferromagnetic resonance (FMR) is a powerful technique for probing the dynamic magnetic properties of materials. In this study, we investigate FMR in Mn_2TiO_4, an inverse spinel oxide. The magnetic Mn^{2+} ions occupy tetrahedrally coordinated (A) sites and half of octahedrally coordinated (B) sites. The space group $P4_322$ possesses a chiral axis along c, which via spin orbit coupling influences the magnetic resonance.

FMR measurements performed across different frequencies allow us to extract resonance fields and linewidths for different crystal orientations. The data can be analysed using Kittel's formula revealing magnetic anisotropy constants and g-factor, while linewidth fitting provides quantitative values of the Gilbert damping parameter. We also utilise circularly polarized microwave excitation to directly address chirality and the resulting non-reciprocity of the magnetic response.

MA 52.37 Thu 15:00 P4

Emergent electromagnetic inductance of nontrivial magnetic textures in $SrRuO_3/SrIrO_3$ bilyers — •Ludwig Scheuchenpflug[1], Sebastian Esser[2], Robert Gruhl[1], Max Hirschberger[2,3], and Philipp Gegenwart[1] — [1]Universität Augsburg, Lehrstuhl für Experimentalphysik VI — [2]Department of Applied Physics, University of Tokyo, Japan — [3]RIKEN Center for Emergent Matter Science, Japan

Emergent electromagnetic induction (EEMI) by current-driven spin dynamics was proposed and observed in the spin helix magnet $Gd_3Ru_4Al_{12}$ [1], where the (current-nonlinear) imaginary impedance at kHz frequency was associated with the motion of helical spin structures.

To explore the possibility of EEMI arising from current-driven dynamics of nontrivial magnetic structures, we fabricated and microstructured epitaxial thin film bilayers of ferromagnetic $SrRuO_3$ and paramagnetic $SrIrO_3$ on STO. This bilayer system is suspected to host DMI-stabilized Néel-skyrmions, indicated by the topological Hall-effect (THE) [2]. We observe in AC-measurements a large and current-linear imaginary impedance at low temperatures over broad current density and frequency ranges, signaling the EEMI of nontrivial textures.

[1] Naoto Nagaosa, Jpn. J. Appl. Phys. (2019) 58 120909, Yokouchi et al., Nature 586, 232 (2020).

[2] J. Matsuno et al., Science Adv. 2 (2016) e1600304, S. Esser et al., Phys. Rev. B 103 (2021) 214430.

MA 52.38 Thu 15:00 P4

SQUID magnetometry of weakly diamagnetic samples using custom 3D-printed sample holders — •Thomas Kerschenbauer, Luca Bischof, and Rüdiger Klingeler — Kirchhoff Institut for Physics, Heidelberg, Germany

Magnetization studies of weakly diamagnetic samples by means of SQUID magnetometers using conventional sample holders often produce background signals comparable to the sample signal. Therefore, accurate background measurement and subtraction processes are necessary, which are challenging with conventional sample holders. Here, we present high-resolution magnetization data on representative diamagnetic samples, including the aromatic compounds naphthalene and anthracene. We obtained these results through SQUID measurements using custom sample holders designed for the Quantum Design MPMS 3 with SLA 3D printing technology. This offers a versatile and cost-effective solution for manufacturing improved sample holders. These sample holders allow us, e.g., to improve the positioning of the sample, which requires high precision for background subtraction. It also allows for flexibility in sample shape, size, and orientation. These improvements can be used to study weakly magnetic materials and enable measurements that are limited by background signals of conventional sample holders.

MA 52.39 Thu 15:00 P4

Quantitative Distance Calibration and Magnetic Noise Imaging with Scanning NV Magnetometry — •Nikhita Khera, Ephraim Spindler, Kristin Kuehl, and Elke Neu Ruffing — RPTU in Kaiserslautern, Rheinland Pfalz, Germany

Nitrogen-vacancy (NV) enters in diamond are widely used as quantum sensors for nanoscale magnetometry and the study of spin dynamics. As part of ongoing work using a Scanning NV Magnetometer, we report progress towards quantitatively calibrated scanning NV measurements and applications to low-magnetisation systems. A central part of this work is the calibration if the sensor sample distance for scanning NV tips, which is essential for reliable spatial resolution. Using perpendicular magnetic anisotropy (PMA) reference sample, we perform distance calibration and aim to determine the NV orientation in the tip. When combined with complementary approaches such as reverse AFM to determine the NV position within the tip, this enables access to the full three-dimensional localisation of the quantum sensor. Beyond calibration, we explore magnetic fluctuations in antiferromagnetic insulators by measuring the NV spin relaxation times T1, giving insight into their local magnetic noise and spin dynamics. We also use scanning NV magnetometers to map stray fields - from exfoliated 2D- hematite flakes revealing nanoscale field structures associated with antiferromagnetic domain structures, and from 3-D printed nickel microstructures. Altogether, this work pushes forward scanning NV magnetometry and showcases its use across a variety of magnetic materials.

MA 52.40 Thu 15:00 P4

User-Interactive Magnetic Field Characterization Employing a 3D Printer as a Three-Axis Motor Stage — •Daniel Feser[1,2], Nikolai Weidt[1,2], Nikita Popkov[2,3], Rico Huhnstock[1,2], and Arno Ehresmann[1,2] — [1]Institute for Physics and CINSaT, University of Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany — [2]AIM-ED, Joint Lab of Helmholtzzentrum für Materialien und Energie, Berlin (HZB) and University of Kassel, Hahn-Meitner-Platz 1, 14109, Berlin, Germany — [3]Intelligent Embedded Systems, University of Kassel, Wilhelmshöher Allee 71-73, 34121, Kassel, Germany

This project presents a flexible, user-interactive system for three-dimensional magnetic field mapping that repurposes a consumer-grade 3D printer as a precise three-axis positioning platform. A teslameter probe is mounted in a custom-designed and 3D-printed printhead, ensuring stable and accurate field measurements. The printer is controlled through Python-generated G-code, with device coordination handled via the Tango server framework. This system allows users to manually configure scan volumes, adjust measurement parameters, and safely map magnetic fields around sensitive samples while avoiding collisions. The acquired magnetic field data are processed and displayed as heatmaps, enabling intuitive analysis of spatial field variations. Overall, the platform demonstrates a low-cost, adaptable approach to magnetic field characterization using accessible hardware and open-source software.

MA 53: Members' Assembly

Time: Thursday 18:00–19:00 Location: HSZ/0002

All members of the Magnetism Division are invited to participate.

MA 54: Altermagnets VI

Time: Friday 9:30–12:30 Location: HSZ/0002

MA 54.1 Fri 9:30 HSZ/0002

A metallic p-wave magnet with commensurate spin helix — Rinsuke Yamada[1], •Jan Masell[2,3], Moritz M. Hirschmann[3], and Max Hirschberger[1,3] — [1]The University of Tokyo, Tokyo, Japan — [2]Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [3]RIKEN Center for Emergent Matter Science (CEMS), Wako, Japan

Antiferromagnetic states with a spin-split electronic structure give rise to spintronic, magnonic and electronic phenomena despite (near-)zero net magnetization. Even-parity spin-split magnets (d, g-wave) can be collinear and are known as altermagnets. Odd-parity magnets (p, f-wave) may be termed antialtermagnets and need co-planar magnetic order.[1] In this talk, we present our recent experimental realization of a metallic p-wave magnet, the simplest odd-parity spin-split magnet. [2] The magnetic texture is a coplanar spin helix whose magnetic period is an even multiple of the chemical unit cell, as revealed by X-ray scattering experiments. This texture breaks space-inversion symmetry but approximately preserves time-reversal symmetry up to a half-unit-cell translation, thereby fulfilling the symmetry conditions for p-wave magnetism. Consistent with theoretical predictions, our p-wave magnet shows a characteristic anisotropy in the electronic conductivity. Spin-orbit coupling and a tiny spontaneous net magnetization further break time-reversal symmetry, resulting in a giant anomalous Hall effect.

[1] A. B. Hellenes et al. arXiv2309.01607 (2024). [2] R. Yamada et al. Nature 646, 837 (2025).

MA 54.2 Fri 9:45 HSZ/0002

Giant Faraday Effect of magnon-polarons in the magnetoelectric altermagnet Fe2Mo3O8 — •Kirill Vasin[1], Sandor Bordács[2], Lilian Prodan[1], Vladimir Tsurkan[3], Istvan Kézsmárki[1], and Joachim Deisenhofer[1] — [1]University of Augsburg, Augsburg, Germany — [2]Budapest University of Technology and Economics, Budapest, Hungary — [3]Moldova State University, Chisinau, Republic of Moldova

We investigate magnetic circular dichroism of magnon-polarons in the polar altermagnet candidate $Fe_2Mo_3O_8$ using time-domain terahertz magnetospectroscopy. From linearly polarized measurements in Faraday geometry we reconstruct right- and left-circular transmission, revealing hybrid magnon-phonon branches which are fully circularly polarized below the Néel temperature. These magnon-polarons are both electric- and magnetic-dipole active and produce exceptionally large Faraday rotations in the terahertz range, with Verdet constant up to $\sim 4100^{\circ}/T/cm$. A suggested minimal circular-birefringent dielectric model captures both the magnitude and field dependence of the response.

MA 54.3 Fri 10:00 HSZ/0002

Mn4As3: a structure-search prediction of altermagnetism in a tetragonal Mn-As compound — •Bo Tai[1], Yu Zhu[1], Weikang Wu[2], and Xiaolong Feng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Straße 40, 01187 Dresden, Germany — [2]Key Laboratory for Liquid-Solid Structural Evolution and Processing of Materials, Ministry of Education, Shandong University, Jinan 250061, China

We predict that 2D Mn4As3 is a dynamically stable altermagnetic Mn-As compound obtained from an ab initio structure search. The search identifies a tetragonal P4/mmm structure as the lowest-energy configuration, and confirming its dynamical stability. Using first-principle calculation, we find 2D Mn4As3 (P4'/mm'm) breaks PT symmetry while preserving zero net magnetization, realizing an altermagnetic state. Spin-resolved band structures reveal characteristic momentum-dependent spin splitting: spin-up and spin-down bands are split along Γ-X and Γ-Y but remain degenerate along Γ-M, leading to a Fermi-surface spin texture with a d-wave-like pattern of spin splitting. Berry-curvature and transport calculations further show that rotating the magnetic moment (Néel vector) direction provides effective control over both the anomalous Hall conductivity and the positions of band crossings near the Fermi level. These results establish structure-searched Mn4As3 as a dynamically stable altermagnet and a promising platform for magnetization-direction control of Berry-phase transport in Mn-pnictides.

MA 54.4 Fri 10:15 HSZ/0002

Antichiral surface states in altermagnets — •Sopheak Sorn — Institute for quantum materials and technology, Karlsruhe Institute of Technology, Karlsruhe, Germany — Institute of theoretical solid state physics, Karlsruhe Institute of Technology, Karlsruhe, Germany

Altermagnets host symmetry-protected nodal lines and nodal planes in their band structures. In this talk, I will show how nodal lines in d-wave altermagnets give rise to unusual surface states that are antichiral. Antichiral surface states on two opposite surfaces of a slab geometry propagate parallel to one another, in contrast to the antiparallel propagation direction of chiral surface states. I demonstrate the presence of antichiral surface states using a tight-binding model. The antichiral character and many important features of the antichiral surface states are explained using a mapping from the altermagnetic model to Su-Schrieffer-Heeger chains: the topological index and the bulk-boundary correspondence of the latter explain the antichiral surface states. This work indicates that altermagnets are one of the few quantum materials that can support such antichiral surface states.

Reference [1] Sopheak Sorn, Antichiral surface states and Su-Schrieffer-Heeger physics in rutile altermagnets, Phys. Rev. B 111, L161109 (2025).

MA 54.5 Fri 10:30 HSZ/0002

Quantum Entanglement Signatures of Altermagnetism — •Mahsa Seyed Heydari, Wolfgang Belzig, and Sebastián A. Díaz — Universität Konstanz

In two-sublattice magnets in an antiferromagnetic configuration, the notion of two-mode squeezing is equivalent to quantum entanglement between the sublattice spins[1]. It has been shown that the logarithmic negativity is linearly related to the squeezing parameter. Altermagnets are a particular class of magnets which have a vanishing total magnetisation but a peculiar spin-polarization texture in momentum space. Using a simple model an altermagnet [2], we determine the magnon spectrum of an altermagnet and show that particular entanglement features witness the altermagnetic nature. Hence, we show that quantum magnonics offers a route towards distinguishing altermagnets from simple antiferromagnets, which is a difficult experimental task to date.

[1] Kamra, A.; Belzig, W. Phys. Rev. Lett. 2016, 116, 146601.
[2] Brekke, B.; Brataas, A.; Sudbø, A. Phys. Rev. B 2023, 108, 224421.

MA 54.6 Fri 10:45 HSZ/0002

Persistent altermagnetic spin polarisation — •Warlley H. Campos[1], Florette C. F. Mbognou[1], Anna B. Hellenes[2,3], Jan Priessnitz[1], and Libor Šmejkal[1,3] — [1]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany — [3]Institute of Physics, Czech Academy of Sciences, 162 00 Praha 6, Czech Republic.

Altermagnets exhibit d-, g-, or i-wave collinear spin polarisation of nonrelativistic exchange origin [1]. Relativistic spin-orbit coupling (SOC) is commonly considered to generate noncollinear spin textures in reciprocal space. Here, we demonstrate that collinear, persistent altermagnetic spin polarisation (PASP) in the full Brillouin zone is possible even in the presence of strong SOC. By combining spin and magnetic layer group analysis, we identify two distinct classes of PASP: one materialising on top of strong exchange spin splitting, and the other accompanying a typically weaker [2], relativistic spin splitting. We then perform *ab initio* calculations to realise the strong and weak types in Lieb-lattice [3-5] and cuprate altermagnets [1], respectively. Finally, we discuss experimental indication of weak PASP in MnTe [2]. PASP could enable strong spintronics currents with long spin lifetimes and efficient spin accumulation [5].

[1] L. Šmejkal *et al.*, Phys. Rev. X **12**, 031042 (2022). [2] Krempasky *et al.*, Nature (2024); A. Dal Din *et al.*, arXiv:2511.01690. [3] R. Jaeschke-Ubiergo *et al.*, arXiv:2503.10797. [4] N. Parthenios *et al.*, arXiv:2502.19270. [5] L.E. Golub *et al.*, arXiv:2503.12203.

15 min. break

MA 54.7 Fri 11:15 HSZ/0002

Spin Orbit Coupling Affecting the Presence of Altermagnetism in $La_2O_2TM_2OSe_2$, TM={Fe, Mn, $Fe_{0.5}Mn_{0.5}$} — •Tillmann Weinhold[1], Cornelius Herrmann[1], Domenic Nowak[2], Rowena Wachtel[2], Felix Seewald[1], Rajib Sarkar[1], Sabine Wurmehl[2], and Hans-Henning Klauss[1] — [1]Institute of Solid State and Materials Physics, IFMP, TUD Dresden University of Technology — [2]Leibniz Institute for Solid State and Materials Research, IFW, Dresden

Altermagnets are a recently discovered type of solid with magnetic order leading to zero net magnetization while providing spin-splitting effects of electron bands of up to multiple eV.

While hundreds of possible candidates have been found by analyzing proposed crystal and magentic structures, only few of them could be experimentally proven to be altermagnets by now.

By the use of local probe techniques we were able to precisely determine the magnetic structure of $La_2O_2Fe_2OSe_2$, a compound isostructural to two proposed altermagnets, namely $La_2O_2FeMnOSe_2$ and $La_2O_2Mn_2OSe_2$.

A comparison of these conclusions with upcoming results of the other two compounds can give strong indications or possibly even experimental verification of whether the magnetic phase of these materials is altermagnetic.

MA 54.8 Fri 11:30 HSZ/0002

Ultrafast carrier dynamics in the g-wave altermagnet $CoNb_4Se_8$ — •Alexander Schmid[1], Gregor Zinke[1,2], Resham B. Regmi[3], Luca Haag[2], Tobias Eul[1], Hans C. Schneider[2], Nirmal J. Ghimire[3], Martin Aeschlimann[2], and Benjamin Stadtmüller[1] — [1]University of Augsburg — [2]RPTU University Kaiserslautern-Landau — [3]University of Notre Dame, USA

Altermagnets have sparked considerable interest as a new type of compensated magnet with an unconventional spin splitting in momentum space that is rooted in the crystal and spin group symmetries of these materials.

In the manifold of altermagnetic candidates, intercalated transition metal dichalcogenides such as $CoNb_4Se_8$ have been identified as altermagnetic materials with characteristic g-wave spin splitting below 168 K. [1]

In our work, we used time- and momentum-resolved photoemission to gain insight into the ultrafast dynamics of the layered altermagnetic $CoNb_4Se_8$. Specifically, we focus on the ultrafast carrier dynamics near the characteristic spin-split bands at the M-point of the band structure, both in the altermagnetic and paramagnetic phases. This direct comparison allows us to uncover the impact of the spin and nodal plane structure of altermagnets on the ultrafast charge and spin carrier scattering. Our findings will be a vital first step toward understanding the optical response of altermagnets on ultrafast timescales.

[1] R. B. Regmi et al., Nat. Commun. 16, 4399 (2025)

MA 54.9 Fri 11:45 HSZ/0002

Emergent d-wave surface altermagnetism in G-type Heusler antiferromagnets V_3Al and V_2TiSi — •Ersoy Sasioglu, Ingrid Mertig, and Samir Lounis — Institute of Physics, Martin Luther University Halle-Wittenberg, 06120 Halle (Saale), Germany

Antiferromagnets that preserve combined inversion and time-reversal symmetry (PT) necessarily exhibit spin-degenerate electronic bands in the absence of spin-orbit coupling. Using density-functional theory, we show that asymmetric surface terminations of centrosymmetric G-type Heusler antiferromagnets lift the PT symmetry and give rise to an exchange-driven, nonrelativistic d-wave spin splitting, a mechanism we term *surface altermagnetism*. In the antiferromagnetic semimetal V_3Al, an experimentally established compound with $T_N \approx 700$ K, and in the antiferromagnetic semiconductor V_2TiSi, the interior layers of the slab retain the conventional compensated G-type order and spin-degenerate electronic structure, whereas inequivalent surface terminations induce pronounced d-wave spin splittings and metallic surface states localized on the outer transition-metal layers that decay exponentially toward the bulk. These results demonstrate that surface altermagnetism arises purely from lattice-symmetry breaking at asymmetric terminations, providing a robust, exchange-driven route to engineer spin-polarized metallic surface states in high-temperature G-type antiferromagnets without invoking spin-orbit coupling.

MA 54.10 Fri 12:00 HSZ/0002

P-wave magnetism with helical order — •Jaafar Ansari[1] and Libor Šmejkal[1,2,3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic

The emergent class of magnetic materials exhibiting p-wave [1] spin polarization represents a critical frontier in condensed matter physics for holding considerable promise for advanced spintronic architectures. Examples have been studied in commensurate and incommensurate p-wave structures with asymmetric spin polarizations [2-4]. This work presents a systematic theoretical classification of systems capable of realizing this unique band-structure symmetry, which is rooted in spin group theory. Our study focuses on helimagnets that do and do not generate p-wave order. By ab initio calculations we investigate the role played by broken inversion symmetry, noncollinearity of the spins, and the robustness of the p-wave polarisation against spin-orbit interaction. Our analysis characterizes the conditions under which the nominal p-wave symmetry is maintained, partially suppressed or entirely lost, and identifies material candidates. [1] Hellenes, A. B., et. al, arXiv.2309.01607 (2023), [2] Chakraborty, A., et al., Nat Commun 16, 7270 (2025), [3] Kim, S.-J, et. al., Adv. Sci. 11, 2307306 (2024), [4] Alvarez, N., Phys. Rev. B 112, 024404 (2025)

MA 54.11 Fri 12:15 HSZ/0002

Evidence for spin split bands in RuO_2 investigated by ultrafast magnetization dynamics — •Kevin Jäckel[1], Holger Grisk[1], Niklas Dornquast[1], Jakob Walowski[1], Markus Münzenberg[1], Maik Gaerner[2], Günter Reiss[2], and Timo Kuschel[2,3] — [1]University of Greifswald, Germany — [2]Bielefeld University, Germany — [3]Johannes Gutenberg University Mainz, Germany

In the search for new materials suitable for spintronic applications, the recently discovered altermagnets open up novel paths of research. In our work we focus on the proposed d-wave altermagnetic material RuO_2 by measuring its magnetic response to circularly polarized ultrashort laser pulses. Hereby we propose a way to link its ultrafast demagnetization dynamics, which are accessed by employing time-resolved magneto-optical Kerr effect measurements, to other, well established material systems such as semiconducting GaAs or topological insulators [1]. Therefore, we measure both the real and imaginary parts of the Kerr rotation, which are the Kerr angle and the Kerr ellipticity related to magnetic circular birefringence and dichroism. We see a strong, transient response, which scatters on a femtosecond timescale and can be described by the Raman coherence time.

[1] https://doi.org/10.1038/srep15304

MA 55: Skyrmions III

Time: Friday 9:30–12:45 Location: HSZ/0004

MA 55.1 Fri 9:30 HSZ/0004

RC circuit based on magnetic skyrmions — •Ismael Ribeiro de Assis, Ingrid Mertig, and Börge Göbel — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany

Skyrmions are nanosized magnetic whirls attractive for spintronic applications due to their innate stability. They can emulate the characteristic behavior of various spintronic and electronic devices such as spin-torque nano-oscillators, artificial neurons and synapses, logic devices, diodes, and ratchets. Here, we show that skyrmions can emulate the physics of an RC circuit-the fundamental electric circuit composed of a resistor and a capacitor-on the nanosecond time scale. The equation of motion of a current-driven skyrmion in a quadratic energy landscape is mathematically equivalent to the differential equation characterizing an RC circuit: the applied current resembles the applied input voltage and the skyrmion position resembles the output voltage at the capacitor. These predictions are confirmed via micromagnetic simulations. We show that such a skyrmion system reproduces the characteristic exponential voltage decay upon charging and discharging the capacitor under constant input. Furthermore, it mimics the low-pass filter behavior of RC circuits by filtering high frequencies in periodic input signals. Since RC circuits are mathematically equivalent to the leaky-integrate-fire (LIF) model widely used to describe biological neurons, our device concept can also be regarded as a perfect artificial LIF neuron.

MA 55.2 Fri 9:45 HSZ/0004

Accelerating Skyrmion-Based Computing via Oscillating Magnetic Fields — •Yuean Zhou[1], Thomas B. Winkler[2], Grischa Beneke[1], Fabian Kammerbauer[1], Robert Frömter[1], Giovanni Finocchio[3], Johan H. Mentink[2], Davi R. Rodrigues[4], and Mathias Kläui[1] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany — [2]Radboud University, Institute for Molecules and Materials, Netherlands — [3]Department of Mathematical and Computer Sciences, Physical Sciences and Earth Sciences, University of Messina, Italy — [4]Department of Electrical and Information Engineering, Politecnico di Bari, Italy

Skyrmion-based unconventional computing architectures, including stochastic, reservoir, and probabilistic computing [1], rely on stochasticity and dynamical transitions. However, pinning effects restrict mobility in realistic device geometries. To stably enhance the dynamics, we apply an additional oscillating out-of-plane magnetic field [2], and quantify the skyrmion motion in confined geometries using Markov State Models constructed from skyrmion trajectories recorded by Kerr microscopy. The diffusion enhancement shows a distinct maximum around 25 Hz and tapers off on either side, suggesting a stochastic-resonance-driven mechanism. Micromagnetic simulations qualitatively reproduce the resonance peak, supporting this interpretation. Controlled periodic driving thus provides an effective route to boost skyrmion dynamics for unconventional computing. [1] T.B. Winkler et al., arXiv:2508.19623 (2025) [2] R. Gruber et al., Adv. Mater. 2208922 (2023)

MA 55.3 Fri 10:00 HSZ/0004

Dipolar Skyrmion Continuum Mechanics — •Kilian Leutner[1], Klaus Raab[1], Grischa Beneke[1], Duc M. Tran[1], Sachin Krishnia[1], Robert Frömter[1], and Mathias Kläui[1,2] — [1]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany — [2]Center for Quantum Spintronics, Norwegian University of Science and Technology, 7491 Trondheim, Norway

Magnetic skyrmions–topological quasiparticle spin textures–offer a platform for both fundamental physics and applications [1]. In multilayer films, micrometer-scale skyrmions can emerge from dipolar interactions, and describing the long-timescale behavior of an ensemble requires multiscale modeling. We extend the Thiele equation by treating the skyrmion radius as a dynamic variable and derive the forces governing changes in both position and size from micromag-

netic theory. As a novel approach to describe ensemble dynamics, we develop a continuum-mechanics framework in which individual skyrmions are replaced by macroscopic fields such as density, velocity, and radius. The equation of state required for this description–relating pressure and density in the basic case–is calculated using dipolar-lattice theory [2]. We validate these two theoretical frameworks by examining how a spin-orbit torque compresses a skyrmion lattice in a Ta/CoFeB/MgO wire in an experiment. The continuum-mechanics model provides deeper insight into dipolar skyrmion ensembles as a hyperelastic medium composed of interacting particles of variable size.

[1] C. Back et al. J. Phys. D: Appl. Phys., 53, 363001 (2020).
[2] E. M. Jefremovas, K. Leutner et al. Newton, 1, 100036 (2025).

MA 55.4 Fri 10:15 HSZ/0004

Magnetoresistance and Planar Hall Effect in Noncollinear Magnets — •Juba Bouaziz[1,2], Hiroshi Ishida[3], Hiroshi Katsumoto[1], and Stefan Blügel[1,4] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich — [2]Faculty of Physics, University of Duisburg-Essen, 47057 Duisburg — [3]College of Humanities and Sciences, Nihon University, Tokyo — [4]Institute for Theoretical Physics, RWTH Aachen University, 52062 Aachen

Magnetotransport measurements are widely used to probe magnetic structures. We study how noncollinear magnetism modifies magnetoresistance (MR) and the planar Hall effect (PHE). In the weak-coupling limit, and using a multiple-scattering expansion of the electron current for Rashba-mediated conduction electrons [1], we show that noncollinearity introduces additional contributions to both MR and PHE. These arise from tilted magnetic moments and include a chiral MR term determined by the chirality of the magnetic structure. We also identify a noncollinear magnetoresistance (NCMR) contribution that persists even without Rashba spin-orbit interaction. Finally, we analyze the form and magnitude of these effects for different nanostructures, including magnetic trimers and topological spin textures such as skyrmions.

[1] J. Bouaziz et al., Phys. Rev. Lett. 126, 147203 (2021).

MA 55.5 Fri 10:30 HSZ/0004

Reorientation of skyrmion lattice with local magnetic field gradients — •Duc Tran[1], Edoardo Mangini[1], Elizabeth Jefremovas[1], Dennis Meier[2,3], Robert Frömter[1], and Mathias Kläui[1,2] — [1]Institute of Physics, Johannes Gutenberg University Mainz, 55128 Mainz, Germany — [2]Centre for Quantum Spintronics, NTNU, 7491 Trondheim, Norway — [3]Faculty of Physics, University of Duisburg-Essen, 45057 Duisburg, Germany

We present a minimally invasive approach for nucleating and manipulating skyrmion lattices in soft CoFeB multilayers using single-pass MFM. By matching the scan-line spacing to the domain periodicity, we drive reversible transitions from stripe domains to isolated skyrmions and locally ordered lattices using the field gradient generated by the magnetic tip. Skyrmion positions are used to calculate the local orientational order parameter ψ_6, allowing quantitative assessment of lattice order[1]. Repeated scanning leads to a systematic increase in $\langle|\psi_6|\rangle$, revealing a progression from a disordered configuration toward a well-ordered hexagonal lattice. We show that the lattice orientation can be directly controlled by altering the scanning direction, as verified through both real-space analysis and fast Fourier transforms. This technique enables on-demand creation, rearrangement, and deletion of metastable skyrmions, offering unprecedented control over lattice symmetry, ordering, and orientation[2].

[1] R. Gruber et al., Nat. Nanotechnol. 20, 1405–1411 (2025).
[2] D. Tran et al., Appl. Phys. Lett. (in press 2025), arXiv:2508.14771.

MA 55.6 Fri 10:45 HSZ/0004

Static and dynamic spin texture manipulation in Fe/Gd multilayers — Tim Titze[1], Sabri Koraltan[2,4], Timo Schmidt[3], Mailin Matthies[1], Florian Bruckner[2], Claas Abert[2], Amalio Fernández-Pacheco[4], Dieter Suess[2], Claus Ropers[5], Manfred Albrecht[3], Stefan Mathias[1], and •Daniel Steil[1] — [1]Georg-August-Universität Göttingen — [2]University of Vienna — [3]University of Augsburg — [4]Technical University of Vienna — [5]Max-Planck Institute for Multidisciplinary Sciences, Göttingen

Topological spin textures can be created, annihilated and manipulated in Fe/Gd multilayers using adiabatic and non-adiabatic external stimuli like temperature, magnetic fields and ultrashort light pulses. In this talk, I will show various ways to control magnetic spin textures statically and dynamically in $[Fe(0.35\ nm)/Gd(0.40\ nm)]_{160}$ multilayers, combining time-resolved magneto-optical Kerr spectroscopy with micromagnetic simulations and static magnetic imaging techniques. In particular, I will discuss different pathways for skyrmion creation [1,3], the use of in-plane fields as an additional control knob [4], as well as tailoring the skyrmion breathing mode using a two pulse excitation sequence [2].

[1] Adv. Funct. Mater. **34**, 2313619 (2024)
[2] Phys. Rev. Lett. **133**, 156701 (2024)
[3] Phys. Rev. B **112**, 064413 (2025)
[4] arXiv:2510.21320 (2025)

15 min break

MA 55.7 Fri 11:15 HSZ/0004

Effects of interlayer Dzyaloshinskii-Moriya interaction on the shape and dynamics of magnetic twin-skyrmions — •Tim Matthies[1], Levente Rózsa[2,3], Roland Wiesendanger[1], and Elena Vedmedenko[1] — [1]University of Hamburg, Hamburg, Germany — [2]Wigner Research Centre for Physics, Budapest, Hungary — [3]Budapest University of Technology and Economics, Budapest, Hungary

Magnetic skyrmions have been proposed as promising candidates for storing information due to their high stability and easy manipulation by spin-polarized currents. Here, we study how these properties are influenced by the interlayer Dzyaloshinskii-Moriya interaction (IL-DMI), which stabilizes twin-skyrmions in magnetic bilayers. We find that the spin configuration of the twin-skyrmion adapts to the direction of the IL-DMI by elongating or changing the helicities in the two layers. Driving the skyrmions by spin-polarized currents in the current-perpendicular-to-plane configuration, we observe significant changes either in the skyrmion velocity or in the skyrmion Hall angle depending on the current polarization. These findings unravel further prospects for skyrmion manipulation enabled by the IL-DMI.

MA 55.8 Fri 11:30 HSZ/0004

Current-Induced Skyrmion Dynamics and Diffusion — •Leonie-Charlotte Dany, Maarten Brems, Simon Fröhlich, Tobias Sparmann, Fabian Kammerbauer, Sachin Krishnia, Peter Virnau, and Mathias Kläui — Institute of Physics, Johannes Gutenberg University Mainz, 55128 Mainz, Germany

Magnetic skyrmions, nanoscale chiral spin textures with particle-like behavior, are promising candidates for information storage and unconventional computing due to their robustness and efficient current-driven motion [1-3]. In Ta/CoFeB/MgO multilayers, we investigate the transition of current-driven skyrmion motion from creep, through depinning, to the viscous flow regime driven by a unipolar, pulsed current. By varying current density, pulse width, and frequency, we demonstrate how external stimulation overcomes pinning potentials and enables skyrmions to enter into a regime characterized by linear velocity-current relations, i.e., the viscous flow regime. Additional studies with an alternating, net-zero current drive reveal an exponential increase of the diffusion coefficient with current density, while higher frequencies suppress diffusion following a power-law dependence. These findings provide quantitative insight into controlling skyrmion mobility and diffusion, essential for spintronic device design [4].

[1] G. Beneke *et al.*, *Nat. Commun.*, **15**, 8103 (2024).
[2] K. Raab *et al.*, *Nat. Commun.*, **13**, 6982 (2022).
[3] K. Everschor-Sitte *et al.*, *J. Appl. Phys.*, **124**, 24, 240901 (2018).
[4] L. Dany *et al.*, under preparation.

MA 55.9 Fri 11:45 HSZ/0004

Correlating on-the-fly Electrical and Optical Skyrmion Readout — •Grischa Beneke[1], Kilian Leutner[1], Nikhil Vijayan[1,2], Fabian Kammerbauer[1], Duc Minh Tran[1], Sachin Krishnia[1], Johannes Güttinger[2], Armin Satz[2], Robert Frömter[1], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Germany — [2]Infineon Technologies Austria AG, Austria

Magnetic skyrmions, topologically stabilized spin textures, are promising candidates for memory devices and non-conventional computing due to their stability, non-linear interactions, and low-power manipulation. However, reliable electrical readout of individual skyrmions remains a fundamental challenge, as current magnetic tunnel junction and anomalous Hall effect techniques fail to reliably detect single moving skyrmions. Our approach leverages thermally activated skyrmions, where a low constant drive current simultaneously drives skyrmion motion and the Hall voltage necessary for detection. We demonstrate reliability through real-time correlation between Hall voltage signals and direct Kerr microscopy imaging. Two consecutive Hall crosses enable skyrmion velocity determination in accordance with Kerr microscopy videos [1]. We present an analytical formula for the skyrmion AHE readout signal, demonstrating scalability from micrometer to nanometer dimensions. These advances establish a robust platform for skyrmion-based sensors, counters, and unconventional computing systems requiring precise individual skyrmion control and detection. [1] G. Beneke et al., Accepted for publication in Appl. Phys. Lett., arXiv:2508.15519 (2025).

MA 55.10 Fri 12:00 HSZ/0004

CNN-Based Classifier for Automated Identification of Magnetic States in Spin Dynamics Simulations — •Amal Aldarawsheh[1], Ahmed alia[2], and Stefan Blügel[1] — [1]Peter Grünberg Institute Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Institute for Advanced Simulation (IAS-7), Forschungszentrum Jülich, 52425 Jülich, Germany

The identification and classification of different magnetic states are essential for understanding the complex behavior of magnetic systems. Traditional approaches that rely on handcrafted features or manual inspection often fall short, particularly when dealing with subtle or topologically complex spin textures. In this study, we present an automated deep learning model that employs an

EfficientNetV1B0 Convolutional Neural Network to classify nine distinct magnetic states, including both FM and, for the first time, AFM spin textures such as AFM skyrmions and AFM stripe domains. The spin configurations are generated through atomistic spin dynamics simulations using the *Spirit* code, then visualized with VFRendering to produce RGB images, which serve as inputs to the classification model. To train and evaluate the model, we created a new dataset of manually labeled RGB images. Experimental results show that the proposed model achieves an accuracy and F1-score of 99%, significantly outperforming established deep learning baselines.

MA 55.11 Fri 12:15 HSZ/0004

Exchange striction model calculations for the skyrmion-containing compound $Gd_3Ru_4Al_{12}$ — •Justus Grumbach[1], Martin Rotter[2], and Mathias Doerr[1] — [1]Institut für Festkörper- und Materialphysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]McPhase Project, Sestiere Cannaregio 2904, 30121 Venezia, Italy

For the compound $Gd_3Ru_4Al_{12}$, we measured the complete dilatometric tensor, enabling a refinement of the phase diagrams in all crystallographic directions (see also the talk by M. Doerr). The most prominent feature is a lattice effect indicating a coupling of skyrmions to the crystal lattice, as previously evidenced by a docking of the propagation vector onto the crystal lattice. In the simulations, an approach for calculating the exchange striction was implemented that takes volume-influences into account and is particularly suitable for Gd-based compounds. Major aspects supporting our experimental results could be reproduced. The presentation will outline the full simulation process - from modeling, through the calculation of general magnetostrictive effects, to the influence of skyrmions - and conclude with a discussion of the volume effect in the skyrmion phase.

MA 55.12 Fri 12:30 HSZ/0004

Volume effect in Gd-containing skyrmion compounds — •Mathias Doerr[1], Justus Grumbach[1], and Maximilian Hirschberger[2] — [1]Technische Universität Dresden, Germany. — [2]University of Tokyo and RIKEN Center for Emergent Matter Science, Japan.

Skyrmions with a smaller characteristic wavelength are currently investigated in centrosymmetric compounds. The interplay between skyrmion lattices (SkL) and underlying crystallographic structures offers the possibility to determine the stability region of skyrmions by dilatometric measurements (thermal expansion and forced magnetostriction). Magnetostriction measurements on the two hexagonal metallic compounds $Gd_3Ru_4Al_{12}$ with a planar breathing kagome lattice and the triangular lattice magnet Gd_2PdSi_3 show a volume change (plateau phase) in the stability region of the skyrmion lattice, indicating the need for an unstrengthened crystal lattice for the formation of skyrmions. Another important result of our investigations was the refinement of the H-T phase diagrams for both investigated materials. The key results of the measurements were verified using a mean field calculation (see talk by J. Grumbach).

MA 56: Focus Session: (Anti)ferroic states – Magnetic and magnetoelectric III (joint session FM/MA)

chair: Morgan Trassin (ETH Zurich, CH)

This focus session explores recent advances in understanding and control of (anti)ferroic states. Emphasis will be placed on theoretical modelling, advanced characterization techniques, and the engineering of emergent properties for use in nano-electronic devices. The session aims to bridge fundamental research with emerging device-relevant functionalities, bringing together experimental, and theoretical perspectives on ferroic materials.

Time: Friday 9:30–11:30 Location: BEY/0E40

See FM 23 for details of this session.

MA 57: Thin Films: Magnetic Coupling Phenomena / Exchange Bias and Magnetic Anisotropy

Time: Friday 9:30–11:00 Location: POT/0112

MA 57.1 Fri 9:30 POT/0112

Angle-dependent magnetization reversal in perpendicular-anisotropy garnet films — •Senyin Zhu, Hanxu Zhang, Xianjie Wang, and Bo Song — Harbin Institute of Technology, Harbin 150001, China

Rare-earth-doped iron garnet (RIG) films with perpendicular magnetic anisotropy (PMA) offer a useful platform for studying angle-dependent magnetization reversal. The hysteresis behavior of Bi/La-doped thin RIG films was measured for magnetic-field orientations ranging from the in-plane direction, defined as 0°, to the out-of-plane direction at 90° and further up to 140°, enabling the identification of two distinct reversal regimes. For field orientations close to the film plane (0-50°), the reversal is governed by a continuous rotation of the magnetization, consistent with a uniform-state instability leading to a second-order phase transition. For field orientations close to the film normal (50-140°), the reversal is driven by domain nucleation with irreversible jumps, which is the characteristic signature of a first-order phase transition. The reversal mechanisms are consistent with the rotation- and nucleation-dominated processes known from metallic films.[1,2] In garnet film systems, however, the angular ranges at which these processes occur are shifted with respect to metallic films, most likely due to their stress-controlled perpendicular anisotropy and the larger exchange lengths.[1] O. Hovorka, A. Berger, and L. Fallarino, Phys. Rev. B 94, 064408 (2016). [2] R. Salikhov, F. Samad, L. Fallarino et al., Phys. Rev. B 110, 024417 (2024).

MA 57.2 Fri 9:45 POT/0112

Tailoring Magnetic Anisotropy Energy (MAE) with ion irradiation on Fe (110) — •Gabriel Gray[1], Kilian Lenz[1], Aleksandra Lindner[1], Fabian Ganss[1], Jürgen Fassbender[1], René Hübner[1], Rodolfo Gallardo[2], Pedro Landeros[2], and Jürgen Lindner[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Dresden, Germany — [2]Universidad Técnica Federico Santa María, Department of Physics, Valparaíso, Chile

Our research focuses on the changes in Magnetic Anisotropy Energies (MAE) in epitaxially grown Fe (110) thin films. We aim to create spatially defined regions with tunable magnetic anisotropies, modified through local ion implantation, in order to engineer spin textures and establish controllable spin-wave channels within the ferromagnetic thin film.

The Fe films were irradiated with Cr ions at varying kinetic energies and fluences. Subsequent magnetic characterization was performed using ferromagnetic resonance, while structural characterization was done by x-ray diffractometry, transmission electron microscopy and energy-dispersive x-ray spectroscopy.

Our results reveal a clear correlation between ion fluence and modifications in uniaxial magneto-crystalline anisotropy, while cubic anisotropy and the effective magnetization remain largely unaffected.

MA 57.3 Fri 10:00 POT/0112

Perpendicular magnetic anisotropy in Pt/Co/Cu heterostructures — •Anastasios Markou[1] and Ioannis Panagiotopoulos[2] — [1]Physics Department, University of Ioannina, 45110 Ioannina, Greece — [2]Department of Materials Science and Engineering, University of Ioannina, 45110 Ioannina,Greece

Magnetic multilayers with perpendicular magnetic anisotropy (PMA) formed by interfacing ferromagnetic layers with heavy-metal spin-orbit-coupled layers have received significant attention due to their tunable magnetic interactions and potential for stabilizing room-temperature topological magnetic textures. Inserting a 3d metal, such as Cu, at the interface between the ferromagnet and the heavy metal can break the symmetry of the adjacent interfaces and give rise to non-compensated asymmetric interactions, enhancing the chiral character of the system [1].

Here, we report on the magnetic properties of magnetron sputtered $[Pt/Co/Cu]_7$ multilayers with optimized deposition parameters to achieve high-quality interfaces and tunable PMA. We show that the magnetic properties can be tuned by varying the thickness of the 3d elements. PMA is observed over a broad range of Co and Cu thicknesses, demonstrating the crucial role of the Pt/Co interface, while the adjacent Cu layer provides an additional degree of freedom to tailor the effective interfacial anisotropy and magnetic coupling. These interfacial contributions are found to govern key properties such as coercivity, loop squareness, and the overall magnetization reversal behavior.

[1] H. Jia et al, Phys. Rev. Mater. 4, 024405 (2020).

MA 57.4 Fri 10:15 POT/0112

Large Microstructure-Dependent Magneto-Ionic Effects in Nanocrystalline Fe-Ni alloys — •Anna Ullrich[1], Florin Leo Hambeck[1], Raphael Kohlstedt[2,3], Sandra Schiemenz[4], Daniel Wolf[4], and Karin Leistner[1,3,4] — [1]Institute of Chemistry, Chemnitz University of Technology, Germany — [2]Institute of Physics, Chemnitz University of Technology, Germany — [3]Research Center MAIN, Chemnitz University of Technology, Germany — [4]Leibniz IFW Dresden, Germany

Magneto-ionic effects offer voltage-driven, energy-efficient control of magnetic properties via electrochemical reactions or ion migration.[1] Most studies focus on Co- or Fe-based systems,[2] recent research has reported similar effects in Ni,[3] prompting exploration in industrial relevant Fe-Ni alloys. We investigated magneto-ionic control in electrodeposited Fe-Ni thin films across the full compositional range using in situ MOKE microscopy.[4] Near-equiatomic films with mixed fcc/bcc phase and ultrafine grains show up to −90 % coercivity reduction at ~ 1 V. In situ Raman spectroscopy and structural characterization attribute the effect to dense grain boundaries and heterogeneous surface oxides, facilitating voltage-induced surface oxide reduction and magnetic softening. Our findings highlight the importance of microstructure in enhancing magneto-ionic functionality, providing guidelines for designing materials for sensing, actuation, and neuromorphic computing. [1] Leighton, Nat. Mater. 2019, 18, 13-18., [2] Nichterwitz et al., APL Mater. 2021, 9, 030903., [3] Kutuzau et al., Phys. Rev. Mater. 2025, 9, 114408., [4] Ullrich et al., Adv. Electron. Mater. 2025, e00654.

MA 57.5 Fri 10:30 POT/0112

Two-component anomalous Hall and Nernst effects in anisotropic $Fe_{4-x}Ge_xN$ thin films — •Jakub Vít[1], Petr Levinský[1], Robin K. Paul[2], Imants Dirba[2], and Karel Knížek[1] — [1]Institute of Physics, Prague, Czechia — [2]TU Darmstadt

50-500 nm thin films of $Fe_{4-x}Ge_xN$ (x=0–1) were fabricated onto MgO substrates by magnetron sputtering. The Hall and Nernst effects were measured, complemented with structural and magnetic characterizations, electron microscopy and DFT calculations. Fe_4N is cubic, whereas a small tetragonal distortion is found in $Fe_{4-x}Ge_xN$ films for x>0.35. The tetragonal samples with x=0.8 and 1 show two-component behavior in the Hall and Nernst effect hysteresis loops, which can be analyzed as a sum of positive and negative loops with different saturation fields. This unusual behavior is due to a combination of several factors: (1) Co-existence of two different crystallographic orientations in the tetragonal thin films. (2) Opposite sign of the anomalous Hall&Nernst effects (AHE&ANE) for the direction of magnetization along the a and c-axis. (3) Strong easy-plane magnetic anisotropy, responsible for different saturation fields for a and c-axis.

The maximum ANE was determined to be 0.9 V/K for x=0 at room temperature, and -0.85 V/K for x=1 at T=50 K. The rapid increase of ANE for Fe_3GeN from low temperatures indicates that, were it not for its low T_C (≈100 K), it could surpass ANE of Fe_4N. This observation is consistent with our theoretical assumptions and motivates further research of doped Fe_4N for which ANE enhancement is predicted by DFT calculations. (Preprint of this research: [arXiv 2511.14305])

MA 57.6 Fri 10:45 POT/0112

Voltage control of exchange bias in coupled spin-valve heterostructures — •Markus Gössler[1], Jonas Zehner[1,2], Rico Huhnstock[3], Falk Röder[2,4], Rico Ehrler[1], Olav Hellwig[1,5], Arno Ehresmann[3], and Karin Leistner[1] — [1]TU Chemnitz, Germany — [2]IFW Dresden, Germany — [3]University of Kassel, Germany — [4]IPF Dresden, Germany — [5]HZDR Dresden, Germany

Exchange bias can be described as a unidirectional magnetic anisotropy that arises at the interface of a ferromagnet and an antiferromagnet, which is commonly used to pin magnetization in magnetic devices. Typically, exchange bias is initiated only once via a field cooling procedure and cannot be easily modified thereafter. Here, we demonstrate the voltage control of exchange bias in a coupled spin-valve heterostructure via a magneto-ionic (i.e. electrochemical) approach. This is accomplished in a sputtered IrMn/Fe/Au/Fe/FeOx layer structure by modifying the Fe/FeOx top layer thicknesses via voltage-triggered electrochemical reduction/oxidation in an alkaline electrolyte.[1] Magnetic interlayer coupling between the exchange-biased (untreated) Fe layer and the top Fe layer through the Au spacer allows controlling exchange bias in this system by a top layer modification only. The reversibility in our heterostructures is significantly improved compared to the direct magneto-ionic treatment of exchange-biased Fe layers. Furthermore, by tailoring the layer structure we also demonstrate a reversible switching between single-step and double-step hysteresis loops,[1] which could pave the way for magnetic field sensors with adjustable sensitivity.

[1] M. Gößler et al., ACS Appl. Mater. Interfaces 17, 49671 (2025)

MA 58: Computational Magnetism II

Time: Friday 9:30–12:45 Location: POT/0151

MA 58.1 Fri 9:30 POT/0151

Prototype for Magnetic Multiscale Modelling Suite (MaMMoS) — •Hans Fangohr[1], Samuel RJ Holt[1], Martin Lang[1], Swapneel Pathak[1], Andrea Petrocchi[1], Wilfried Hortschitz[2], Santa Pile[2], Alena Vishina[3], M Nur Hasan[3], Georgia A Marchant[3], Timoteo Colnaghi[4], Christina Winkler[4], Jonas Winkler[5], Nora Dempsey[6], Thomas G Woodcock[5], Andreas Marek[4], Heike C Herper[3], and Thomas Schrefl[2] — [1]MPSD, Hamburg, Germany — [2]UWK, Krems, Austria — [3]Uppsala University, Sweden — [4]MPCDF, Garching, Germany — [5]IFW, Dresden, Germany — [6]Institute Neel, Grenoble, France

Magnetic materials require multiscale modelling across electronic, atomistic, micromagnetic and device levels. MaMMoS provides a unified Python framework that links these steps and avoids manual data translation. Based on ground-state magnetic parameters from DFT databases, it computes their temperature dependence using atomistic spin-dynamics, and passes them directly to micromagnetic solvers for modelling hysteresis and switching. Common analysis tools (e.g., coercivity, remanence) are included, and benchmarking and optimisation are possible. Planned extensions include machine-learning based modules to replace simulations with faster, approximate estimates. We present the current prototype to attract early adopters and invite community feedback.

Acknowledgements: This work is supported by the European Union's Horizon Europe research and innovation programme under grant agreement No. 101135546 (MaMMoS).

MA 58.2 Fri 9:45 POT/0151

A Fourier-Space Approach to Physics-Informed Magnetization Reconstruction from Nitrogen-Vacancy Measurements — •Alexander Setescak[1], Florian Bruckner[1], Dieter Suess[1], Young-Gwan Choi[2,3], Hayden Binger[2], Lotte Boer[2], Claire Donnelly[2], Uri Vool[2], and Claas Abert[1] — [1]University of Vienna, Vienna, Austria — [2]Max Planck Institute for the Chemical Physics of Solids, Dresden, Germany — [3]University of Ulsan, Ulsan, Republic of Korea

Reconstructing complex magnetization textures from nitrogen-vacancy (NV) magnetometry stray-field measurements presents a challenging inverse problem. In this work, we introduce a physics-informed method that addresses this by incorporating the full micromagnetic energy directly into the variational formulation.

Built on a PyTorch backend, our forward model integrates an auto-differentiable micromagnetic framework with FFT-based stray-field calculations and Fourier-space upward continuation. This enables efficient gradient-based optimization via the adjoint method and allows the sensor-sample distance to be treated as an optimization parameter. By doing so, we eliminate the experimental uncertainty arising from unknown NV implantation depths and surface oxidation layers.

Validation on synthetic data demonstrates high-fidelity reconstruction of spin textures and precise sensor height estimation. Furthermore, when applied to experimental NV measurements of the van der Waals magnet $Fe_{3-x}GaTe_2$, the framework reconstructs skyrmion bubbles that are consistent with theoretical micromagnetic behavior.

MA 58.3 Fri 10:00 POT/0151

First principals calculation of current-induced spin-transfer and spin-orbit torques — •Tamás Véber[1], László Oroszlány[1,2], Zoltán Tajkov[1,3], Marcell Sipos[1], and Branislav K. Nikolic[4] — [1]Eötvös Loránd University, Budapest, Hungary — [2]Wigner Research Centre for Physics, Budapest, Hungary — [3]HUN-REN Centre for Energy Research, Budapest, Hungary — [4]University of Delaware, USA

The study of two dimensional magnetic materials - especially those possessing strong spin-orbit coupling - has great promise both in terms of providing new theoretical discoveries, as well as practical applications like smaller and more energy efficient magnetoresistive RAM (MRAM) technologies. The theoretical study of such systems has been well-established in recent decades. However, no single ecosystem exists in which all the simulation and post-processing steps can be performed in a cohesive way. We aim to fill this gap by providing a chain of cross-compatible software for this purpose - and where it is possible, do this in the form of open-source libraries. In this work we lay out such an implementation for obtaining current-induced spin torques - like spin-transfer torque (STT) and spin-orbit torque (SOT) - in the linear response regime from ab initio results. We demonstrate this method on a set of magnetic two dimensional few-layer materials, comparing our results with the literature.

MA 58.4 Fri 10:15 POT/0151

Multi-spin Hamiltonians from symmetry considerations — •Levente Rózsa — HUN-REN Wigner Research Centre for Physics, Budapest, Hungary — Budapest University of Technology and Economics, Budapest, Hungary

Spin Hamiltonians are central to modeling magnetic materials. These Hamiltonians must reflect the symmetry of the underlying crystal [1]. Going beyond the most extensively studied two-spin interaction terms, for example the introduction of the isotropic biquadratic exchange interaction, has proven successful in describing special types of magnetic ordering in classical and quantum magnets. Four-spin generalizations of the anisotropic Dzyaloshinsky-Moriya interaction have also been proposed [2,3].

Here, we present a general formalism for deriving symmetry-adapted multi-spin interactions up to arbitrary order in the spin Hamiltonian. This method provides an alternative to perturbative expansions [2] which become difficult to tract as the number of spins and the complexity of the interactions increases. We identify all possible interaction terms containing four spins, and describe their transformation properties under rotations. We propose procedures for deriving these interactions from first-principles calculations, and for calculating the magnetic ground states stabilized by them.

[1] J. Bouaziz et al., Phys. Rev. B 112, 014406 (2025). [2] S. Brinker et al., New J. Phys. 21, 083015 (2019). [3] A. Lászlóffy, L. Rózsa et al., Phys. Rev. B 99, 184430 (2019).

MA 58.5 Fri 10:30 POT/0151

Above-Room-Temperature Magnetism in the Fe3GeTe2 and Fe3GaTe2 monolayer — •Anjali Jyothi Bhasu[1], Bendegúz Nyári[1], László Oroszlány[2], László Udvardi[1], and László Szunyogh[1] — [1]Department of Theoretical Physics, Budapest University of Technology and Economics, Budafoki ut 8., HU-1111 Budapest, Hungary — [2]Department of Physics of Complex Systems, Eötvös Loránd University, 1117 Budapest, Hungary

Room-temperature ferromagnetism that remains robust at the nanoscale is a key requirement for next-generation spintronic and information storage technologies. Using density-functional methods, we investigate monolayers of the van der Waals magnets Fe3GeTe2 and Fe3GaTe2, both of which exhibit magnetic ordering under ambient conditions. We compute the magnetic interaction parameters using the LKAG torque formalism as well as the spin-cluster expansion combined with the relativistic disordered local moment formalism. Special emphasis is placed on how these interactions vary with the Hubbard parameter U, which controls electron-electron correlations within the DFT+U framework. We then estimate the energetically favored magnetic structure by evaluating the Fourier transform of the tensorial coupling matrices. The order-disorder transition temperatures are obtained from large-scale Monte Carlo simulations, and we find that the simulated transition temperatures depend sensitively on the value of U.

MA 58.6 Fri 10:45 POT/0151

Micro and macroscopic quantum details of complex spin-textures — •Wenhan Chen[1,2], Sangeeta Sharma[1,3], and John Kay Dewhurst[2] — [1]Max-Born-Institut (MBI) im Forschungsverbund Berlin e.V,Max-Born-Str 2A, Berlin — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle (saale) — [3]Freie Universität Berlin, Berlin

Studying large-scale systems from first principles remains challenging because conventional DFT becomes prohibitively expensive. The recently proposed ultra-long-range DFT (ULR-DFT) aims to address this systematically while retaining full quantum-mechanical detail.

In our preliminary work, ULR-DFT successfully reproduces micrometre-scale ferromagnetic domains and domain walls, while also providing quantum-level information such as band structures and response functions. Applied to B20 chiral magnets, it captures helical states and skyrmion textures in agreement with experiments. Overall, ULR-DFT is promising for both fundamental research and device modelling, including band-structure engineering for spintronic applications.

15 min break

MA 58.7 Fri 11:15 POT/0151

Automated Defect Detection in Magnetic Imaging Data Using Latent Measures and U-Net Segmentation — •Ross Knapman[1,2], Nasim Bazazzadeh[1,3], Kübra Kalkan[1], Atreya Majumdar[1], and Karin Everschor-Sitte[1] — [1]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany — [2]Institute of Mechanics, Faculty of Engineering, University of Duisburg-Essen, 45141 Essen, Germany — [3]Radiology Department, Massachusetts General Hospital, 175 Cambridge St., Boston, MA 02114, USA

Detecting and characterising local inhomogeneities is essential for understanding and optimising magnetic materials. We present an automated framework that combines physics-based latent measures with deep convolutional segmentation for robust defect identification in magnetic imaging data. Time-resolved micromagnetic simulations with randomly distributed defects are used to compute three per-pixel descriptors: temporal mean, temporal standard deviation, and a latent-entropy measure that quantifies local dynamical complexity [1,2]. Each measure serves as input to a U-Net architecture trained for pixel-level segmentation of defect regions. Performance is evaluated under additive and multiplicative noise to test robustness. This approach demonstrates how integrating physics-motivated feature construction with deep learning enables reliable automated analysis of magnetic textures and defect landscapes in simulation and experiment.

[1] Horenko, I. et al., Comm. App. Math. and Comp. Sci 16, 267 (2021). [2] Rodrigues, D. R. et al., iScience 24, 102171 (2021).

MA 58.8 Fri 11:30 POT/0151

Dynamical mean-field theory for spin systems at finite temperature: cluster extension — •Przemyslaw Bieniek[1], Timo Grässer[2], and Götz Uhrig[1] — [1]Condensed Matter Theory, TU Dortmund University, Otto-Hahn-Str. 4, 44227 Dortmund, Germany — [2]Institute of Molecular Physical Science, ETH Zürich, Vladimir-Prelog-Weg 1-5/10, 8093 Zürich, Switzerland

Dynamical mean-field theory (DMFT) is an established numerical technique for approximately solving fermionic many-body problems. It maps the full quantum system to an impurity problem and uses a self-consistency condition to connect back to expectation values of the original model. In recent years, a method inspired by DMFT applicable to spin systems (spinDMFT) was developed. It is in agreement with numerical techniques and has already proven successful in explaining nuclear magnetic resonance experiments. However, it was derived only in the case of infinite temperature.

Based on spinDMFT, we develop a dynamical mean-field theory for spin systems at finite temperatures. The algorithm computes spin correlations in imaginary time. It maps the spin system to a single-site problem with a time-dependent mean field and uses a self-consistency condition to connect the values of the mean-field to quantum expectation values. The single-site approach is extended to a cluster algorithm, allowing for the computation of nonlocal expectation values. We benchmark the algorithm by comparing the resulting correlations with numerical approaches. We discuss the potential applications of the method and possible extensions.

MA 58.9 Fri 11:45 POT/0151

A Computational Framework for Bare and Interacting Longitudinal Susceptibility in Magnetic Materials — •Rohit Pathak[1], Vladislav Borisov[1,2], Mikhail I. Katsnelson[2,3], Anna Delin[4,5], and Olle Eriksson[1,2] — [1]Uppsala University, Sweden — [2]Wallenberg Initiative Materials Science for Sustainability, Uppsala, Sweden — [3]Radboud University, Netherlands — [4]KTH Royal Institute of Technology, Sweden — [5]Wallenberg Initiative Materials Science for Sustainability, Stockholm, Sweden

We present a computational framework for calculating the non-interacting and interacting spin susceptibilities in magnetic materials using the Relativistic Spin-Polarized Toolkit (RSPt) [1]. The ground-state electronic structure is obtained from self-consistent DFT calculations, followed by the computation of site-resolved Matsubara Green's functions, whose convolution yields the bare susceptibility. The interacting χ^{zz} is evaluated by solving the ADA–TDDFT Dyson equation $K = (1 - XU)^{-1}X$, based on previously developed theory [2]. Applications to bcc Cr, $BaFe_2As_2$, and FeSe show that the calculated $\chi(\mathbf{q})$ peaks reproduce the known magnetic ordering vectors. This framework enables systematic exploration of spin-density-wave phenomena in correlated electron systems.

[1] J. M. Wills, M. Alouani, P. Andersson, A. Delin, O. Eriksson, and O. Grechnyev, Full-Potential Electronic Structure Method (Springer, 2010).

[2] M. I. Katsnelson and A. I. Lichtenstein, J. Phys.: Condens. Matter 16, 7439 (2004).

MA 58.10 Fri 12:00 POT/0151

Proximity-Induced Magnetic Phases in CrI3 Monolayers Coupled to Transition-Metal Dichalcogenide Monolayer — •Zoltan Tajkov[1], Laszlo Oroszlany[1], Amador Garcia Fuente[2], Jaime Ferrer[2], Jaroslav Fabian[3], and Daniel Pozsar[1] — [1]Eotvos Lorand University, Budapest, Hungary — [2]University of Oviedo, Oviedo, Spain — [3]University of Regensburg, Regensburg, Germany

We investigate the emergence of altered magnetic phases in a CrI3 monolayer induced by proximity effects with WTe2. Using density functional theory (DFT) calculations within the SIESTA framework, we analyze the magnetic properties via a novel approach for extracting the magnetic exchange interaction and on-site anisotropy tensors in extended Heisenberg spin models, explicitly incorporating relativistic effects. This method, based on the Liechtenstein-Katsnelson-AntropovGubanov torque formalism, evaluates energy variations upon infinitesimal spin rotations. Our results provide insight into how a 2D magnet is influenced when coupled to a material with strong spin-orbit coupling. Additionally, we explore the impact of varying twist angles, considering the incommensurability of the CrI3 and WTe2 unit cells.

MA 58.11 Fri 12:15 POT/0151

Acoustic Wave Group Velocity under Magnetic Field — •Dominik Legut[1,2], Ievgeniia Korniienko[1], and Pablo Nieves[3] — [1]IT4Innovations, VSB-TU Ostrava, Ostrava, Czechia — [2]Charles University, Prague, Czechia — [3]University of Oviedo, Oviedo, Spain

Recently, we derived a spin-lattice model for ferromagnetic cubic crystals[1]. Then we analyzed the effect of the magneto-elasticity on the group velocities for high symmetry directions[2]. Here we present a different approach to determine the group velocity of the acoustic waves in any crystals and under the effects an external magnetic field for cubic and hexagonal symmetry. The group velocity is obtained by calculating Christoffel matrix elements and their partial derivative with respect to the phase velocity direction, and inserting them in an analytical expression for the group velocity. The effect of that external magnetic field is computed through the induced effective corrections to the elastic tensor which depend on the magnetic susceptibility tensor and the magnetoelastic constants. We present examples of dry sandstone, cubic CoPt and hcp Co to show complex landscapes of fractional change in group velocity as a function of ray direction, as well as a field dependence consistent with the Simon effect[3]. We have developed web-based applications where these effects can be analyzed and visualized in 3D[4].

[1] P. Nieves et al.: Phys. Rev. B **103**, 094437 (2021)
[2] P. Nieves et al.: Phys. Rev. B **105**, 134430 (2022)
[3] I. Korniienko, et al.: Results in Physics, **73**, 108264 (2025)
[4] P. Nieves et al.:, SoftwareX **33**, 102472 (2026)

MA 58.12 Fri 12:30 POT/0151

machine learning prediction of magnetic ordering in chiral induced multiferroic hybrid MOFs — •Gayathri Palanichamy, Biplab Sanyal, and Jonas Fransson — Materials Theory Division, Angstrom Laborartory, Uppsala Univesity, Sweden

Chiral hybrid metal organic frameworks with Ruddlesden Popper type halide layers provide a versatile platform for engineering multiferroicity by combining molecular chirality with transition metal magnetism. In this work, we develop a machine learning framework to identify multiferroic candidates in systems where chiral A-site organic molecules break inversion symmetry to induce ferroelectricity, while B-site transition metal centers govern magnetic ordering. First principles calculations confirm that the chiral distortion stabilizes a spontaneous polarization, and selected compositions exhibit coexisting ferroelectricity and ferromagnetism. To efficiently explore this large chemical and structural space, we construct feature descriptors capturing molecular chirality, distortion modes, metal ligand coordination metrics, and octahedral connectivity. Random Forest and Deep Neural Network models are trained to classify magnetic ground states (FM, AFM A, AFM C, AFM G) and achieve an R* score of 0.94, enabling reliable prediction of magnetic ordering across diverse chiral MOFs. Our approach also identifies previously unexplored chiral Ruddlesden Popper candidates with potential multiferroic behavior. This work establishes a data driven strategy toward building a chiral magnetic MOF repository, providing design principles for future spintronic and multifunctional materials.

MA 59: Magnonics III

Time: Friday 9:30–12:30 Location: POT/0361

MA 59.1 Fri 9:30 POT/0361

Magnetization dynamics in RMn_6Sn_6 crystals investigated by broadband ferromagnetic resonance spectroscopy — •Philipp Schwenke[1], David Weffling[1,3], Kyle Fruhling[2], Vitaliy Vasyuchka[1], Fazel Tafti[2], and Mathias Weiler[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]Department of Physics, Boston College, Chestnut Hill, MA 02467, USA — [3]Present address: Department of Physics and Materials Science, University of Luxembourg, L-4362 Esch-sur-Alzette, Luxembourg

The RMn_6Sn_6-material family is known for hosting complex magnetic orders [1]. Their Kagome and triangular lattices give rise to an unconventional band structure forming flat bands and Dirac cones leading to significant anomalous Hall- and Nernst-effects [2,3]. In this study, we investigate the magnetization dynamics of $ErMn_6Sn_6$ and $YbMn_6Sn_6$. We track characteristic phase transitions of the materials and the accompanying signatures in the magnetization dynamics over temperature. We find that the phase transitions are in agreement with previous results, while the spin dynamical signatures have not been discussed before. This study highlights the potential of using broadband ferromagnetic resonance spectroscopy to investigate the magnetic properties in RMn_6Sn_6

[1] L. Nil, *et. al*, Phys. Rev. B **111**, 054410 (2025)
[2] A. Bolens and N. Nagaosa, Phys. Rev. B **99**, 165141 (2019)
[3] K. Fruhling, *et. al*, Phys. Rev. Mat. **8**, 094411 (2021)

MA 59.2 Fri 9:45 POT/0361

Anisotropic magnon transports in van der Waals altermagnetic and ferromagnetic insulators — •Qirui Cui — Department of Applied Physics, School of Engineering Sciences, KTH Royal Institute of Technology, AlbaNova University Center, SE-10691 Stockholm, Sweden

Based on state-of-the-art first-principles calculations and model analysis [Nat. Rev. Phys. 5, 43-61 (2023)], we report the spin Seebeck effect (SSE) and spin Nernst effect (SNE) in vdW altermagnetic and ferromagnetic insulators, which are entirely independent of magnetic fields and spin-orbit coupling [Phys. Rev. B 108, L180401 (2023)]. In altermagnetic monolayers Cr2Te2O and Cr2Se2O, the breaking of combined symmetries of space inversion P, time reversal T, and translation τ, while preserving the combined symmetry of mirror M and τ, renders magnons with anisotropic spin-momentum locking, i.e., altermagnetic magnons. Interestingly, this spin-momentum locking gives rise to the SSE and SNE, with very efficient generation of longitudinal and transverse spin currents when the thermal gradient is aligned with and deviates from the main crystal axes, respectively. Moreover, anisotropic magnon dispersions are also realized in synthesized ferromagnetic monolayers CrPS4 and CrSBr, arising from C4 symmetry breaking-induced anisotropic exchange couplings [Adv. Funct. Mater. 35, 2407469 (2025)]. Consequently, without the magnetic field, the anisotropic SSE and the SNE emerge. These nontrivial magnonic transports can be further manipulated by the temperature and gate current.

MA 59.3 Fri 10:00 POT/0361

Magnon Shake-Up Enabling Quantum Features and Devices — •Vahid Azimi Mousolou — Department of physics and astronomy, Uppsala University

Shake-up effects, based on the sudden approximation and many-body quantum dynamics, reveal fundamental aspects of quantum systems and have broad applications in molecular spectroscopy and electronic structure analysis. Here, we present magnon shake-up patterns within magnetic systems [1], highlighting their significance in generating and detecting magnon entanglement and squeezing. This study offers new insights into shake-up phenomena in quantum magnonics and paves the way for novel developments in quantum technology.

[1] V. Azimi-Mousolou, A. Delin, E. Sjöqvist, O. Eriksson, Magnon Shake-up: Entanglement Generation and Sensing, arXiv:2503.20063 (2025).

MA 59.4 Fri 10:15 POT/0361

Optical vortex generation by magnons with spin-orbit-coupled light — •Ryusuke Hisatomi[1,2], Alto Osada[3], Kotaro Taga[1], Haruka Komiyama[1], Takuya Takahashi[1], Shutaro Karube[1,2], Yoichi Shiota[1,2], and Teruo Ono[1,2] — [1]Institute for Chemical Research, Kyoto University, Uji, Japan — [2]Center for Spintronics Research Network, Institute for Chemical Research, Kyoto University, Uji, Japan — [3]Center for Quantum Information and Quantum Biology (QIQB), Osaka University, Toyonaka, Osaka, Japan

Magneto-optic effects are generally described as the interaction between spin systems and collimated light (paraxial light). However, in many real-world systems studied in magneto-optics research, light focused by an objective lens (non-paraxial light) is utilized, which inherently exhibits optical spin-orbit coupling. Such spin-orbit-coupled light possesses a longitudinal electric-field component. Recently, we found that the interaction between spin-orbit-coupled light and collective spin dynamics (i.e., magnons) leads to optical vortex scattering, and we developed a theoretical framework to reproduce this phenomenon. The result provides the first step toward a comprehensive magneto-optics study incorporating optical vortices.

MA 59.5 Fri 10:30 POT/0361

Magnetization dynamics in YIG optomechanical crystals — •Matthias Grammer[1,2], Jonny Qiu[3], Sebastian Sailler[4], Sebastian T.B. Goennenwein[4], Matthias Althammer[1,2], Stephan Geprägs[1], Michaela Lammel[4], Eva Weig[3], and Hans Huebl[1,2] — [1]Walther-Meißner-Institut, BAdW, Garching, Germany — [2]School of Natural Sciences, TUM, Garching, Germany — [3]School of Computation, Information and Technology, TUM, Garching, Germany — [4]Department of Physics, University of Konstanz, Konstanz, Germany

Efficient transduction between microwave and optical photons is a key requirement for future quantum network applications. Recent studies have focused on freestanding magnetic nanostructures such as optomechanical crystals (OMC) based on yttrium iron garnet (YIG). These devices allow for co-localizing magnonic, elastic and photonic exitations in a single nanostructure. While the optical properties of a YIG OMC have already been experimentally shown [1], its magnonic and phononic modes have so far only been explored

through simulations. In this talk, we present an experimental investigation of the magnetic modes in a YIG OMC. For our proof of principle study, we fabricated a non-suspended YIG OMC on a GGG substrate using sputtering and lift-off techniques. We investigate the collective magnon modes using spacially resoved micro-focused magneto-optical Kerr effect measurements and categorize the observed modes using micromagnetic simulations.

[1] A. Rashedi et al., Phys. Rev. Applied 24, 054017(2025).

MA 59.6 Fri 10:45 POT/0361

Direct observation of magnetic vortex resonances on curvilinear surfaces — •Sabri Koraltan[1], Takeaki Gokita[1], Michal Krupinski[2], Sebastian Wintz[3], and Amalio Fernández-Pacheco[1] — [1]Insitute of Applied Physics, TU Wien, Vienna, Austria — [2]Institute of Nuclear Physics, Polish Academy of Sciences, Krakow, Poland — [3]Institute for Nanospectroscopy, Helmholtz-Zentrum Berlin, Berlin, Germany

Spin waves in magnonic systems offer energy-efficient alternatives to conventional electronics [1], with low-frequency magnetic vortex resonances being particularly relevant for microwave applications [2]. While planar magnetic vortices have been extensively studied [2], their dynamics in three-dimensional curvilinear architectures remain largely unexplored. Here, we present the direct experimental observation of vortex core gyration on a 3D curvilinear surface [3]. Using a stripline antenna on a SiN membrane, we excite self-assembled polystyrene spheres coated with NiFe, which host a vortex lattice state at remanence. Time-resolved scanning transmission X-ray microscopy (TR-STXM) at BESSY II [4] captures real-space, time-resolved dynamics, revealing complex spin-wave modes due to curvature-induced field gradients. Our results highlight the potential of curvilinear magnetic architectures for next-generation magnonic devices.

[1] Chumak, Andrii V., et al. Nature physics 11.6 (2015): 453-461. [2] Yu, Haiming, et al. Physics Reports 905 (2021): 1-59. [3] Koraltan, Sabri, et al. In Preparation (2026). [4] Koraltan, Sabri, et al. Science Advances 10.39 (2024): eado8635.

15 min break

MA 59.7 Fri 11:15 POT/0361

Direction Selective Spin Waves Imaging in Microstructures — •Roméo Beignon[1], Chris Köerner[2], Rouven Dreyer[2], Zeling Xiong[3], Katrin Schultheiss[3], Helmut Schultheiss[3], Vincent Jacques[1], Georg Woltersdorf[2], and Aurore Finco[1] — [1]Laboratoire Charles Coulomb, Université de Montpellier, CNRS, Montpellier, France — [2]Martin Luther University Halle-Wittenberg, Halle, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Institut für Ionenstrahlphysik und Materialforschung, Dresden, Germany

Spin waves can be generated and manipulated at the nanoscale using patterned microstructures and magnetization features. Harnessing these effects is key to the development of magnonic devices. With scanning NV microscopy, we are able to image spin waves with a spatial resolution of about 50 nm. Simultaneously, we probe the stray field produced by non-uniform static magnetic textures hosted in the microstructures and explore their interactions with spin wave modes.

Here, we apply this technique to observe spin waves in Permalloy microstructures. We first investigate spin waves generated via scattering and measure their dispersion relation. Then, we show that the NV center is sensitive to the handedness of the circularly polarized field emitted by spin waves. We can thus selectively image spin waves propagating in different directions and study how they interact with the edges of the Py structure. Finally, we observe discrete magnon modes with high azimuthal indices in disks featuring a vortex state. These measurements open the way to understanding complex non-linear dynamic phenomena in magnetic microstructures.

MA 59.8 Fri 11:30 POT/0361

Time domain correlation spectroscopy of thermal and nonequilibrium magnons — •F. S. Herbst[1], M. A. Weiss[1], C. Runge[1], N. Beaulieu[2], J. B. Youssef[2], A. Leitenstorfer[1], M. Lammel[1], R. Schlitz[1], and S. T. B. Goennenwein[1] — [1]Department of Physics, University of Konstanz, Germany — [2]LabSTICC, CNRS, Université de Bretagne Occidentale, France

Yttrium iron garnet (YIG) is a prototypical material for spintronics and magnonics due to its low magnetic damping and high spin wave propagation velocities. The properties of coherently excited, standing spin waves are well understood. However, much less is known about the interplay between coherently excited magnons and incoherent fluctuations, as schemes simultaneously resolving both coherent and incoherent contributions in a single measurement are scarce. In this work, we probe bismuth doped YIG with femtosecond noise correlation spectroscopy (FemNoC), an optical technique probing magnetization dynamics in the time domain. This method enables us to simultaneously investigate both the thermal magnon noise background and the coherent magnon response induced by microwave excitation. Using a phenomenological model, we can fit both the waveform and amplitude of the experimental data. This step allows us to quantify and disentangle the respective contributions by their correlation signature. Consequently, FemNoC gives access to the absolute magnon number of a magnetic system in the time domain.

MA 59.9 Fri 11:45 POT/0361

Nonlinearly controllable magnonic mode-converter in a synthetic antiferromagnet — •Mujin You[1,2], Moojune Song[2], Jun Seok Seo[2], Sanghoon Kim[3], Yoichi Shiota[4], Teruo Ono[4], Se Kwon Kim[1], Albert M. Park[2], Kab-Jin Kim[2], Mathias Weiler[1], and Philipp Pirro[1] — [1]Fachbereich Physik and Landesforschungszentrum OPTIMAS, Rheinland-Pfälzische Technische Universität Kaiserlautern-Landau, Germany — [2]Department of Physics, Korea Advanced Institute of Science and Technology (KAIST), Korea — [3]Department of Nanosemiconductor Engineering, University of Ulsan, Korea — [4]Institute for Chemical Research, Kyoto University, Uji, Japan

Exploring and controlling nonlinear regimes enables new functionalities in hybrid magnonic systems, including phenomena such as nonlinear anticrossing gap closure and bistability in magnon dispersion. In this work, we observe mode hopping between acoustic and optic modes in a SAF, occurring at the magnetic field where the optic frequency becomes twice the acoustic frequency-consistent with a three-magnon interaction process. Based on this nonlinear mode-hopping behavior, we demonstrate an electrically tunable, nanoscale GHz-range mode-converter. These findings reveal a promising application via nonlinear coupling between acoustic and optic magnons in SAFs, paving the way for energy-efficient, reconfigurable magnonic devices.

MA 59.10 Fri 12:00 POT/0361

$\mathbb{Z}$ Topological Index for 3D Hamiltonians based on Lattice Gauge Theory — Nastaran Salehi and •Manuel Pereiro — Department of Physics and Astronomy, Uppsala University, Box 516, SE-751 20 Uppsala, Sweden

The characterization of topological phases in three-dimensional (3D) systems often requires extending concepts well-established in two dimensions (2D). We propose a robust method for calculating an integer topological invariant, akin to the Chern number, for 3D Hamiltonians with periodic boundary conditions. This approach utilizes conceptual elements derived from lattice gauge theory, defining the invariant over a discretized Brillouin zone (a 3-torus, T^3). By constructing U(1) link variables from the Bloch wavefunctions, we define a gauge-invariant quantity from Wilson loops over elementary 3D plaquettes (cubes) in k-space. The resulting topological index is an integer, reflecting the classification of principal fiber bundles $T^3 \times U(1)$ and related to the homotopy group $\pi_3(\mathbb{P}^2(\mathbb{R})) \cong \mathbb{Z}$. This method is general and computationally efficient, avoids issues with band degeneracies, and provides a unique integer invariant for each band. We adapt the method for magnetic Hamiltonians and showcase its effectiveness with two examples: firstly, a 3D Kagome lattice model, and secondly, a realistic material, Mn_3Se, for which the magnon spectra is obtained by employing electronic structure first-principles calculations.

MA 59.11 Fri 12:15 POT/0361

Second-Chern Topology of 3D Magnon Bands via a Field-Angle Pump — •Nastaran Salehi and Manuel Pereiro — Department of Physics and Astronomy, Uppsala University, Box 516, SE-751 20 Uppsala, Sweden

We present a general framework to realize second-Chern topology in three-dimensional (3D) bosonic Bogoliubov-de Gennes (BdG) bands by augmenting the Brillouin zone with a slow, cyclic control parameter, yielding a 4D manifold $\mathbf{T}^3 \times S^1$. Using the bosonic metric Σ_3 and paraunitary gauge, we define the non-Abelian Berry connection/curvature for isolated positive-norm band bundles and an integer invariant $C_2 \in \mathbf{Z}$. We prove that C_2 quantizes an adiabatic transport: across a slab, the pumped conserved quantity (spin for magnons) per 2π cycle is an *integer* set by C_2, and the corresponding current is proportional to $\dot{\phi}$. We introduce a stable lattice algorithm, based on Σ_3-polar link variables, that is gauge covariant and robust in the presence of degeneracies. For the sake of concreteness and pedagogical clarity, we carry out the full derivation in a kagome-based 3D magnet, where a field-angle cycle drives a topological spin flow detectable via inverse spin Hall voltages in Pt contacts on opposing faces. Although illustrated for magnons, the construction applies broadly to quadratic bosonic BdG systems, including phononic and photonic analogues.

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Overview of Invited Talks and Sessions

(Lecture halls SCH/A215, SCH/A216, SCH/A251, and SCH/A315; Poster P5)

Invited Talks

MM 2.1	Mon	9:30–10:00	SCH/A251	**Deep-Learning and Generative AI for the Discovery of Electron-Phonon Superconductors** — •Richard Hennig
MM 6.1	Mon	15:00–15:30	SCH/A251	**Transformation-induced plasticity in zirconia ceramics: simulations and experiments** — •David Rodney
MM 10.1	Tue	9:30–10:00	SCH/A251	**Chemically graded materials for accelerated exploration of the TRIP-TWIP Ti-alloy family** — •Lola Lilensten
MM 24.1	Wed	15:00–15:30	SCH/A251	**Recent advances in processing of rare-earth free MnBi magnets by severe plastic deformation** — •Andrea Bachmaier, Lukas Weissitsch-Reiner, Martin Kraus, Michael Meindlhumer, Stefan Wurster
MM 29.1	Thu	9:30–10:00	SCH/A251	**Three dimensional sub-Ångström resolution imaging from 4D-STEM experiments** — •Philipp Pelz
MM 33.1	Thu	15:00–15:30	SCH/A251	**LPBF with Ultrashort Laser Pulses - Additive Manufacturing Beyond Current Limits** — •Stefan Nolte, Hagen P. Kohl, Lisa Matthäus, Tobias Ullsperger, Dongmei Liu, Stephanie Lippmann
MM 38.1	Fri	9:30–10:00	SCH/A251	**Alloy design and deformation behaviour of Mo-based silicide materials** — •Manja Krueger

Invited Talks of the joint Symposium SKM Dissertation Prize 2026 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	HSZ/0002	**Stochastic-Calculus Approach to Non-equilibrium Statistical Physics** — •Cai Dieball
SYSD 1.2	Mon	10:00–10:30	HSZ/0002	**Nonuniform magnetic spin textures for sensing, storage and computing applications** — •Sabri Koraltan
SYSD 1.3	Mon	10:30–11:00	HSZ/0002	**Anomalous Quantum Oscillations beyond Onsager's Fermi Surface Paradigm** — •Valentin Leeb
SYSD 1.4	Mon	11:00–11:30	HSZ/0002	**Coherent Control Schemes for Semiconductor Quantum Systems** — •Eva Schöll
SYSD 1.5	Mon	11:30–12:00	HSZ/0002	**On stochastic thermodynamics under incomplete information: Thermodynamic inference from Markovian events** — •Jann van der Meer

Invited Talks of the joint Symposium The Sustainability Challenge: A Decade of Transformation (SYSC)

See SYSC for the full program of the symposium.

SYSC 1.1	Mon	15:00–15:30	HSZ/AUDI	**Open-Endedness and Community-Based Approaches to Sustainability Challenges** — •Hiroki Sayama
SYSC 1.2	Mon	15:30–16:00	HSZ/AUDI	**Education as a Social Tipping Element: Evidence from Climate and Physics Education Research** — •Thomas Schubatzky
SYSC 1.3	Mon	16:00–16:30	HSZ/AUDI	**Mechanistic and Material Perspectives on Enzymatic Hydrolysis of Semicrystalline Polyesters** — •Birte Höcker
SYSC 1.4	Mon	16:45–17:15	HSZ/AUDI	**Decarbonization Options for Industry** — •Uwe Riedel
SYSC 1.5	Mon	17:15–17:45	HSZ/AUDI	**Impacts of Cosmic Dust and Space Debris in the Terrestrial Atmosphere** — •John Plane

Invited Talks of the joint Symposium AI and Data Challenges behind Emerging Self-Driving Laboratories (SYAI)

See SYAI for the full program of the symposium.

SYAI 1.1	Thu	9:30–10:00	HSZ/AUDI	**Data and Experimental Foundations for Reliable Self-Driving Laboratories** — •Dr. Marcus Tze-Kiat Ng
SYAI 1.2	Thu	10:00–10:30	HSZ/AUDI	**Digital Catalysis - AI for Experiment Planning and Control** — •Christoph Scheurer
SYAI 1.3	Thu	10:30–11:00	HSZ/AUDI	**Autonomous, Data-Driven Workflows for Materials Acceleration Platforms with pyiron** — •Jan Janssen, Joerg Neugebauer
SYAI 1.4	Thu	11:15–11:45	HSZ/AUDI	**Machine Learning for Autonomous Optimization and Discovery of Materials** — •Pascal Friederich
SYAI 1.5	Thu	11:45–12:15	HSZ/AUDI	**Transforming Our View on Transformers in the Sciences** — •Kevin Maik Jablonka

Sessions

MM 1.1–1.1	Sun	16:00–18:15	TRE/MATH	**Hands on tutorial: Linking Large Language Models with Digital Workflows for Materials Science Simulations (joint session MM/TUT)**
MM 2.1–2.1	Mon	9:30–10:00	SCH/A251	**Invited Talk: Richard Hennig**
MM 3.1–3.9	Mon	10:15–12:45	SCH/A215	**Mechanical Properties and Alloy Design I**
MM 4.1–4.9	Mon	10:15–13:00	SCH/A216	**Materials for the Storage and Conversion of Energy I**
MM 5.1–5.7	Mon	10:15–12:45	SCH/A251	**Topical Session: Physics-driven Artificial Intelligence for Materials I**
MM 6.1–6.1	Mon	15:00–15:30	SCH/A251	**Invited Talk: David Rodney**
MM 7.1–7.10	Mon	15:45–18:30	SCH/A215	**Mechanical Properties and Alloy Design II**
MM 8.1–8.10	Mon	15:45–18:30	SCH/A216	**Materials for the Storage and Conversion of Energy II**
MM 9.1–9.9	Mon	15:45–18:30	SCH/A251	**Topical Session: Physics-driven Artificial Intelligence for Materials II**
MM 10.1–10.1	Tue	9:30–10:00	SCH/A251	**Invited Talk: Lola Lilensten**
MM 11.1–11.6	Tue	10:15–11:45	SCH/A215	**Structurally and Chemically Complex Alloys**
MM 12.1–12.9	Tue	10:15–12:45	SCH/A216	**Materials for the Storage and Conversion of Energy III / Functional Materials I**
MM 13.1–13.9	Tue	10:15–12:45	SCH/A251	**Data-driven Materials Science: Big Data and Workflows I**
MM 14.1–14.5	Tue	11:30–12:45	SCH/A315	**Liquid and Amorphous Materials I**
MM 15.1–15.7	Tue	14:00–15:45	SCH/A215	**Phase Transformations I**
MM 16.1–16.7	Tue	14:00–15:45	SCH/A216	**Functional Materials II**
MM 17.1–17.7	Tue	14:00–15:45	SCH/A251	**Data-driven Materials Science: Big Data and Workflows II**
MM 18.1–18.6	Tue	14:00–15:30	SCH/A315	**Liquid and Amorphous Materials II**
MM 19.1–19.49	Tue	18:00–20:00	P5	**Poster Session**
MM 20.1–20.1	Wed	9:30–10:00	SCH/A251	**Topical Talk: Shigenobu Ogata**
MM 21.1–21.10	Wed	10:15–13:00	SCH/A215	**Phase Transformations II**
MM 22.1–22.9	Wed	10:15–12:45	SCH/A216	**Data-driven Materials Science: Big Data and Workflows III**
MM 23.1–23.5	Wed	10:15–11:30	SCH/A251	**Topical Session: Dislocations in Functional Materials I (joint session MM/FM)**
MM 24.1–24.1	Wed	15:00–15:30	SCH/A251	**Invited Talk: Andrea Bachmaier**
MM 25.1–25.5	Wed	15:45–17:00	SCH/A215	**Interface Controlled Properties, Nanomaterials, and Microstructure Design I**
MM 26.1–26.5	Wed	15:45–17:00	SCH/A216	**Transport in Materials: Diffusion, Charge, or Heat Conduction I**
MM 27.1–27.5	Wed	15:45–17:15	SCH/A251	**Topical Session: Dislocations in Functional Materials II (joint session MM/FM)**
MM 28	Wed	17:15–18:45	SCH/A251	**Members' Assembly**
MM 29.1–29.1	Thu	9:30–10:00	SCH/A251	**Invited Talk: Philipp Pelz**
MM 30.1–30.6	Thu	10:15–11:45	SCH/A215	**Interface Controlled Properties, Nanomaterials, and Microstructure Design II**
MM 31.1–31.10	Thu	10:15–13:00	SCH/A216	**Transport in Materials: Diffusion, Charge, or Heat Conduction II**
MM 32.1–32.6	Thu	10:15–12:45	SCH/A251	**Topical Session: Advanced Nanomechanics – Accelerating Materials Physics from the Bottom I**
MM 33.1–33.1	Thu	15:00–15:30	SCH/A251	**Invited Talk: Stefan Nolte**
MM 34.1–34.7	Thu	15:45–17:30	SCH/A215	**Hydrogen in Materials I**
MM 35.1–35.7	Thu	15:45–17:30	SCH/A216	**Additive Manufacturing / Transport in Materials III**
MM 36.1–36.5	Thu	15:45–17:15	SCH/A251	**Topical Session: Advanced Nanomechanics – Accelerating Materials Physics from the Bottom II**
MM 37.1–37.5	Thu	15:45–17:00	SCH/A315	**Development of Calculation Methods I**

MM 38.1–38.1	Fri	9:30–10:00	SCH/A251	**Invited Talk: Manja Krüger**
MM 39.1–39.9	Fri	10:15–12:45	SCH/A215	**Hydrogen in Materials II**
MM 40.1–40.8	Fri	10:15–12:30	SCH/A216	**Transport in Materials: Diffusion, Charge, or Heat Conduction IV**
MM 41.1–41.9	Fri	10:15–12:45	SCH/A251	**Development of Calculation Methods II**

Members' Assembly of the Metal and Material Physics Division

Wednesday 17:15–18:45 SCH/A251

- discussion of MM activities
- announcement of the poster awards
- exchange of ideas for the next DPG meeting

Sessions

– Invited Talks, Topical Talks, Tutorials, Contributed Talks, and Posters –

MM 1: Hands on tutorial: Linking Large Language Models with Digital Workflows for Materials Science Simulations (joint session MM/TUT)

Advanced computational simulations often require chaining several models and software packages together, a process that demands careful workflow management. In this tutorial you can gain hands-on experience with the Python based workflow environment pyiron (www.pyiron.org). Participants in the tutorial will be able to run all the examples shown in the presentation interactively on their own laptops. There is no need to install any code, just a standard web browser to explore the applications interactively.

Time: Sunday 16:00–18:15 Location: TRE/MATH

Tutorial MM 1.1 Sun 16:00 TRE/MATH

Hands on tutorial: Linking large language models with digital workflows for materials science simulations — •Jörg Neugebauer[1], Tilmann Hickel[1,2], and Ralf Drautz[3] — [1]Max Planck Institute for Sustainable Materials — [2]Bundesanstalt für Materialforschung und -prüfung — [3]ICAMS, Ruhr Universität Bochum

Advanced computational simulations now reliably predict material properties, but they often require chaining several models and software packages together, a process that demands expert knowledge and careful workflow management. Efficient, reproducible research therefore hinges on automated workflow tools that can handle this complexity. In this tutorial we introduce pyiron (www.pyiron.org), a Python based workflow environment for building and executing fully automated simulation pipelines. We show how complex simulations workflows can be constructed programmatically via Python code as well as via a flow-based graphical user interface. We further introduce how large language models (LLMs) can be embedded to streamline the "human in the loop" tasks. After a brief overview of pyiron's core concepts, we construct workflows for computing ab initio thermodynamic bulk phase diagrams. The necessary steps, such as density functional theory calculations, training ACE-based machine learning potentials, and exploring phase stability using foundational models like GRACE, are all performed within pyiron workflows. Participants will learn how to develop and integrate such workflows into their own materials science simulations, thereby enabling faster, more transparent, and more reproducible research.

MM 2: Invited Talk: Richard Hennig

Time: Monday 9:30–10:00 Location: SCH/A251

Invited Talk MM 2.1 Mon 9:30 SCH/A251

Deep-Learning and Generative AI for the Discovery of Electron-Phonon Superconductors — •Richard Hennig — University of Florida, Gainesville, Florida, USA

The search for new superconductors with higher critical temperatures, T_c, and critical fields, H_c, is limited by the cost of electron-phonon calculations and the vastness of compositional and structural space. To overcome both obstacles, we develop an integrated deep-learning workflow for conventional, electron-phonon-mediated superconductors.

First, we introduce BEE-NET, an ensemble of equivariant graph neural networks trained to predict the Eliashberg spectral function $\alpha^2F(\omega)$ and T_c directly from crystal structures, optionally augmented by the phonon density of states. Unlike traditional approaches that learn T_c directly, predicting $\alpha^2F(\omega)$ treats superconductors and non-superconductors on equal footing and, together with explicit phonon-spectrum information, leverages electron-phonon physics to improve predictions for rare superconducting materials. Embedded in a multi-stage screening pipeline that combines elemental substitution strategies with machine-learned interatomic potentials, BEE-NET scans over 1.3×10^6 candidate structures and down-selects to 741 dynamically and thermodynamically stable compounds with DFT-confirmed $T_c > 5$ K, including two experimentally realized new superconductors.

Finally, I will briefly show how guided diffusion models for crystal structures and our Open Materials Generation (OMatG) framework based on stochastic interpolants extend this physics-informed, data-driven approach to the generative design of new superconductors.

MM 3: Mechanical Properties and Alloy Design I

Time: Monday 10:15–12:45 Location: SCH/A215

MM 3.1 Mon 10:15 SCH/A215

Mechanical Properties of Disordered Fe-Co Nanoparticles — •Yarden Nathan — Technion, Haifa, Israel

We synthesized Fe- 50 at.% Co nanoparticles (NPs) via solid-state dewetting of Fe-Co bilayers deposited on a sapphire substrate at the temperature of 900 *C followed by slow cooling. By employing X-ray diffraction and electron diffraction in transmission electron microscope (TEM) we demonstrated that the NPs are fully disordered α-FeCo body centered cubic (BCC) phase. We demonstrated that the size and orientations of the disordered BCC NPs can be controlled by varying their fabrication parameters. Most of the NPs were faceted single crystals with their top (110) facet oriented parallel to the substrate. The mechanical properties of the NPs were measured by employing in-situ micro compression tests in the scanning electron microscope (SEM). The near-theoretical strength of α-FeCo NPs was demonstrated. We propose that the fully disordered NPs behave similarly to the defect-free NPs of pure metals. The plasticity of these NPs is controlled by the dislocation nucleation requiring near-theoretical stress. This mechanism explains the near-theoretical strength and the distinct "smaller is stronger" size effect observed in this metastable phase.

MM 3.2 Mon 10:30 SCH/A215

Role of Structural Hierarchy on Tensile Properties of Nanoporous Metals — •Wei-Che Chang[1], Yong Li[1], Henry Ovri[1], and Shan Shi[1,2] — [1]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany — [2]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, Hamburg, Germany

Nanoporous gold (NPG) is drawing significant attention as functional, lightweight material due to its low density, high surface area, and tunable structures. Despite the inherent ductility of bulk gold, NPG often exhibits brittleness under tension [1]. Recently, hierarchical nanoporous gold (HNPG) with multiple levels of well-defined porosities has attracted significant interest for its enhanced functional performance and improved compressive properties at reduced solid fraction [2]. However, whether these mechanical enhancements under compression also extend to tension, particularly whether structural hierarchy can mitigate the intrinsic brittleness of nanoporous networks under tension, remains an important open question. In this work, we introduce an in-situ micro-tensile setup for real-time observation of deformation and fracture behaviors in a scanning electron microscope (SEM). Our results show that the hierarchical structure improves ductility by a factor of five. The mechanism of tensile deformation is further revealed by molecular dynamics simulations.

[1] N. Badwe, X. Chen, K. Sieradzki, Acta Mater. 129 (2017) 251-258 [2] S. Shi, Y. Li, B. Ngo-Dinh, J. Markmann, J. Weissmüller, Science 371 (2021) 1026-1033

MM 3.3 Mon 10:45 SCH/A215

Mechanical shielding of holes in elastic solids — •Kanka Ghosh and Andreas M. Menzel — Institut für Physik, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Holes inside an elastic solid reduce its overall mechanical stiffness. We examine whether a stiff shell around the hole can act as a shield under external loading, maintaining overall mechanical properties of the solid as if the hole were absent. For this purpose, an isotropic, homogeneous, linearly elastic material, loaded uniformly under plane strain with low concentrations of holes is considered. Instead of changing the materials to conceal a hole, we suggest to adjust the thickness of the shell for given elasticity parameters. A corresponding analytical expression for the thickness of the shell is derived. We extend this idea to the atomistic level using molecular dynamics simulations of model Lennard-Jones solids. Consistency of the resulting shell thickness for mechanical shielding at the atomistic scale attests the robustness of our continuum elasticity predictions. The concept is crucial for light-weight construction without compromising elastic materials properties.

We acknowledge support of this work through the European Union (EFRE) and the State Saxony Anhalt through project no. ZS/2024/02/184030.

Reference: K. Ghosh and A. M. Menzel, Mechanically concealed holes, arXiv:2511.00135

MM 3.4 Mon 11:00 SCH/A215

Synthesis and mechanical properties of multi-scale hierarchical Ni and Cu foams — •Ulrike Dette[1,2] and Shan Shi[1,3] — [1]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, 21073 Hamburg, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, 21073 Hamburg, Germany — [3]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany

As functionalized materials gain importance and component miniaturisation advances, there is an increasing demand for optimized structured materials. This talk presents a novel and straightforward alloying-dealloying approach to fabricate metals such as Ni and Cu with two- and three-level hierarchical network structures. Due to the significant difference in vapour pressures between the target metals, vapor phase alloying (VPA) of a metal foam with Zn resulted in Zn-based intermetallic alloy foams. This is then followed by vapor phase dealloying (VPD) which removes Zn and creates a finer porosity, resulting in a second level. A subsequent VPA-VPD cycle produces a third hierarchical level. Compression tests on these hierarchical foams with varying solid fractions were performed to determine Young's modulus and strength. The experimental results align well with the predictions of our new scaling law.

15 min. break

MM 3.5 Mon 11:30 SCH/A215

Formation and properties of crystalline and amorphous high-entropy ZrTiTaMoWNi thin films using magnetron sputtering of a segmented target — •Anna Kornyushchenko[1,2], Vyacheslav Perekrestov[2], Marilena Tomut[1,3], Harald Rösner[1], Martin Peterlechner[4], and Gerhard Wilde[1,5] — [1]Institute of Materials Physics, University of Muenster, Muenster, Germany — [2]Laboratory of Vacuum Nanotechnologies, Sumy State University, Sumy, Ukraine — [3]GSI Helmholtz Center for Heavy Ion Research, 64291 Darmstadt, Germany — [4]Karlsruhe Institute of Technology, Laboratory for Electron Microscopy, 76131 Karlsruhe, Germany — [5]Herbert Gleiter International Institute, Liaoning Academy of Materials, Shenyang, China

Using direct current magnetron sputtering of a segmented target under conditions of thermodynamical equilibrium, single-phase bcc or amorphous ZrTiTaMoWNi high entropy alloy layers have been formed. The crystalline layers have been obtained in the form of nano-patterns, with crystal growth occurring preferentially on the basis of (310) crystallographic plane, which aligns parallel to the substrate surface. The amorphous layers have smooth surface, featureless morphology and demonstrate structural stability. TEM studies have shown that their crystallization into a single bcc phase occurs at the annealing temperature of 800 C. The microhardness of the amorph and the crystalline films has measured to be 10 GPa and 4.6 GPa, correspondingly. Resistance to impact of swift heavy Au ions irradiation with energies 4.8 MeV/u have been compared for amorph and crystalline layers.

MM 3.6 Mon 11:45 SCH/A215

Microstructural and Chemical Analysis on MoSiTi samples with PDC coating for High Temperature Application — •Ingrit Nurak[1], Daniela Camacho[2], Lukas Korell[3], Giorgia Guardi[1], Heike Störmer[1], Svetlana Korneychuk[1], Yolita M. Eggeler[1], Astrid Pundt[1], and Samuel A. Kredel[2] — [1]Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Technische Universität Darmstadt, Darmstadt, Germany — [3]Dechema Forschungszentrum, Frankfurt, Germany

MoSiTi material is of high interest for high temperature applications, such as Mo-20Si-52.8Ti [Schliephake et. al., 2019]. In this presentation, we investigate the combination of this material with a Cr-bond coat and a Si(Hf, Ta)BCN(O)-polymer derived ceramic (PDC) upper layer. The structural and chemical evolution of the layered material, depending on the specific synthetic routes used and additional thermal treatments will be addressed by using different scanning and transmission electron microscopy (SEM, TEM) techniques. TEM will be applied to the (i) polymer-derived ceramic nanocomposites coating, to the development of (ii) ultra-high temperature silicides and to the (iii) Cr bond coat layer. Heat treatments will be addressed at 1200˚C and 1400˚C both in air and in argon atmosphere. The experimental outcomes demonstrate that the Materialsystem exhibits the capacity to withstand temperatures of 1200˚C for an hour without delamination. Notwithstanding the application of heat treatment at 1400˚C, there is no oxygen penetration into the MoSiTi substrate occurred. Moreover, the PDC coating was found to remain partially amorphous.

MM 3.7 Mon 12:00 SCH/A215

Understanding Alloying Effects on Grain Boundary Adhesion in Nickel Alloys by Atomistic Simulation — •Aljoscha F. Baumann[1], Reyhaneh Ghassemizadeh[1], and Daniel F. Urban[1,2] — [1]Fraunhofer IWM, Freiburg, Germany — [2]Freiburger Materialforschungszentrum, Freiburg, Germany

When increasing the in-service performance of engineering metallic materials, interfaces such as phase or grain boundaries (GB) may act as the weakest links. For the nickel-base superalloy Alloy 718 intergranular cracking can be a relevant damage mechanism as a result of high-temperature fatigue in an oxygen-rich environment. The reliable prediction of adhesion and mechanical stability at grain boundary interfaces from atomistic calculations remains a challenge due to the high-dimensional parameter space of chemical compositions and GB structures. Recently developed machine learning interatomic potentials (MLIPs) such as GRACE offer a promising solution to explore this parameter space by combining high accuracy with computational efficiency. Here we use a MLIP to perform cleavage simulations on grain boundaries in fcc Ni with Cr and Fe as alloying elements at varying concentrations and statistical distributions. This approach provides a pathway for atomistic simulations towards a more comprehensive modelling of alloys and their interface mechanical properties, thereby providing insights into intergranular failure mechanisms. Our results can be used to parametrize traction separation laws used in finite element modelling, allowing for microstructure-sensitive modelling of fatigue crack formation and growth.

MM 3.8 Mon 12:15 SCH/A215

Phase stability and surface segregation in multinary noble-metal alloys: an atomistic study with universal models — •Quentin Bizot, Matous Mrovec, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, 44780 Bochum, Germany

Multinary alloys are complex solid solutions composed of several elements. They rarely behave like ideal solid solutions due to differences in phase stability, atomic size, and crystalline preferences. In bulk, short-range order can therefore be significant, leading to the formation of specific phases or distortions across the lattice. In addition to the effects in the volume, surface segregation affects the order and composition of the few first layers at the surface. A detailed understanding of these effects at the atomic scale is essential to predict and control the distribution and ordering of surface atoms, as well as their influence on material properties.

In this work, we investigate complex solid solutions based on noble metals with atomistic simulations demonstrating the formation of stable phases in the bulk as well as the segregation of specific elements at the surface. For this purpose, we used tailored GRACE model capable of describing interactions for 25 transition metals as well as universal GRACE models trained on diverse datasets.

MM 3.9 Mon 12:30 SCH/A215

First-principles study of aluminum alloy - polymer interfaces: From surface structures to adsorbate interactions — •Zhengqing Wei[1], Inna Plyushchay[2], Nebahat Bulut[1], Florian Lehmann[4], Philip Grimm[5,6], Maik Gude[4], Julia Hufenbach[5,6], and Sibylle Gemming[1,3] — [1]Inst. Physics, TU Chemnitz, Germany — [2]Natl. Taras Shevchenko University of Kyiv, Ukraine — [3]MAIN Center, TU Chemnitz, Germany — [4]ILK, TU Dresden, Germany — [5]IFW Dresden, Germany — [6]Inst. Materials Science, TU-BA Freiberg, Germany

Aluminum alloy surfaces face strict demands regarding extreme environmental conditions. The joining of aluminum alloy materials with engineering plastics enhances the overall resilience of composite. This study employs density functional theory (DFT) to model aluminum alloy surfaces while including electronic structure considerations. The surface stability was investigated as functions of alloying composition particularly on surfaces doped with Mg, Zr, and Si. The study includes the alloy's diffusion tendency, which shows that differential electron density variations occur simply at the outermost surface layer in contact with vacuum. Surface vacancy and migration barriers, and when the surface is bonded to the polymers, the interactions between atomic species of polymer side chains and aluminum alloy surfaces as well as surface vacancy sites were also analyzed. The modeled adsorbates on aluminum alloy surfaces provides modified local potential parameters for classical modeling of large-scale aluminum alloy–polymer surface and interfacial regions.

MM 4: Materials for the Storage and Conversion of Energy I

Time: Monday 10:15–13:00 Location: SCH/A216

Topical Talk MM 4.1 Mon 10:15 SCH/A216

Photoelectric properties of dislocations in SrTiO3 single crystals — •Marin Alexe — University of Warwick

Dislocations are one-dimensional crystallographic line defects traditionally regarded as detrimental to the functional properties of conventional semiconductors. However, it has been recently shown on Fe-doped SrTiO3 single crystals containing well-ordered, high-density dislocation structures that dislocations can significantly enhance photoconductivity. Local photoconductivity measurements using atomic force microscopy (AFM) revealed that regions surrounding dislocation cores exhibit up to a fourfold increase in photoconductivity compared with dislocation-free areas of the crystal. Furthermore, macroscopic in-plane surface measurements using microcontacts aligned along dislocation slip bands showed orders-of-magnitude enhancement in photoconductivity. This might be due a significant increase of the carrier density at the core of dislocation due to a to a non-chemical local doping induced by the strain or strain gradient.

These results provide unambiguous evidence that dislocations in oxide semiconductors can be beneficial for specific functional properties. The anisotropic enhancement of photoconductivity along dislocation cores highlights their potential as active elements in future one-dimensional oxide electronic and optoelectronic devices.

MM 4.2 Mon 10:45 SCH/A216

Defect-driven carrier dynamics in tantalum nitride photoelectrodes — •Lukas M. Wolz[1], Johannes Dittloff[1,2], Laura I. Wagner[1,2], Julius Kühne[1,2], Luc-Fabrice Tremel[1], Lina M. Todenhagen[1,2], Lissa Eyre[1,2], Felix Deschler[1,2,3], Ian D. Sharp[1,2], and Johanna Eichhorn[1] — [1]Physics Department, TUM School of Natural Sciences, Technische Universität München, Germany — [2]Walter Schottky Institute, Technische Universität München, Germany — [3]Institute for Physical Chemistry, Heidelberg University, Germany

Tantalum nitride (Ta_3N_5) is a widely studied semiconductor for solar-driven water splitting. Yet, experimentally realized efficiencies often remain below theoretical limits largely because native and impurity-related defect states alter charge carrier dynamics by promoting trapping and recombination. Here, we investigate how distinct defect properties in Ta_3N_5 thin films govern ultrafast photocarrier behavior using femtosecond transient absorption spectroscopy, complemented by photoluminescence (PL) and PL excitation measurements. Ta_3N_5 photoelectrodes were synthesized by annealing TaO_x, TaN_x, and Ta precursor films in NH_3, enabling systematic control over shallow and deep defect state concentrations. The controlled defect properties allow us to disentangle the roles of nitrogen vacancies and oxygen-related defects in shaping carrier dynamics. Our results reveal that deep defects function as efficient trapping and recombination centers for free carriers. Here, we correlate ultrafast spectroscopy with complementary optical and photoelectrochemical data.

MM 4.3 Mon 11:00 SCH/A216

Probing Defect-State Photoionization in Ta_3N_5 Thin Films via Photocurrent Excitation Spectroscopy — •Luc-Fabrice Tremel[1], Lukas M. Wolz[1], Johannes Dittloff[1,2], Ian D. Sharp[1,2], and Johanna Eichhorn[1] — [1]Physics Department, TUM School of Natural Sciences, Technische Universität München, Germany — [2]Walter Schottky Institute, Technische Universität München, Germany

Transition-metal nitrides are a highly interesting material space for solar-energy conversion due to their suitable bandgap for visible light absorption and high theoretical solar-to-hydrogen efficiencies. A prominent example is Ta_3N_5, which combines a bandgap of 2.2 eV with favorable band alignment for solar water splitting. In practice, however, its photoelectrochemical performance is strongly constrained by shallow and deep defects. Here, we use photocurrent excitation spectroscopy, complemented by power-dependent photocurrent measurements, to determine how these defect states shape the spectral photocurrent response of Ta_3N_5. By tracking photocurrent as a function of photon energy, light intensity, and applied potential, we distinguish the sharp band-edge transition from a broadened onset dominated by defect-assisted photoionization into the conduction band. These insights into the defect-controlled photoresponse of Ta_3N_5 provide guidance for improved fabrication strategies and the development of higher-performing nitride-based solar-fuel devices.

MM 4.4 Mon 11:15 SCH/A216

Piezoresponse force microscopy on substituted BaTiO3-relaxors — •Markus Kratzer[1], Philipp Fahler-Muenzer[2], Christian Maier[4], Klaus Reichmann[3], Marco Deluca[5], and Christian Teichert[1] — [1]Chair of Physics, Department of Physics, Mechanics and Electrical Engineering, TU Leoben, Leoben, Austria — [2]University of Warwick - Department of Physics, Coventry, United Kingdom — [3]Institute for Chemistry and Technology of Materials, Graz, Austria — [4]Materials Center Leoben GmbH, Leoben, Austria — [5]Silicon Austria Labs GmbH, Sandgasse 34, 8010 Graz, Austria

Relaxor ferroelectrics are key materials in electrostatic capacitors for energy storage but also for high-performance actuators and transducers. Classical relaxor ferroelectric systems often contain lead, which is environmentally unsound. Thus, lead free relaxors are highly desired. A promising route is via substituted barium titanate (BaTiO3). In this study we focus on B-site-substituted polycrystalline BaTiO3, where the central Ti ion in the perovskite lattice is partially substituted by Zr or Nb. In such systems, information on the microscopic ferroelectric domain structure is still lacking, even though detailed macroscopic characterization using a variety of techniques has been undertaken. We use piezoresponse force microscopy to investigate domain structure and local polarization switching at different temperatures and compositions. We find that temporal stabilization of domains with limited volume is still possible, even though long-range ferroelectric order is strongly supressed with increasing levels of substitution. This suggests the presence of residual highly unstable polar nanoregions.

15 min. break

MM 4.5 Mon 11:45 SCH/A216

Tunable TiO_xN_y Photoelectrodes for Efficient Solar Energy Conversion — •Sebastian Trautschold and Johanna Eichhorn — TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany

Oxynitrides have recently emerged as a versatile material class for photoelectrochemical energy conversion, offering a pathway to combine the stability of oxides with the visible-light absorption and favorable charge transport of nitrides. Their key advantage lies in the continuous tunability of optical and electronic properties via adjusting the O/N ratio. TiO_xN_y provides a particularly illustrative platform: while TiO_2 is limited by a wide bandgap and TiN is metallic, TiO_xN_y can be tuned into an intermediate semiconducting regime, enabling improved utilization of the solar spectrum without sacrificing transport.

Here, we deposit TiO_xN_y thin films by pulsed gas reactive sputtering, enabling precise stoichiometric control over a broad composition range. Post-annealing in ammonia and nitrogen is then used as an additional handle to tailor crystallinity, phase evolution, and defect chemistry. By correlating deposition and annealing parameters with structural, chemical, and optoelectronic characteristics - particularly bandgap and defect properties - we identify processing windows that optimize qualities relevant for solar harvesting. Our results demonstrate the strong sensitivity of TiO_xN_y to both growth kinetics and thermal treatment, and establish practical guidelines for engineering oxynitride photoelectrodes toward efficient and durable solar energy conversion systems.

MM 4.6 Mon 12:00 SCH/A216

In Situ Scanning Transmission Electron Microscopy Investigation of Solid-State Batteries Under Realistic Processing Conditions — •Thomas Demuth, Shamail Ahmed, and Kerstin Volz — Philipps Universität Marburg, Department of Physics and mar.quest, Marburg, Germany

Solid-state batteries promise safer energy storage with higher energy density compared to conventional lithium-ion batteries with liquid electrolytes. To ensure good ionic conductivity between the cathode active material (CAM) and solid electrolyte (SE), the interface area must be maximized. This can be achieved by co-sintering the materials at elevated temperatures. However, high-temperature treatment can induce secondary phase formation at the SE - CAM interface. To optimize material stability, a fundamental understanding of the materials' structure and the processes occurring at the interface are required. Here, in situ (scanning) transmission electron microscopy ((S)TEM) offers insights into nanoscale reaction processes. In our study, we have heated the CAM LiNiO2 (LNO) as a model system in an oxygen atmosphere, utilizing a closed gas cell heating holder, which enables heating the sample in a gaseous atmosphere of 1 bar to temperatures of up to 1000 °C. Using a scanning nanobeam mode allows rapid switching between live imaging for the observation of morphological changes and recording of 4D diffraction pattern datasets for structural analysis. Our findings indicate that the onset temperature for phase degradation is significantly higher in an oxygen atmosphere compared to vacuum, highlighting the importance of replicating realistic processing conditions.

MM 4.7 Mon 12:15 SCH/A216

Voltage-Dependent CEI Development on LMO Cathodes in-situ monitored via Langasite Microgravimetry — •Robert Löser and Guido Schmitz — University of Stuttgart, Stuttgart, Germany

Understanding the formation and evolution of the cathode-electrolyte interphase (CEI) is essential for improving the stability of high-voltage lithium-ion battery materials such as LiMn2O4 (LMO). In this work, we investigate the CEI formation and composition in-situ on sputtered LMO thin films using an electrochemical microbalance based on a Langasite (La3Ga5SiO14) resonator. Unlike conventional quartz crystal microbalances, Langasite substrates enable high-temperature annealing of sputtered oxide films while keeping their piezoelectric properties, making them uniquely suited for preparing crystalline cathode layers directly on the resonator surface. LMO films were cycled to different upper voltage cutoffs to investigate how oxidative potentials influence CEI formation. The coupled electrochemical-gravimetric data reveal clear voltage-dependent mass changes associated with electrolyte decomposition, surface reconstruction, and dissolution processes. By correlating frequency shifts with electrochemical signatures, we quantify the onset, magnitude, and reversibility of CEI species formation dependent of the upper voltage boundary. This study demonstrates that Langasite-based microgravimetry enables powerful, in-situ investigation of CEI evolution and interphase dynamics on annealed cathode films such as LMO, opening the way for systematic studies across a broader range of high-temperature processed electrodes.

MM 4.8 Mon 12:30 SCH/A216

Tuning electronic structure of CoNi LDHs via surface Fe doping for achieving effective oxygen evolution reaction — •Yunli Shi[1,2], Huaping Zhao[1], Junqi Li[2], and Yong Lei[1] — [1]Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]School of Materials Science and Engineering, Shaanxi University of Science and Technology, Xian 710021, China

Cobalt and nickel based layered double hydroxides (LDHs) are promising oxygen evolution reaction (OER) catalysts, but their performance is limited by poor conductivity and low intrinsic catalytic activity. In this study, CoNi LDHs were used as a matrix, with iron sites introduced onto the surface via cation replacement (Fe-CoNi LDHs). Unlike ternary Fe-CoNi LDHs synthesized through conventional one-step methods, the iron sites in Fe-CoNi LDHs are primarily located on the surface and edges of nanosheets, ensuring abundant exposure of reactive sites. Surface doping was found to optimize the coordination environment and electronic structure, reducing the binding energy between reactants and active sites. As a result, Fe-CoNi LDHs exhibit an overpotential of only 260 mV at 10 mA cm**, demonstrating superior OER performance. This study elucidates the electronic structure and mechanism of enhanced activity, highlighting the potential of surface doping to advance electrocatalytic applications.

MM 4.9 Mon 12:45 SCH/A216

NiCo2O4/Fe3O4 Nanocomposite with a Sea Urchin-like Morphology as a High-Performance Dual-Functional Material for Advanced Lithium-Ion Batteries and Supercapacitors — •Amina Zafar, Amjad Nisar, and Mashkoor Ahmad — Pakistan Institute of Nuclear Science and Technology (PINSTECH), Islamabad, Pakistan

The development of advanced electrode materials with multifunctional electrochemical properties is critical for next-generation energy storage systems. In this study, mesoporous sea urchin-like nickel cobaltite/magnetite (NiCo2O4/Fe3O4) composite was synthesized and systematically investigated for lithium-ion batteries and supercapacitors. The resulting composite offers high specific surface area, improved conductivity, abundant active sites and favorable structural characteristics. DFT calculations reveal that the composite exhibits enhanced redox kinetics and improved charge transfer compared to pristine NiCo2O4, leading to superior electrochemical performance. As an anode for lithium-ion batteries, the NiCo2O4/Fe3O4 electrode delivers a high reversible capacity of around 730 mAh/g at 0.3 A/g with excellent cycling stability, retaining 87.1 % of its capacity after 1000 cycles. For supercapacitor, the electrode exhibits an enhanced specific capacitance of 1330 F/g at 1 A/g, outperforming both NiCo2O4 and Fe3O4. The assembled (NiCo2O4/Fe3O4//activated carbon) device achieved a specific capacitance of 221 F/g and an energy density of 69.6 Wh/kg, along with excellent cycling stability, retaining around 94 % capacitance after 8000 cycles.

MM 5: Topical Session: Physics-driven Artificial Intelligence for Materials I

Time: Monday 10:15–12:45 Location: SCH/A251

Topical Talk MM 5.1 Mon 10:15 SCH/A251

Machine Learning for Materials Discovery: from Big Data to Predictive Insights — •Silvana Botti — Research Center Future Energy Materials and Systems and Interdisciplinary Centre for Advanced Materials Simulation, Ruhr University Bochum, Universitätsstraße 150, D-44801 Bochum, Germany

Machine learning (ML) models for materials science are rapidly evolving, driven by large-scale, high-quality datasets and innovative neural network architectures. This talk explores critical challenges in improving the accuracy and reliability of complex ML models, examining the interplay between the quality and quantity of training data and model performance across material properties. Recent advances have been marked by the creation of extensive FAIR databases, such as Alexandria (https://alexandria.icams.rub.de/), which provides over 7 million density-functional theory calculations spanning periodic compounds of various dimensionalities. These comprehensive datasets enable systematic investigation of the relationship between training data volume/quality and model accuracy.

J. Schmidt, T.F.T. Cerqueira, A.H. Romero, A. Loew, F. Jäger, H.-C. Wang, S. Botti, M.A.L. Marques, Improving machine-learning models in materials science through large datasets, Mater. Today Phys. 48, 101560 (2024).

MM 5.2 Mon 10:45 SCH/A251

Screening of high-entropy oxides as oxygen conductors for fuel cells — •Jesper R. Pedersen, Ciku Parida, Benjamin H. Sjølin, and Ivano E. Castelli — Department of Energy Conversion and Storage, Technical University of Denmark, Kgs. Lyngby 2800, Denmark

High-entropy materials are at the cutting edge of materials design and this work investigates their suitability for use in fuel cells. However, screening high-entropy materials is computationally demanding, especially for properties such as oxygen migration barriers which are critical for components used in fuel cell cathodes. We aim to address this challenge by fine-tuning the MACE foundation model to a generated database containing more than 400 nudged elastic band (NEB) calculations spanning the chemical space of double perovskites. We show this new model achieves accuracy similar to the DFT calculations not only on structural relaxations, but also for the more complex task of saddle-point discovery. This enables the continued rapid exploration of the chemical space beyond the initial screening, leading to new insights into factors governing oxygen migration in fuel cell cathodes.

MM 5.3 Mon 11:00 SCH/A251

Interpretable Bayesian Optimization for Autonomous Materials Discovery — •Akhil S. Nair[1,2], Lucas Foppa[1], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at the FHI of the Max Planck Society, Berlin, Germany — [2]Institut für Chemie und Biochemie, Freie Universität Berlin, Germany

Bayesian Optimization (BO) can accelerate materials discovery by exploring complex design spaces using surrogate models and acquisition functions [1]. Its efficiency, however, relies on identifying a small set of key parameters or features that are potentially correlated with the target property. Existing feature-selection methods often fall short, as they struggle to capture nonlinearities and interactions among features [2], limiting BO's performance in high-dimensional spaces. To overcome this challenge, we introduce the Sparse Adaptive Representation-based Bayesian Optimization (SARBO) framework, which integrates BO with the Sure-Independence Screening and Sparsifying Operator (SISSO) method [3]. By capturing the non-linear interactions, SARBO identifies the most relevant features and adaptively updates their selection during the BO cycles, ensuring the optimization is continuously guided by the features that matter most. We demonstrate SARBO's effectiveness through the simulated discovery of single-atom alloy catalysts for CO_2 activation.

[1] Y. Tian, et al., npj Comput. Mater. 11, 209 (2025)
[2] M. R-. Kochi et al., Chem. Sci. 16, 5464 (2025)
[3] R. Ouyang et al., Physical Review. M 2, 8 (2018)

MM 5.4 Mon 11:15 SCH/A251

Fantastic Polaronic Peaks and Where to Find Them: Learning Vibrational Spectra of a Disordered Energy Material — •Christoph Dähn[1], Yang Wang[2], Risov Das[2], Bettina V. Lotsch[2], Karsten Reuter[1], and Christian Carbogno[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]MPI für Festkörperforschung, Stuttgart

Vibrational Raman and infrared spectroscopy offers unique opportunities for characterizing microscopic structural and dynamical properties. For energy materials and in particular for solar batteries [1], a straightforward interpretation of such spectra is however hindered by the intrinsic structural and occupational disorder, which includes defects and polarons. At the same time, this also prevents their accurate *ab initio* simulation, which would require extensive calculations at a hybrid level of density-functional theory (DFT) in a multitude of disordered supercells. In this work, we discuss how machine-learning interatomic potentials trained on high-level DFT data can be used to capture the otherwise inaccessible vibrational dynamics. We demonstrate this approach for a

two-dimensional titanium niobate featuring partially occupied metal sites and polarons. By Monte Carlo sampling its configurational disorder, we are able to disentangle polaronic signatures and disorder induced contributions in the spectra. This reveals how local atomic environments control polaron stability and offers insights on how doping can be used to control charge retention in such compounds.

[1] M. Rinaldi *et al.*, J. Phys.: Mater. **8**, 031003 (2025).

15 min. break

Topical Talk MM 5.5 Mon 11:45 SCH/A251

Leveraging data science technologies to enable AI-driven materials design — •Tilmann Hickel[1,2], Han Mai[2], Shankha Nag[1], Sarath Menon[3], Osamu Waseda[2], Liam Huber[1,2], Jan Janssen[2], and Jörg Neugebauer[2] — [1]Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany — [2]MPI für Nachhaltige Materialien, Düsseldorf, Germany — [3]Ruhr University Bochum, Germany

The handling of materials data is of key importance in designing and producing engineering systems. Therefore, consortia such as NFDI MatWerk aim to develop a sustainable infrastructure for the digital representation of materials science and engineering. The goal is to seamlessly integrate decentralized data and metadata, experimental and computational workflows, and a materials ontology to maximize interoperability and reproducibility of materials data processing. Many AI techniques particularly benefit from structured workflows for data generation and exploitation. For example, the generation and application of machine-learning interatomic potentials becomes accessible for many materials scientists via workflow-management systems such as pyiron. In conjunction with semantic technologies and large-language models they allow to design and validate novel, complex workflows solutions in materials science. We will demonstrate these advantages in the context of atomistic approaches to chemo-structural couplings in metallic alloys. To this end, a high-throughput analysis of the segregation behaviour to grain boundaries will be introduced. Further, hydrogen solubility trends in alloys will be discussed. We will conclude future perspectives in materials informatics.

MM 5.6 Mon 12:15 SCH/A251

Unveiling the Core of Materials Properties via SISSO and Sensitivity Analysis: Use-case Demonstration for Perovskites — •Lucas Foppa and Matthias Scheffler — The NOMAD Laboratory at the Fritz Haber Institute of the Max Planck Society, Berlin, Germany.

Interpretable AI can help reveal the physical principles governing intricate material properties and functions. In particular, the sure-independence screening and sparsifying operator (SISSO) symbolic-regression approach identifies analytical expressions correlating a target materials performance to a small set of physical descriptive parameters, termed materials genes, selected from a vast pool of primary features. However, the identified genes influence the SISSO models to different degrees. Here, we use the gradient-based partial-effect sensitivity analysis to pinpoint the most influential genes, thus enhancing SISSO's interpretability and enabling deeper physical insights. This analysis also highlights that different combinations of genes can yield equally accurate descriptions of the correlation. The approach is demonstrated for the bulk properties of perovskites.

MM 5.7 Mon 12:30 SCH/A251

Towards automated calculation of phase diagrams with machine learning interatomic potentials — •Sarath Menon and Ralf Drautz — ICAMS, Ruhr University Bochum, Germany

Calculation of thermodynamic properties and phase diagrams through atomistic simulations provides valuable insights for the design and assessment of new materials. Accurate phase diagram prediction requires determining the Helmholtz and Gibbs free energies for relevant phases and understanding their dependence on thermodynamic state variables, yet conventional approaches remain technically complex and computationally demanding.

In this work, we introduce algorithms that streamline the computation of multicomponent phase diagrams. Relevant phases are identified using a combination of materials databases and machine learning interatomic potentials, and their free energies are computed with atomic cluster expansion potentials. Temperature and composition effects are assessed through non-equilibrium thermodynamic integration and alchemical sampling, including both vibrational and configurational entropy contributions.

We demonstrate the methodology by computing unary pressure-temperature and several binary temperature-composition phase diagrams as well as phase equilibria in ternary materials. We provide all corresponding computational tools. The workflows are designed to be independent of the interatomic potential and material system, supporting broader use and advancing the accessibility of thermodynamic phase diagram computation in atomistic simulations.

MM 6: Invited Talk: David Rodney

Time: Monday 15:00–15:30 Location: SCH/A251

Invited Talk MM 6.1 Mon 15:00 SCH/A251

Transformation-induced plasticity in zirconia ceramics: simulations and experiments — •David Rodney — Insitut Lumière Matière, University of Lyon, France

Similar to steels, zirconia ceramics display transformation-induced plasticity (TRIP) through an stress-induced tetragonal-to-monoclinic phase transformation. However, the conditions under which TRIP occurs remain unclear, owing to the intrinsic complexity of the transformation, which involves multiple variants and intermediate phases, and to experimental and computational limitations. Experimentally, the transformation is difficult to track in situ and classical interatomic potentials do not capture zirconia's polymorphism.

We present a combined experimental and numerical study addressing these challenges. Experimentally, we perform in situ Laue micro-diffraction on ceria-doped zirconia micropillars compressed along different crystallographic directions. We replicate the same loading conditions in atomistic simulations using a neural-network interatomic potential (NNIP) trained on extensive DFT data and capable of describing the phase behavior of pure and ceria-stabilized zirconia.

Comparison between experiments, NNIP simulations, and DFT calculations provides new insights into the transformation mechanisms. The results clarify the origin of tetragonal stabilization by ceria and show that TRIP proceeds through a complex sequence of stable and metastable phases, including multiple monoclinic and orthorhombic structures, revealing a richer transformation landscape than previously recognized.

MM 7: Mechanical Properties and Alloy Design II

Time: Monday 15:45–18:30 Location: SCH/A215

MM 7.1 Mon 15:45 SCH/A215

On-the-Fly Machine Learning of Interatomic Potentials for Elastic Property Modeling in Al-Mg-Zr Solid Solutions — •Lukas Volkmer[1], Leonardo Medrano Sandonas[1], Philip Grimm[2,3], Julia Kristin Hufenbach[2,3], and Gianaurelio Cuniberti[1,4] — [1]Institute for Materials Science and Max Bergmann Center of Biomaterials,TUD Dresden University of Technology — [2]Institute of Materials Science, Technische Universität Bergakademie Freiberg — [3]Leibniz Institute for Solid State and Materials Research Dresden — [4]Dresden Center for Computational Materials Science, TUD Dresden University of Technology

Aluminum-based alloys offer exceptional mechanical performance due to their low density, high specific strength, and strong resistance to oxidation and corrosion. In this work, we develop a scalable and transferable machine-learning interatomic potential (MLIP) capable of accurately predicting thermodynamic, mechanical, and microstructural properties across a broad concentration space of Al-Mg-Zr alloys. The MLIP is trained using an active-learning workflow that combines ab initio molecular dynamics, Bayesian uncertainty quantification, and kernel ridge regression, enabling efficient exploration of diverse atomic environments. Additionally, we model an Al/Al3Zr grain-boundary system using experimentally observed orientation relationships and calculate the stress-strain behavior. This framework provides a computationally efficient strategy for exploring the phase space of Al-based alloys and guiding the design of materials with optimized mechanical properties.

MM 7.2 Mon 16:00 SCH/A215

Atomistic modelling of Ni-based superalloys at real chemical complexity — •Aditya Vishwakarma, Sarath Menon, Thomas Hammerschmidt, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr University Bochum, Germany

Ni-based superalloys are critical high-temperature high-load materials for jet-engine turbine blades. While *ab-initio* computation has been essential for fundamental understanding (e.g., in binary NiAl), simulating the full chemical complexity of commercial superalloys has remained computationally infeasible. In this work, we demonstrate how Graph Atomic Cluster Expansion (GRACE) foundational models overcome this limitation to investigate the complex phase stability of the γ and γ' phases in industrially relevant Ni-based superalloys. We compute the binary NiAl phase diagram, successfully reproducing the critical γ-γ' phase coexistence. We then extend these phase stability calculations to a CMSX-4 type multi-component composition using hybrid Molecular Dynamics/Monte Carlo simulations. Our results reveal the short-range order (SRO) in the γ phase and quantify long-range order (LRO) in the γ' phase. We specifically find that refractory alloying elements (Ta, W, Ti) exhibit strong LRO alongside Al across the operational temperature range. These findings validate that foundational machine learning interatomic potentials are now capable of calculating complex phase diagrams and capturing subtle ordering and clustering phenomena in multi-component alloys. This capability marks a crucial step toward realizing faster, computationally-driven design of next-generation, single-crystal Ni-based superalloys.

MM 7.3 Mon 16:15 SCH/A215

A machine-learning approach to investigate deformation mechanisms in Mo-Si-based alloys — •Julie Hammoud and Karsten Albe — Technische Universität Darmstadt, Darmstadt, Germany

Mo-Si-X alloys have gained significant attention for high-temperature applications such as turbine blades, due to their outstanding creep resistance, thermal stability and corrosion resistance. In general, Mo-Si-X alloys include three phases: two intermetallic phases (Mo_3Si and Mo_5SiX_2) and a Mo solid solution phase Mo_{ss}. Despite its limited oxidation resistance, the solid solution phase enhances the room temperature fracture toughness of the system. However, the Mo solid solution also incorporates Si-rich subphases with a complex microstructure that leads to an unconventional and still insufficiently understood solid solution strengthening behaviour. Previous studies indicate that small additions of Si (0.1 wt.%) soften Mo, motivating a closer examination of this effect. In this study, we employ a machine-learning interatomic potential (MLIP) based on the Atomic Cluster Expansion (ACE) formalism for the Mo-Si binary system. MLIPs have demonstrated their capability to combine first principles calculations accuracy with the scalability characteristic of empirical potentials. To investigate how Si affects the mechanical response of Mo, we examine two aspects: (i) the concentration dependence of Si on the elastic moduli, analyzed within the framework of the Fleischer model, and (ii) the influence of Si on the behaviour of screw dislocations activity under external loading.

MM 7.4 Mon 16:30 SCH/A215

Jog-Pair Formation and Climb Mechanisms of Dissociated Dislocations in FCC Metals — •Erik Bitzek[1], Sergei Starikov[2], and Daria Smirnova[1,2] — [1]Max Planck Institute for Sustainable Materials, Düsseldorf, Germany — [2]ICAMS, Ruhr-Universität Bochum, Germany

Jogs on dislocations are preferred sites for vacancy segregation and thus play a critical role in dislocation climb. Under conditions of high point-defect supersaturation – such as after quenching or irradiation – the availability of jogs along the dislocation line can become the rate-limiting factor for climb. Understanding jog-pair nucleation is therefore essential for modeling the kinetics of dislocation creep. Jog pair formation on split edge dislocations in fcc metals was first investigated by Thomson and Balluffi [J. Appl. Phys. 1962] and atomistic simulations [Sarkar et al., PRB 2012] confirmed the suggested mechanism. However, both studies assumed a certain vacancy configuration at the dislocation as the initial nucleus.

Using high-temperature molecular dynamics simulations of dislocations in vacancy supersaturated nickel, we identify an alternative pathway that takes place without predefined nuclei. We demonstrate the role of ⟨110⟩-oriented vacancy tubes in the climb of edge and 60° dislocations and propose a new climb mechanism for 30° dislocations involving double cross-slip of the screw partial dislocation. These findings highlight how atomistic simulations can inform mesoscale models of creep and annealing.

MM 7.5 Mon 16:45 SCH/A215

Seeking descriptors for predicting mechanical properties of transition-metal light-element compounds — •Rui Zhang[1,2], Xinlei Gu[1], Kan Zhang[1], Chang Liu[3], and David Holec[2] — [1]Department of Materials Science, Jilin University, Changchun 130012, China — [2]Department of Materials Science, Montanuniversity Leoben, Franz Josef-Straße 18, 8700 Leoben, Austria — [3]College of Physics, Jilin University, Changchun 130012, China

Mechanical strength and durability are key properties that dictate service life. To meet requirements of modern technological and industrial applications, it is essential to screen, sort and predict targeted mechanical properties via finding descriptors that can effectively identify materials with specific application needs. Transition-metal light-element (TMLE) compounds show superb mechanical, chemical and thermal properties. We focus on the analysis of the intrinsic physical/chemical parameters of the component elements and structure factors to identify the key factors affecting the mechanical properties of TMLE. In this presentation, we will introduce two research works: (1) Core electron count as a versatile and accurate new descriptor for sorting mechanical properties of diverse transition metal compounds; and (2) Nitrogen vacancy regulated lattice distortion improvement of mechanical properties and wear resistance of (NbMoTaW)Nx thin films. Ultimately, our work yielded a universal descriptor incorporating core electron count and established nitrogen-vacancy-driven lattice distortion as a key structural factor, offering two distinct pathways to guide the design of high-performance materials.

15 min. break

MM 7.6 Mon 17:15 SCH/A215

Atomistic-to-Mesoscale Computational and Experimental Analysis of the Interactions between Dislocations, Precipitates, Grain and Phase Boundaries in Complex Alloys — •Liming Xiong — NC State University, Raleigh, NC, USA

In this talk, we will present multiscale computational and experimental analysis on the deformation behavior of complex alloys. In experiments, polycrystalline nickel, alloy 709, and Ni3Al-NiCr (γ/γ') alloys are deformed in a transmission electron microscope (TEM). Microstructure evolution is imaged through in-situ TEM. Local stress build up at the slip-GB/PBs are measured by electron backscattering diffraction (EBSD). Meanwhile, concurrent atomistic-continuum (CAC) simulations are performed to understand how a queue of dislocations interacts with the atomically structured precipitates, coherent twin boundaries (CTBs), GB, and γ/γ' PB. One unique feature of CAC is to accommodate the microscale slip containing a large population of dislocations together with the atomistic structure nearby the precipitates/GB/PBs all within one model. Our several findings are: (i) the sequential dislocation-precipitates differs from the single dislocation-precipitates. It is history dependent and has a mechanism cross-over from Orowan bowing out to cross-slip; (ii) the CTBs don't block dislocations. They can accommodate incoming dislocations by allowing them to migrate and form a pileup on the CTB; (iii) dislocation motion is smooth in γ phase but jerky in γ' phase. Such insight will support the design of high-performance alloys by configuring the precipitates, CTBs, GBs, and PBs in them appropriately.

MM 7.7 Mon 17:30 SCH/A215

The Effect of Rhenium on Irradiation Induced Defects in Tungsten-Rhenium Alloys Studied by Positron Annihilation Spectroscopy — •Lisa-Marie Krug[1], Danny R. Russell[1], Maximilian Suhr[1], Leon Chryssos[1], Lucian Mathes[1], Mikhail Zibrov[2], Thomas Schwarz-Selinger[2], and Christoph Hugenschmidt[1] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technical University of Munich, Garching, Germany — [2]Max Planck Institute for Plasma Physics, Garching, Germany

The plasma-facing components in a nuclear fusion reactor have to withstand irradiation by 14 MeV neutrons. Tungsten is considered to be the most suitable plasma-facing material, due to its high melting point, high thermal conductivity and low erosion under fusion reactor operating conditions. In addition to radiation damage, neutron irradiation of tungsten induces nuclear transmutation reactions, resulting in the formation of rhenium. We investigated the effect of Re on the defects produced during the irradiation of W. We provide bench-marking data at extremely high damage doses using ion-irradiation. Transmutation to Re is substituted by Re-ion irradiation or the use of W-Re alloys. Positrons provide a non-destructive, atomic scale resolution of defect analysis of the irradiation damage. Positron Annihilation Spectroscopy (PAS) is a suitable method to determine the defect type, concentration and chemical surrounding. We observe a positive effect of Re on the radiation damage after irradiation at both room temperature and 1350 K. We have found evidence that fewer vacancy clusters are present after irradiation of W-3%Re alloys.

MM 7.8 Mon 17:45 SCH/A215

Understanding the influence of residual elements on the toughness of martensitic steels towards recycled steels — •Eloho Okotete, Subin Lee, and Christoph Kirchlechner — Karlsruhe Institute of Technology, Karlsruhe, Germany

Martensitic steels are critical for many load-bearing applications due to their inherent microstructure, giving rise to unique mechanical properties. However, traditional steelmaking routes produce high greenhouse gas emissions, posing a long-term threat to our environment. Cleaner steel production alternatives aim to use recycled iron scrap as input to electric arc furnaces used in steelmaking. A significant concern for key stakeholders in the steel industry and academia is the presence of residual elements, including Cu, Sn, Sb, As, and P, in iron scrap. Hence, an in-depth analysis of the role of the residual elements on the local and global mechanical properties of martensitic steel would provide relevant insights for the development of environmentally friendly steelmaking alternatives. Small-

scale mechanics using indentation-based techniques can help locally probe how the critical microstructural features of lath martensite, such as prior austenite grain boundaries, packets, blocks, and laths, are affected by residual elements.

In this talk, we use nanoindentation, micro-pillar compression, and micro-cantilever bending experiments to identify the residual element that has the most detrimental effect on the microstructure and properties of our lath martensite. Then, proceed to determine the most impacted microstructural feature of our microstructure as well as the predominant damage mechanism in the steel samples.

MM 7.9 Mon 18:00 SCH/A215

Martensitic phase transformation and anomalous hardening of CrMnFeCoNi high-entropy alloy deformed by high pressure torsion — Robert Chulist[1], Aurimas Pukenas[2], Anton Hohenwarter[3], Reinhard Pippan[3], and •Werner Skrotzki[2] — [1]AGH University of Science and Technology, Krakow, Poland — [2]Technische Universität, Dresden, Germany — [3]Montanuniversität, Leoben, Austria

Under hydrostatic pressure, the CrMnFeCoNi high-entropy alloy (HEA) undergoes a phase transformation from face-centered cubic to hexagonal close-packed. The onset pressure is strongly reduced by high pressure torsion (HPT): shear stress promotes partial dislocation slip. HPT of the low stacking fault energy HEA leads to a nanocrystalline microstructure. The hardness anomaly is due to the extreme nanostructuring, with grain boundary/interphase boundary sliding acting as predominant deformation mechanism: inverse Hall-Petch regime, in which hardness increases with increasing grain size. In submicrocrystalline materials, conventional Hall-Petch hardening dominates, i.e., hardness decreases with increasing grain size.

MM 7.10 Mon 18:15 SCH/A215

Insights into loading condition and microstructural evolution under tribological load — •Antje Dollmann, Robin Freville, Patric Gruber, Christoph Kirchlechner, and Christian Greiner — IAM, KIT, Karlsruhe, Germany

Tribological loading changes the microstructure of materials in contact, e.g. in coarse-grained metals, grain refinement occurs, followed by cracks formation and wear particles removal leading to component failure. This requires an adequate description of the stress field to understand the ongoing microstructural evolution. Due to the complexity of tribological loading, two approaches were explored, both on single-crystalline face-centred cubic metallic materials:

(1) The experiments on CoCrFeMnNi were designed in such a fashion that in some crystal orientations deformation twins were formed. These served as probes to validate various stress field models. General trends regarding the influence of different materials parameters can be identified. The most significant mismatch is between the experimentally observed deformation layer depth and the calculated depth by the stress field. (2) In copper, one deformation layer was analysed by *Laue. Based on its higher sensibility towards small deformations, the deformation layer thickness was greater than what had been detected previously. The combination of those approaches gives deep insight into the so far hidden stress field, which will support future efforts in designing materials to withstand tribological loading.

MM 8: Materials for the Storage and Conversion of Energy II

Time: Monday 15:45–18:30 Location: SCH/A216

MM 8.1 Mon 15:45 SCH/A216

Self-Consistent Hubbard Corrections for Accurate Modelling of Li- and Na-Ion Cathodes — •Valentina Sanella[1,2], Stefan Schären[1,3], Cristiano Malica[4], Livia Giordano[5], Nicola Marzari[1,3,4], Claude Ederer[2], and Iurii Timrov[1] — [1]PSI, Switzerland — [2]ETHZ, Switzerland — [3]EPFL, Switzerland — [4]U Bremen, Germany — [5]UniMiB, Italy

Accurate first-principles modelling of layered transition-metal oxides is essential for understanding and optimizing cathode materials for Li- and Na-ion batteries.

In this work, we investigate two widely studied systems: $LiCoO_2$ and P2-Na_xMnO_2, using density-functional theory (DFT) with self-consistent Hubbard corrections (DFT+U+V). We apply onsite U parameters to both transition-metal 3d orbitals and oxygen 2p states, together with intersite V derived from density-functional perturbation theory (DFPT), enabling a consistent treatment of electron localization and metal-oxygen hybridization.

For $LiCoO_2$, we show that including a U correction on oxygen significantly improves predictions of the intercalation voltages, resolving known inaccuracies associated with standard DFT approaches. In Na_xMnO_2, the extended Hubbard formalism provides a more realistic description across varying sodium concentrations, leading to reliable predictions of structural stability and electrochemical trends.

Our results demonstrate that self-consistent U and V parameters provide significant improvements over empirical or fixed values, enabling reliable predictions of structural and electronic properties.

MM 8.2 Mon 16:00 SCH/A216

Voltage Profile Predictions for Na-Ion Cathodes: A Hybrid MLIP / PBEsol+U+V approach — •Stefan Schären[1,2], Valentina Sanella[1,3], Manuel Dillenz[4], Nicola Marzari[2], and Iurii Timrov[1] — [1]PSI, Villigen, Switzerland — [2]EPFL, Lausanne, Switzerland — [3]ETHZ, Zürich, Switzerland — [4]DTU, Copenhagen, Denmark

Sodium-ion batteries are emerging as a sustainable alternative to lithium-ion batteries, but are limited by the lack of a cathode that offers high voltage, energy density and long-term stability. Here, we present a computational approach that accelerates the prediction of voltage profiles during cathode discharge, using a combination of self-consistent Hubbard-corrected DFT (PBEsol+U+V), and foundational machine-learning interatomic potentials (MLIPs). Using $Na_xV_2(PO_4)_3$ (NVP) as a test case, we show that MLIP-based pre-screening reduces the number of required DFT calculations to a fraction of those needed for a traditional cluster expansion, while retaining comparable accuracy. Furthermore, the self-consistent Hubbard U and V corrections yield electronic occupations that closely match the chemical intuition for oxidation states, enabling a direct analysis of vanadium redox activity and associated volume changes during desodiation. Altogether, the approach delivers a useful and predictive toolkit for identifying high-performance Na-ion cathodes in the future.

MM 8.3 Mon 16:15 SCH/A216

Electronic structure of perovskite oxides calculated with dynamical mean field theory — •Daniel Mutter[1], Jannis Ehrlich[1], Frank Lechermann[2], Daniel F. Urban[1], and Christian Elsässer[1] — [1]Fraunhofer IWM, Freiburg — [2]Institut für Theoretische Physik III, Ruhr-Universität Bochum

Perovskite oxide materials containing first-row transition-metal (TM) elements are regarded as promising alternatives to platinum-based electrodes for high-temperature solid-oxide fuel and electrolyser cells. This is due to the strong electronic correlation effects of the localized 3d electrons of the TM, which directly influence the mechanism and activity of the oxygen reduction reaction. We analyze the electronic structure of perovskite oxides by means of a combined approach of density functional theory and the dynamical mean field theory (DFT+DMFT) to account for the correlation of the electrons in the TM-3d orbitals. We exemplarily demonstrate the influences of static versus dynamic correlation. In addition, we consider correction methods to treat the correlation in the O-2p orbitals, namely the self-interaction correction (SIC) or the DFT-1/2 method. A systematic study of different A- and B-site occupations of the ABO_3 perovskite phases will be presented.

MM 8.4 Mon 16:30 SCH/A216

Unraveling the connection between Jahn-Teller dynamics and charge transport in $LiMn_2O_4$ — •Manuel Dillenz, José Maria Castillo Robles, Mikkel Agerbo Essendrop, Ivano Eligio Castelli, and Juan Maria García Lastra — Department of Energy Storage and Conversion, Technical University of Denmark, Kgs. Lyngby, DK-2800, Denmark

Future energy storage solutions demand batteries that are energy-dense, fast-charging, and based on abundant materials. However, ultrafast dynamics in battery electrodes remain insufficiently characterized despite their crucial role in energy storage performance. Moreover, charge transport in Mn- or Ni-based cathodes is strongly influenced by local structural distortions originating from Jahn-Teller active centers. $LiMn_2O_4$ (LMO) exemplifies this behavior, featuring a ferrodistortive tetragonal ground state that undergoes an order-disorder transition at 290K, where pseudorotations continuously reorient the Jahn-Teller axis. These processes occur on timescales relevant for to polaron and ion transport in the electrode. By combining ab initio molecular dynamics (AIMD) simulations with nudged elastic band (NEB) calculations, we reveal that the interplay of JT and polaron dynamics governs the kinetics of charge transfer in LMO. Our work provides essential mechanistic understanding for enhancing charge transport in Jahn-Teller active electrode materials.

MM 8.5 Mon 16:45 SCH/A216

Defect Landscape of $Ba_2In_2O_5$: The Role of Oxygen Interstitials — •Rachele Sciotto and Karsten Albe — achgebiet Materialmodellierung, Institut für Materialwissenschaft, Technische Universität Darmstadt, Otto-Berndt-Str. 3, D-64287 Darmstadt, Germany

$Ba_2In_2O_5$ (BIO) is a promising n-type mixed ionic and electronic conductor (MIEC) for oxygen permeation membranes and solid oxide fuel cells (SOFCs).

At ambient conditions, BIO adopts an orthorhombic brownmillerite structure with alternating InO_6 octahedral and InO_4 tetrahedral layers that can host interstitial oxygen atoms at sites of structural vacancies. Existing defect thermodynamics models consider only this type of oxygen interstitial; however, oxygen interstitials forming O-O dumbbells, found in oxides like ZnO and In_2O_3, are also possible. In this work, we investigate the potential existence of O-O dumbbells in BIO using density functional theory (DFT). By calculating formation enthalpies as a function of Fermi level and concentrations as a function of oxygen chemical potential, we identify two distinct classes of interstitial configurations. Neutral O-O dumbbells are stabilized over a wide Fermi-level range, while negatively charged interstitials at the structural oxygen vacancy site become favorable under *n*-type conditions. Although the neutral dumbbells do not contribute to charge compensation, they form in high concentrations. They could therefore serve as intermediate positions for oxygen diffusion pathways, thereby influencing the material's ionic and electronic conductivity.

15 min. break

MM 8.6 Mon 17:15 SCH/A216

Interplay of Dynamic Defects and Ultrafast Carrier Dynamics in Lead-Free Double Oxide Perovskites Toward Stable, High- Performance Photovoltaics — •Manasa Gattavadi Basavarajappa, Arijeet Sarangi, and Sudip Chakraborty — Harish-Chandra Research Institute, Chhatnag Road, Jhunsi, Prayagraj - 211019, India

Oxide-based double perovskites are gaining increasing attention as stable and environmentally benign alternatives to halide perovskites in photovoltaic and optoelectronic devices. Their structural versatility and chemical flexibility open pathways for fine-tuning both electronic and lattice properties, yet their carrier dynamics and defect behavior remain less understood. In this work, we investigate these aspects using a combination of first principles calculations and advanced simulation techniques. Non-adiabatic molecular dynamics is employed to capture ultrafast carrier relaxation and to quantify the role of electron*phonon coupling in determining charge transport and recombination lifetimes. The results highlight efficient charge separation and suppressed nonradiative recombination channels, which are essential for high photovoltaic efficiency. To establish the dynamical stability of the materials, we carry out a phonon-based symmetry analysis that confirms the absence of imaginary modes and reveals the interplay between structural distortions and vibrational spectra. In parallel, we explore the formation and dynamic evolution of intrinsic point defects through defect-mediated molecular dynamics simulations.

MM 8.7 Mon 17:30 SCH/A216

Morphological study of $LiNi_{0.5}Mn_{1.5}O_4$ synthesized with alkali molybdates by density functional theory — •Liang-Yin Kuo[1], Tavinder Singh[1], Rio Akbar Yuwono[2], Fu-Ming Wang[2], and Harald Oberhofer[1] — [1]Chair for Theoretical Physics VII and Bavarian Center for Battery Technologies, University of Bayreuth — [2]Graduate Institute of Applied Science and Technology, National Taiwan University of Science and Technology

High-voltage spinel $LiNi_{0.5}Mn_{1.5}O_4$ (LNMO) has emerged as a promising cathode active material for next-generation lithium-ion batteries due to its high operating voltage (~ 4.7 V vs. Li/Li^+), manganese abundance, and potential for high energy density. Single-crystal (SC) LNMO has attracted particular interest because it offers enhanced structural integrity, reduced surface area for electrolyte interaction, and improved cycling stability. Among the synthesis methods, molten-salt synthesis has shown promise for producing SC LNMO. However, the role of the precursor salts remains unclear. In this study, the effects of alkali molybdates, specifically Li_2MoO_4 and Na_2MoO_4, on the SC LNMO formation mechanism are investigated by density functional theory (DFT). Surface energies of various facets are calculated to analyze the resulting Wulff shapes. Our results indicate that LNMO synthesized with Li_2MoO_4 tends to form a truncated octahedron shape, whereas Na_2MoO_4 leads to an octahedron morphology with aggregation into polycrystalline structures. Furthermore, the influence of surface energy on nucleation is discussed, providing insight into morphology control in SC LNMO synthesis.

MM 8.8 Mon 17:45 SCH/A216

Thermodynamic Stability of $MgSc_2Se_4$ Surfaces — •Sebastian Utz[1] and Axel Gross[1,2] — [1]University Ulm, Ulm, Germany — [2]Helmholtz Institute Ulm, Ulm, Germany

$MgSc_2Se_4$ represents a promising candidate for post-lithium battery technologies as a solid-state magnesium ion conductor. With magnesium being significantly more abundant and cheaper than lithium, magnesium-based materials could offer sustainable alternatives for next-generation energy storage systems. While the bulk properties and ion diffusion of $MgSc_2Se_4$ have already been studied extensively, its surface structure and properties remain largely unexplored. However, understanding its surface behaviour is crucial as surfaces and interfaces can behave substantially differently from the bulk. In real applications, like batteries, the properties of surfaces and their interfaces may be limiting factors for stability and mass transfer. This work addresses this gap in the literature by investigating the low-index surfaces of $MgSc_2Se_4$ using grand-canonical density functional theory. Our computational approach enables the characterisation of thermodynamic surface stability and structure under varying chemical potentials. The results provide fundamental insights into surface terminations and their stability in different chemical environments. Combined with experimental validation, these findings could enable detailed atomistic studies of mass transfer at and through $MgSc_2Se_4$ surfaces, supporting the rational assesment of $MgSc_2Se_4$ as a battery material.

MM 8.9 Mon 18:00 SCH/A216

LDH Under Stress: Assessing Degradation Pathways of Ni-Fe-V Catalysts Under Technical Operating Conditions — •Juan Manuel Lombardi, Charles Pare, Karsten Reuter, and Christoph Scheurer — Fritz-Haber-Institut der MPG, Berlin

The transition to a sustainable energy landscape relies on electrocatalysts that are not only active and affordable but also structurally robust under operating conditions. Ni-based layered double hydroxides (LDHs) doped with Fe and V are among the most promising OER candidates for anion-exchange membrane water electrolyzers (AEMWE), owing to their tunable lattice chemistry and rich redox behavior. However, the mechanistic influence of these dopants and how they reshape catalytic performance and structural stability remains insufficiently understood due to the immense configurational complexity.

In this contribution, we present an integrated strategy tailored to address this complexity directly. Our evolutionary exploration framework EZGA provides a systematic route through the high-dimensional composition-structure landscape, employing chemically informed operators and explicit diversity control to generate physically meaningful structural candidates. Machine-learning interatomic potentials (MLIPs) enable high-throughput sampling of thermally accessible configurations with near first-principles fidelity, revealing how dopants modulate stability and reactivity. Together, these elements deliver a predictive workflow that reveals how dopants reshape the accessible configurational landscape and provides a mechanistic picture of their influence on stability and reactivity.

MM 8.10 Mon 18:15 SCH/A216

Quantum-mechanical study of miscibility of Sn in $LaNi_5$ — •Martin Friák[1], Petr Čípek[2,1], Anna Huňařová[2,1], Kateřina Dočkalová[2,1], Jana Pavlů[2,1], and Ondřej Zobač[1] — [1]Institute of Physics of Materials, v. v. i., Czech Academy of Sciences, Žižkova 22, Brno, 61600, Czech Republic — [2]Institute of Chemistry, Masaryk University in Brno, Kotlářská 2, Brno, 61137, Czech Republic

The $LaNi_5$ compound is a prototypical hydrogen-storage material intended for future energy applications. Some of its properties have not been sufficiently studied so far, and some critically important data are missing. In particular, there are conflicting literature reports related to the substitution of Ni atoms with Sn atoms in $LaNi_5$. We have employed quantum-mechanical calculations implementing the density functional theory (DFT) within the generalised gradient approximation (GGA) to determine the ground-state structural, electronic, thermodynamic, and vibrational properties of several substituted $La(Ni,Sn)_5$ phases. Our computational cell containing 48 atoms allowed for simulating different Sn/Ni ratios as well as different configurations of substituting Sn atoms. Our results indicate that the free energy of formation is concave and there is a miscibility gap and a decomposition into two phases, one with a low and one with a high Sn concentration. Our theoretical study was complemented by experiments which found a similar miscibility gap, too.

MM 9: Topical Session: Physics-driven Artificial Intelligence for Materials II

Time: Monday 15:45–18:30 Location: SCH/A251

Topical Talk MM 9.1 Mon 15:45 SCH/A251

Atomistic simulations in the ternary Fe-O-H system: interatomic potential development and applications — •Baptiste Bienvenu[1], Mira Todorova[1], Matous Mrovec[2], Ralf Drautz[2], Dierk Raabe[1], and Jörg Neugebauer[1] — [1]Max Planck Institute for Sustainable Materials, Düsseldorf, Germany — [2]Interdisciplinary Centre for Advanced Materials Simulation, Ruhr Universität Bochum, Germany

Atomistic modeling of iron oxides is challenging, requiring accurate electronic structure calculations and extensive length and time scales to simulate elementary mechanisms such as the extraction of metallic iron from its oxides through hydrogen-based reduction. To enable atomic scale modeling of these and other technologically relevant processes within the ternary Fe-O-H system (e.g., hydrogen embrittlement, water splitting), an accurate yet efficient interatomic potential is needed, something that is currently lacking in the literature. First, we focus on the binary Fe-O system, for which we previously developed a robust and transferable Atomic Cluster Expansion (ACE) machine-learning potential with an explicit account of magnetism, to study bulk diffusion and the structure and stability of various surfaces of iron oxides. We then extend the model to include hydrogen and show that the resulting ACE potential can faithfully reproduce key mechanisms of the Fe-O-H system: (i) surface reactions and microstructure evolution during hydrogen reduction of iron oxides, (ii) surface reactions of iron and its oxides with water and (iii) hydrogen trapping, interaction with extended defects and permeation in metallic iron.

MM 9.2 Mon 16:15 SCH/A251

Learning long-range interactions with equivariant charges — •Marcel F. Langer, Egor Rumiantsev, Tulga-Erdene Sodjargal, Michele Ceriotti, and Philip Loche — Laboratory of Computational Science and Modeling, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Machine-learning interatomic potentials trained on first-principles data have become key tools across computational physics, chemistry, and biology. Equivariant message-passing neural networks, including transformer variants, now deliver state-of-the-art accuracy, but their cutoff-based graphs restrict the treatment of long-range physics such as electrostatics, dispersion, and electron delocalisation. Existing long-range corrections based on inverse-power laws of distances capture only scalar interactions and cannot convey higher-order geometric information, limiting their applicability. To address this, we propose the use of equivariant (rather than scalar) charges to mediate long-range interactions and build a graph neural-network architecture, LOREM [1], around this equivariant message-passing scheme. The talk will outline the architecture, present results on several benchmark datasets, and discuss our work on universal long-range interatomic potentials.

[1] Egor Rumiantsev, Marcel F. Langer, Tulga-Erdene Sodjargal, Michele Ceriotti & Philip Loche, arXiv:2507.19382 (2025).

MM 9.3 Mon 16:30 SCH/A251

Physics-informed Hamiltonian-learning for large-scale electronic-structure calculations — •Martin Schwade, Shaoming Zhang, Frederik Vonhoff, Frederico P. Delgado, and David A. Egger — Physics Department, TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany

Exploring the optoelectronic properties of large-scale materials systems across a wide temperature range using conventional density functional theory (DFT) is often prohibitively computationally expensive. Recent advances in deep neural network approaches offer a promising route to efficiently predict accurate effective Hamiltonians, yet incorporating temperature dependence remains challenging, largely due to the substantial volume of training data typically required. In this work, we introduce HAMSTER [1], a physics-informed Hamiltonian-learning framework that achieves high accuracy with exceptional data efficiency, requiring only a small fraction of the training data demanded by alternative machine-learning models. We demonstrate the capabilities of Hamster on several halide perovskite systems, known for their soft lattices and strong electron-phonon coupling, and show that it reliably reproduces their optoelectronic properties across a broad range of temperatures.

[1] M. Schwade, S. Zhang, F. Vonhoff, F. P. Delgado, D. A. Egger, Physics-informed Hamiltonian learning for large-scale optoelectronic property prediction, arXiv:2508.20536 (2025)

MM 9.4 Mon 16:45 SCH/A251

Making equivariant graph neural network prediction of electronic structure properties fast and accurate — •Chen Qian[1], Valdas Vitartas[1], James Kermode[1], and Reinhard J. Maurer[1,2] — [1]University of Warwick, UK — [2]University of Vienna, AT

Machine learning predictions of band structures and equivariant electronic properties, such as real-space density functional theory (DFT) operator matrices and response properties, have the potential to accelerate electronic structure prediction while avoiding expensive ab initio calculations. However, most current models struggle to strike a balance between prediction accuracy and inference speed. Following our previous work on the equivariant graph neural network MACE-H [arXiv:2508.15108], we assess the model's performance on DFT operator matrices and, subsequently, on a property based on electron-phonon response, the electronic friction tensor. We compare its applications across various datasets. Furthermore, we analyze several existing algorithm- and hardware-based acceleration methods for the computationally intensive Clebsch-Gordan tensor product in terms of accuracy and computational efficiency, and discuss their respective suitable application scenarios. To this end, we present the MACE-H2 framework, which features an O(3) equivariant graph neural network with many-body expansion and suitable acceleration approaches and provides separate routines for DFT operator matrices and electron-phonon response prediction. The model achieves high accuracy and inference speed and is suitable for high-throughput band-structure calculations and material discovery.

15 min. break

MM 9.5 Mon 17:15 SCH/A251

Predicting the Thermal Properties of Semiconductor Defects with Equivariant Neural Networks — •Jonas A. Oldenstaedt, Manuel Grumet, Xiangzhou Zhu, Patrick Rinke, and David A. Egger — Physics Department, TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany

Predicting temperature-dependent properties of defects in semiconductors remains computationally challenging, even with density functional theory (DFT), due to the large supercells and long simulation times required for the calculations. In our recent work [1], we developed an active-learning workflow to accelerate defect calculations by combining two equivariant graph neural networks, trained using DFT calculations: MACE for predicting energies and forces needed in molecular dynamics, and DeepH-E3 for predicting electronic Hamiltonians needed for computing electronic properties across many thermally-excited configurations. We discuss the performance of our approach for predicting structural and electronic properties of intrinsic defects in the prototypical semiconductor GaAs, and demonstrate calculation accuracy comparable to DFT at much reduced computational cost. Furthermore, we discuss extensions of our approach to predict the thermal behavior of defects in more complex semiconductors such as halide perovskites.

[1] X Zhu, P. Rinke and D. A. Egger, arXiv:2511.18398 (2025).

MM 9.6 Mon 17:30 SCH/A251

Learning exact exchange with symbolic regression — •Noah Hoffmann, Santiago Rigamonti, and Claudia Draxl — Humboldt-Universität zu Berlin, Berlin, Deutschland

Density functional theory (DFT) is the most widely used method for the ab-initio prediction of material properties. It is used for computing structural, vibrational, and electronic properties and more. One important factor influencing the accuracy of the predictions is the choice of the exchange-correlation functional. PBE is the de-facto standard functional because of its good results for ground-state properties at comparatively low computational cost. The most prominent downside of this functional, however, is the underestimation of electronic band gaps. Hybrid functionals like PBE0 compensate this by mixing PBE with the non-local exact-exchange (EXX) energy. This improves band-gaps but comes with a drastic increase in computational cost. We apply symbolic regression (SR), a machine-learning technique, to find inexpensive yet accurate exchange potentials as a surrogate for the EXX potential. This enables computationally efficient DFT calculations with an accuracy close to that of hybrid functionals. To generate the training data for the SR models, we used the optimized effective potential (OEP) method, in which a local approximation to the EXX potential is constructed. The OEP method provides rather accurate electron densities. The SR models are then validated with respect to their numerical stability and their ability to predict band gaps. Compared to PBE, the SR models show improved band gap predictions on OEP band gaps with comparable computational cost.

MM 9.7 Mon 17:45 SCH/A251

Development of a GRACE Machine-Learning Potential for Modeling SiC Epitaxial Growth — •Anders Vesti, Thomas Hammerschmidt, and Ralf Drautz — Ruhr Universtät Bochum, Bochum, Germany

Silicon carbide (SiC) is a highly attractive wide band-gap semiconductor for power electronics due to its high breakdown field and low on-state resistance. However, the widespread adoption of SiC-based devices is hindered by challenges in epitaxial growth, including uncontrolled polytype switching and defect formation, which ultimately increase production costs.

In this work, we present the development and benchmarking of a physics-driven machine-learning interatomic potential for SiC based on the GRACE formalism. Starting from a general-purpose foundational model, we refit the potential using comprehensive C, Si, and SiC datasets to construct a specialized model tailored for simulating SiC epitaxy.

We validate the resulting GRACE potential against density functional theory (DFT) calculations and available experimental data for Si, C, and SiC. The developed model provides a basis for testing proposed growth mechanisms in SiC epitaxy.

MM 9.8 Mon 18:00 SCH/A251

Integrating FlashMD into LAMMPS for Efficient Long-Timestep Molecular Dynamics — •Johannes Spies, Filippo Bigi, and Michele Ceriotti — Laboratory of Computational Science and Modeling, Institut des Matériaux, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

FlashMD [1] is a machine-learning model that predicts future molecular configurations from the current state, reducing the need to call machine-learning interatomic potentials at every timestep and enabling larger effective integration steps.

I present its integration into LAMMPS. The implementation acts as a drop-in replacement for standard integrators and makes FlashMD directly available to the molecular simulation community. The interface is modular and extensible through the metatomic ecosystem, allowing new predictor models to be added with minimal effort.

The contribution outlines the integration strategy and initial performance results, focusing on usability, extensibility, and compatibility with existing MLIP workflows. The approach provides a practical route to accelerating large-scale atomistic simulations by reducing the frequency of expensive potential evaluations while maintaining physical reliability.

[1] Filippo Bigi, Sanggyu Chong, Agustinus Kristiadi & Michele Ceriotti, arXiv:2505.19350 (2025).

MM 9.9 Mon 18:15 SCH/A251

Learning to Converge: ML-based Initialization for Fast DFTB Simulations — •Maximilian L. Ach, Karsten Reuter, and Chiara Panosetti — Fritz-Haber-Institut der MPG, Berlin

Density Functional Tight-Binding (DFTB) [1], a class of semiempirical electronic structure methods, captures the electronic structure of a material, unlike conventional machine-learned (ML) interatomic potentials, at a significantly lower computational cost compared to *ab initio* methods. Despite this gain in efficiency, for many processes, DFTB does not scale favorably with the number of atoms, and simulations of realistic material systems often represent a significant challenge due to the associated computational overhead. A large portion of this cost can be attributed to the difficulty of converging these calculations efficiently. To address this, we introduce an ML-enhanced scheme, which significantly accelerates and improves the DFTB self-consistent charge convergence. Our approach leverages state-of-the-art ML methods to provide improved initializations for DFTB calculations, hence reducing the overall cost. We demonstrate the effectiveness of this method on small molecules and a range of materials.

[1] B. Hourahine *et al.*, J. Phys. Chem. A **129**, 5373 (2025).

MM 10: Invited Talk: Lola Lilensten

Time: Tuesday 9:30–10:00 Location: SCH/A251

Invited Talk MM 10.1 Tue 9:30 SCH/A251

Chemically graded materials for accelerated exploration of the TRIP-TWIP Ti-alloy family — •Lola Lilensten — IRCP - CNRS, Paris, France

Twinning induced plasticity (TWIP) and transformation induced plasticity (TRIP) in β-metastable titanium alloys provide remarkable work hardening, enhancing ductility and strength, opening up new possibilities for titanium alloys. These mechanisms depend on the metastability of the retained β phase and thus on the alloy composition.

However, the development of these alloys is still limited. Current design approaches are mostly empirical, relying on datasets that focus on composition and deformation mechanisms, neglecting factors like processing conditions, grain size, and oxygen content. This leads to inconsistencies and overlooks optimization opportunities through microstructure engineering.

The chemically graded materials approach is proposed to tackle this problem, enabling quick identification of compositional ranges where specific deformation mechanisms occur, and consistent results since all compositions share the same processing. This method accelerates the study and development of TRIP/TWIP Ti-alloys.

MM 11: Structurally and Chemically Complex Alloys

Time: Tuesday 10:15–11:45 Location: SCH/A215

MM 11.1 Tue 10:15 SCH/A215

Quantifying chemical short-range order in Ti–Zr–Nb alloys — Yujun Zhao[1,2], Andrea Fantin[3], Yue Li[1], Tong Li[2], and •Yilun Gong[4] — [1]Max-Planck-Institut für Nachhaltige Materialien, Düsseldorf, Germany — [2]Ruhr Universität Bochum (RUB), Bochum, Germany — [3]Bundesanstalt für Materialforschung und -prüfung (BAM), Berlin, Germany — [4]University of Oxford, Oxford, UK

Chemical short-range order (CSRO) is expected to influence phase stability and defect interactions in Ti–Zr–Nb alloys, yet its direct quantification in equiatomic TiZrNb has remained unresolved. Here, we apply X-ray absorption spectroscopy (XAS) and X-ray pair-distribution-function (PDF) analysis to experimentally probe local chemical environments in single-phase bcc TiZrNb. Nanometre-scale compositional fluctuations and elemental pair distributions are further explored using orientation-specified atom-probe tomography (APT). XAS and PDF measurements reveal small but systematic local distortions in element-specific partial coordination shells (from XAS), consistent with emerging CSRO, and ensemble-averaged structural distortions in the atomic network (from PDF). To interpret these findings, we develop density functional theory-trained interatomic potentials and perform on-lattice Monte Carlo simulations to obtain the temperature-dependent equilibrium CSRO pair correlations. Together, these results provide the first quantitative CSRO map for TiZrNb, capturing its temperature and crystallographic dependence. This establishes TiZrNb as a reference system for understanding how CSRO influences phase stability, interstitial accommodation, and mechanical behaviour in refractory alloys.

MM 11.2 Tue 10:30 SCH/A215

Radiation Tolerance in High Entropy Alloys — •Jyoti Verma[1], Paul Chekhonin[2], Andreas Worbs[1], Cornelia Kaden[2], Maciej Oskar Liedke[3], and Gregor Hlawacek[1] — [1]Institute of Ion Beam Physics and Material Research,Helmholtz Zentrum Dresden Rossendorf, Bautzner Landstrasse 400 — [2]Institute of Resource Ecology,Helmholtz Zentrum Dresden Rossendorf, Bautzner Landstrasse 400 — [3]Institute of Radiation Physics,Helmholtz Zentrum Dresden Rossendorf, Bautzner Landstrasse 400

High-entropy alloys (HEAs), or compositionally complex alloys (CCAs), are near-equiatomic multicomponent materials forming single-phase solid solutions with exceptional mechanical strength, thermal stability, and radiation resistance, making them strong candidates for structural use in advanced nuclear systems. In Generation IV fission and future fusion reactors, materials must endure 500*600 $^{\circ}$C, high neutron fluxes, and helium and hydrogen generated by 14 MeV neutrons, which significantly influence irradiation-induced defect evolution. We are investigating the irradiation response of Co-free (CrFeMnNi) CCAs using Fe-ion irradiation at 300°C to 1, 3, and 10 dpa. Transmission electron microscopy revealed typical dislocation loops, while positron annihilation spectroscopy identified vacancy-type defects and vacancy-dislocation complexes, whose concentration decreased with dose, suggesting progressive interaction and annihilation between vacancies and dislocations at higher irradiation levels. These results demonstrate the promising irradiation tolerance of Co-free CCAs for structural use in next-generation reactors.

MM 11.3 Tue 10:45 SCH/A215

Preparation of an impurity-free quinary alloy surface without significant changes in composition — •Yong-He Pan[1], Niklas Osterloh[1], Wun-Chang Pan[1], Natalia Pukhareva[2], Alfred Ludwig[2], and Karina Morgenstern[1] — [1]Physical Chemistry I, Ruhr University Bochum, Universitätsstr. 150, 44780 Bochum, Germany — [2]Centre for Interface-Dominated High-Performance Materials (ZGH), Ruhr University Bochum, Universitätsstr. 150, 44780 Bochum, Germany

Compositionally Complex Solid Solutions (CCSSs) are a promising new pathway to electrochemical catalysts [1,2]. Their complex surface offers multiple adsorption sites for different reaction steps simultaneously [3]. We investigated the composition of the surface elements and impurities using X-ray photoelectron spectroscopy. The quinary alloy sample Ag-Au-Ir-Pd-Pt was prepared in ultra-high vacuum by argon sputtering and annealing. Surface impurities were removed by sputtering, and the alloy composition remained stable even during prolonged thermal treatment. Optimal sputtering and annealing parameters for achieving a clean surface were established. This study clarifies the effects of these processes on the surface composition ratio of Ag-Au-Ir-Pd-Pt alloys.

[1] H. J. Qiu et al., J. Mater. Chem. A, 2019, 7, 6499 [2] T. Löffler et al., Angew. Chem. Int. Ed. 2021, 60, 26894 [3] J. K. Pedersen et al., ACS Catal. 2020, 10, 2169

MM 11.4 Tue 11:00 SCH/A215

Effect of partial occupancy on the properties of FeCr σ-phase — •Mariano Forti[1], Guillaume Laplanche[1], Wenhao Zhang[2], Ralf Drautz[1], and Thomas Hammerschmidt[1] — [1]Ruhr Universität Bochum, Germany — [2]LINK, CNRS-Saint-Gobain- NIMS

The σ-phase forms in Fe-Cr alloys over 870K at about 50 at.% Cr, strongly affecting their performance. Atomistic studies usually assume a sublattice model, but experiments show fractional occupancy of the Whyckoff sites, creating many possible local atomic configurations. This complexity limits direct sampling with DFT and opens questions about the effect of partial occupancy on properties of the σ-phase.

We address the problem using a combination of DFT and MLIPs for a $Fe_{16}Cr_{14}$ σ-phase with experimentally observed site occupancy. We use a GRACE potential to screen all possible configurations of the intermetallic and validate the predictions with DFT calculations of a representative selection of configurations.

This approach enables a direct comparison between the traditional sublattice models and explicit disorder. Our results show that partial occupancy stabilizes the σ-phase, while mechanical properties differ roughly 10% from those predicted by sublattice models.

These findings provide a clearer picture of the local chemical disorder effects on the mechanical response of the σ-phase.

MM 11.5 Tue 11:15 SCH/A215

Accurate temperature-dependent Gibbs free energies of point defects in B2 MoTa — •Xiang Xu[1], Xi Zhang[1], Sergiy V Divinski[2], and Blazej Grabowski[1] — [1]University of Stuttgart, Stuttgart, Germany — [2]Universität Münster, Münster, Germany

Controlling order-disorder motifs is proven to be a key strategy for tuning performance in complex concentrated alloys. To this end, understanding ordered configurations is particularly important, as they represent the theoretical boundary of atomic diffusion, phase stability, and order-disorder phenomena. Since point defects like vacancies and antisites control diffusion and thereby affect ordering and phase evolution, their thermodynamic properties provide critical insight into the fundamental mechanisms behind property tuning. However, difficulties in stabilizing highly ordered refractory phases and the computational complexity of finite-temperature free energy calculations have limited quantitative understanding of their defect thermodynamics. To address this gap, we employ first-principles methods to investigate vacancy thermodynamics in the prototype B2-ordered MoTa alloy systematically. By explicitly accounting for electronic excitations and thermal vibrational contributions, particularly the explicit anharmonicity, we reveal distinct temperature-dependent Gibbs energies for vacancies and antisites in the B2-ordered MoTa. Vibrational pair distribution analysis, performed using an accurate machine-learning potential, demonstrates that the difference in thermal contributions arises from the vibrational phase spaces of the investigated point defects.

MM 11.6 Tue 11:30 SCH/A215

Modelling Bulk and Confined High-entropy Materials — •Chen-Chen Er[1,2], Tom Barnowsky[1,2], and Rico Friedrich[1,2] — [1]TU Dresden — [2]Helmholtz-Zentrum Dresden Rossendorf, Dresden

High-entropy materials (HEMs) are single-phase multi-component disordered systems with unique electronic, mechanical, and thermal properties that are promising for applications in the energy and electronics sectors. HEMs include disordered ceramics such as carbides, nitrides, or oxides with ordered anion sublattices and disorder on the metal cation sites. Generally, five or more cation species are required to maximize configurational entropy.

In our work, efficient modelling of the disordered systems is conducted based on an ensemble of ordered structures as implemented in the partial occupation algorithm (POCC) [1] within the AFLOW framework [2,3]. Predictive descriptors including the entropy forming ability (EFA) [4] and disordered enthalpy-entropy descriptor (DEED) [5] are crucial to assess synthesizability. Here, we present new results for several bulk and confined high-entropy ceramics.

[1] K. Yang *et al.*, Chem. Mater. **28**, 6484 (2016).
[2] M. Esters *et al.*, Comput. Mater. Sci. **216**, 111808 (2023).
[3] S. Divilov *et al.*, High Entropy Alloys Mater. **3**, 178 (2025).
[4] P. Sarker *et al.*, Nat. Commun. **9**, 4980 (2018).
[5] S. Divilov *et al.*, Nature **625**, 66 (2024).

MM 12: Materials for the Storage and Conversion of Energy III / Functional Materials I

Time: Tuesday 10:15–12:45 Location: SCH/A216

MM 12.1 Tue 10:15 SCH/A216

Harmonising Symmetry and Spin: Unveiling Giant Rashba Splitting and Diverse Topological Phases in Composite Quantum Materials — •Arijeet Sarangi, Rajib Sarkar, and Sudip Chakraborty — Harish-Chandra Research Institute, Chhatnag Road, Jhunsi, Prayagraj - 211019, India

We present a systematic theoretical study of ABX-type composite quantum materials crystallizing in non-centrosymmetric hexagonal structures, carried out through high-throughput DFT calculations. Approximately 50 candidate systems were screened to explore the interplay between structural symmetry breaking, strong SOC and emergent electronic properties. Our investigation reveals a striking coexistence of Rashba spin splitting and topologically nontrivial band topology across this materials family, with Rashba coefficients and band inversions strongly dependent on atomic ordering and chemical composition. To complement the band-structure analysis, we perform Berry phase calculations, which confirm the topological character of selected states and identify Berry curvature hotspots near avoided crossings. Building upon this, we evaluate the spin Hall conductivity and orbital Hall conductivity for representative compounds, demonstrating substantial intrinsic values comparable to those in established topological semimetals. These findings point to a strong potential for dissipationless spin and orbital current generation, key ingredients for next-generation spintronic and orbitronic devices. These results establish a promising design space for multifunctional applications, bridging spintronics and topological electronics.

MM 12.2 Tue 10:30 SCH/A216

TiO_2 meets water: Band alignment and spectral properties for solar-driven catalysis using Koopmans spectral functionals — •Marija Stojkovic[1], Edward Linscott[2,3], and Nicola Marzari[1,2,3] — [1]Theory and Simulations of Materials (THEOS), École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland — [2]Center for Scientific Computing, Theory and Data, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland — [3]National Centre for Computational Design and Discovery of Novel Materials (MARVEL), Paul Scherrer Institute, 5232 Villigen PSI, Switzerland

Photocatalytic water splitting has drawn considerable attention for renewable energy production. Thanks to its favorable band gap and band-edge positions, titanium dioxide has remained one of the most promising materials since its first reported photocatalytic water splitting. However, conventional computational approaches often struggle to accurately predict band gaps and band alignments. Here, we showcase the capabilities of Koopmans spectral functionals for evaluating photocatalysts* properties, showing how these can accurately predict band structures and level alignments for rutile, anatase, and brookite TiO_2. Furthermore, we investigate the impact of explicit water on band alignment at TiO_2-water interface by combining advanced molecular dynamics methods with electronic-structure Koopmans calculations.

MM 12.3 Tue 10:45 SCH/A216

Theoretical Calculation of Finite-Temperature X-Ray Absorption Fine Structure: Application to Sodium K-Edge in NaCl — Philipp Hönicke[1,2], Yves Kayser[3], and •Pouya Partovi-Azar[4] — [1]Helmholtz-Zentrum Berlin (HZB), Hahn-Meitner-Platz 1, 14109 Berlin, Germany — [2]Physikalisch-Technische Bundesanstalt (PTB), Abbestr. 2-12, 10587 Berlin, Germany — [3]Max Planck Institute for Chemical Energy Conversion, Stiftstr. 34-36, 45470 Mülheim an der Ruhr, Germany — [4]Institute of Chemistry, Martin Luther University Halle-Wittenberg, Von-Danckelmann-Platz 4, 06120 Halle (Saale), Germany

A comprehensive computational framework for calculating the full X-ray absorption fine structure (XAFS) through quantum-chemical simulations is presented. The near-edge region is accurately captured using time-dependent density-functional perturbation theory applied to core excitations, while *ab initio* molecular dynamics provides sampling of core-excitation energies and interatomic distance distributions for interpreting extended X-ray absorption fine structure (EXAFS) features. Owing to the efficiency of the approach, the total spectrum can be decomposed into contributions from bulk, defective, and surface environments, which commonly coexist in experimental systems. The methodology is demonstrated for sodium at the Na K-edge in NaCl, where the predicted spectra show good agreement with experimental measurements on thin film samples. This strategy offers a practical route to generating chemically specific XAFS cross-section data for elements that remain challenging to characterize experimentally.

MM 12.4 Tue 11:00 SCH/A216

Spin-Charge Coupling at Mixed Fe/Cr Nodes Governs Optical Gaps in MIL-100 Photocatalysts — •Sabuhi Badalov[1], Patrick Länger[2], Jürgen Senker[2], and Harald Oberhofer[1] — [1]Chair for Theoretical Physics VII and Bavarian Center for Battery Technologies, University of Bayreuth — [2]Chair for Inorganic Chemistry III and Northern Bavarian NMR Centre, University of Bayreuth

With a view on photocatalytic CO_2 reduction, we investigate how mixed metal Fe/Cr nodes in MIL-100 metal organic frameworks (MOFs) influence the MOFs electronic and optical response. Using hybrid level density functional theory (DFT) on models of Fe_3O, Fe_2CrO, $FeCr_2O$ and Cr_3O, we map the evolution of spin-resolved edge levels and Kohn-Sham holes during the stepwise substitution of Fe with Cr. Time-dependent DFT calculations reveal dense $O(2p)\rightarrow M(3d)$ ligand-metal charge transfer (LMCT) bands, appearing between approximately 3.5 and 4.5 eV. From these we derive composition-dependent optical band gaps and λ_{max} values. The calculated trends, modest red/blue shifts of the first bright excitation and systematic hardening of the LMCT manifold with increasing Cr content, quantitatively agree with the experimentally obtained gaps. Our combined theoretical/experimental approach provides a deep microscopic insight into the influence of the Fe/Cr mixed metal centers on spin topology, band edges, and optical absorption. Ultimately, our work points the way towards a rational design of MIL-100 for maximal CO_2 conversion.

15 min. break

MM 12.5 Tue 11:30 SCH/A216

Beyond Ion Dynamics: Efficient Charge Transport Simulations including Electrons at Battery Scales — Matteo Rinaldi, Karsten Reuter, and •Christian Carbogno — Fritz-Haber-Institut der MPG, Berlin

Small polarons, i.e., atomically localized excess charges, are fundamental for charge transport in energy materials. A quantitative modeling of their dynamics is challenging, though, since it typically requires not only long time and length scales, but also an account of electronic degrees of freedom at an *ab initio* level. In this work, we overcome this hurdle via a machine-learning interatomic potential that explicitly accounts for small polarons, which are incorporated as semi-classical degrees of freedom that adiabatically follow the nuclei. Using HSE06 calculations [1] as training data, we validate the approach for $BiVO_4$ and further demonstrate its power for lithium titanium oxide (LTO), a prototypical anode material featuring polarons [2]. By running accelerated sampling and large-scale molecular dynamics simulations, we clarify the mechanisms that drive ionic and polaronic transport as well as their coupling in LTO. This reveals that polarons do not merely serve as spectators, but thermodynamically adapt to the much slower ionic motion. This results in an increase of ionic conductivity, in line with experimental measurements. For the first time, this theoretically corroborates the occurrence of a correlated polaron-ion dynamics with profound implications for the design of energy materials.

[1] S. Kokott *et al.*, J. Chem. Phys. **161**, 024112 (2024).
[2] M. Kick *et al.*, ACS Appl. Energy Mater. **4**, 8583 (2021).

MM 12.6 Tue 11:45 SCH/A216

Ion Transport in Mixed-Halide Lithium Argyrodites from Machine Learning Potentials — •Yufeng Xu, Takeru Miyagawa, Waldemar Kaiser, and David A. Egger — Physics Department, TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany

Lithium argyrodites Li_6PS_5X (X=Cl, Br, I) are structurally and chemically complex solid electrolytes. Their ionic conductivity is strongly affected by static forms of disorder, including sulfur-halide anti-site defects [1] and compositional disorder introduced through halide mixing [2]. In this study, we use the MACE message-passing architecture [3] together with machine-learning molecular dynamics to examine ion transport mechanisms in both pure and mixed-halide Li_6PS_5X. We analyze how static and dynamic disorder in mixed-halide systems shapes Li ion diffusion, and how these changes in ion conduction are reflected in the vibrational spectra of the argyrodites. References: [1] B.J. Morgan, Chem. Mater., 2021, 33, 6, 2004-2018. [2] S.V. Patel et al. Chem. Mater., 2021, 33, 4, 1435-1443. [3] I. Batatia et al. J. Chem. Phys., 2025, 163, 184110.

MM 12.7 Tue 12:00 SCH/A216

Positron Annihilation Studies of Nuclear and Highly Oriented Pyrolytic Graphite — •Jagoda Urban-Klaehn, Arvin Cunningham, and William Windes — Idaho National Laboratory, 1955 Fremont Ave, Idaho Falls, ID 83415 USA

Graphite is a life-limiting component in nuclear reactor design thus its microstructure characterization and the effects of extreme conditions are of great importance.

We examined nuclear graphite materials of different origin, porosity and grain sizes by use of Positron Annihilation Lifetime Spectroscopy (PALS).

We determined that each type of graphite has its specific signature with trapping lifetimes in the range: 360-410 ps, and the most important factor was the grain size. Graphite with the coarse grain showed less positron trapping compared to fine grain which agrees with literature.

Graphite that was heat-treated (2300 C) showed a significant increase in positron trapping thus changes in the microstructure. PALS studies on Highly Oriented Pyrolytic Graphite (HOPG) polycrystalline specimens showed less trapping due to its polycrystalline nature. We are planning to use ELBE slow positron beam at different temperatures to study isotropic graphite defects formation enthalpy as well as crystalline graphite*s depth profiling.

MM 12.8 Tue 12:15 SCH/A216

Positron annihilation spectroscopy for atomic defects in functional materials — •Maciej Oskar Liedke, Eric Hirschmann, Jyoti Verma, Sebastian Klug, and Andreas Wagner — Institute of Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328, Germany

Positron annihilation spectroscopy (PAS) is a highly effective method for the characterization of point defects and their agglomerates in functional bulk materials and thin films. The method provides access to defect concentration in the range of 0.01-100 ppm, which is common for most material classes, including metals, semi-, and superconductors. The utilization of the radiation source ELBE at HZDR in Dresden, which delivers a pulsed positron beam, enables depth profiling by varying the kinetic energy of positrons. The integration of PAS techniques with density functional theory calculations facilitates understanding of defect types and local chemistry at the defected crystal sites. In this contribution, we will present few highlights from positron studies and discuss the role of defects in wide-bandgap semiconductors, such as Ga2O3, in addition to superconducting Nb-based coatings, and high-entropy alloys intended for fusion applications. The presentation will emphasize the control over transitions between different polymorphs of Ga2O3 driven by ion irradiation and resulting defect microstructure. Furthermore, we will demonstrate the correlations between deposition parameters and defect landscapes in Nb alloys. We will conclude discussing healing processes in CrFeMnNi subjected to Fe-ion irradiation, which is analogous to neutron radiation in nuclear systems.

MM 12.9 Tue 12:30 SCH/A216

Operando X-ray Absorption Spectroscopy studies of the X-ray exposed active and passive fiber preforms and their recovery properties upon UV-laser light — •Ali KARATUTLU[1,2], Esra KENDIR TEKGÜL[1], Iremnur DURU[1,2], Timuçin Emre TABARU[2], Latif Ullah KHAN[3], Messaoud HARFOUCHE[3], and Bülend ORTAÇ[1] — [1]Bilkent University, Institute of Materials Science Nanotechnology and National Nanotechnology Research Center (UNAM), Ankara, 06800 Turkey — [2]Sivas University of Science and Technology, Department of Engineering Basic Sciences, Sivas, 58100 Turkey — [3]Synchrotron-light for Experimental Science and Applications in the Middle East (SESAME), Allan, 19252, Jordan

In the development of active fiber preforms and active fibers containing rare-earth (RE) ions such as Yb+3 ions for 1-micron laser applications, the determination of the local environment around the Yb+3 ions is of paramount importance for their high optical-optical efficiency. In the long-term operation or when exposed to the gamma or X-ray exposures, the unwanted structural units are usually associated with the defects called color centers. This study demonstrates the formation of photodarkening upon gamma and X-ray exposures and operando X-ray absorption spectroscopy to determine the structural change around Yb+3 ions or Ge+4 ions with different doping levels before and after the irradiation of X-rays.

MM 13: Data-driven Materials Science: Big Data and Workflows I

Time: Tuesday 10:15–12:45 Location: SCH/A251

MM 13.1 Tue 10:15 SCH/A251

Surface reconstruction via automated LEED analysis based on Bayesian optimization — •Xiankang Tang and Hongbin Zhang — Institute of Materials Science, Technische Universitat Darmstadt, 64287 Darmstadt, Germany

Recent advances in machine learning have enabled the automation of many material characterization processes, which are essential for realizing autonomous experimentation for solid-state materials in the near future. Low-energy electron diffraction (LEED) is a fundamental technique in surface science, providing structural reconstruction information encoded in the energy-dependent intensity modulation of diffracted beams. However, the complexity of data analysis and the computational demands have limited the broader adoption of quantitative LEED in routine surface structure determination. In this work, we implement a Bayesian optimization-based approach to automatize the LEED I(V) analysis, where the best matching structures can be obtained for the experimental I(V) curves by minimize the R-factor between the experimental and simulated I(V) data. This approach can bee combined with density functional calculations or atomisitic simulations to further accelerate the recommendation of plausible structures by minimizing total energies.

MM 13.2 Tue 10:30 SCH/A251

Structural relaxations for nonstoichiometric alloys without forces — •Luca Numrich and Hongbin Zhang — Insitute of Materials Science, Technische Univerität Darmstadt, Darmstadt, Germany

Advances in machine learning and first-principles electronic-structure methods are accelerating materials design, focusing on stoichiometric compounds. Coherent potential approximation (CPA) is a standard approach for alloys with chemical disorder but there is no compatible implementation for forces, hindering the investigation of structural relaxations for nonstoichiometric alloys. For example, in many Ni-based Heusler alloys, a high-temperature disordered B2 phase transforms into the fully ordered $L2_1$ structure upon cooling via a second-order B2-$L2_1$ order-disorder transition.

In this work, we integrate Bayesian optimization (BO) with CPA as implemented in the exact muffin-tin orbitals (EMTO) code to identify low-energy crystal structures for nonstoichiometric alloys, as demonstrated for Ni-Mn-Ga-X Heusler alloys. Symmetry analysis is used to reduce the number of independent Wyckoff coordinates, which serve as parameters for BO, while the energy per atom computed via EMTO-CPA defines the objective function to be minimized. Using a Gaussian process surrogate model with a parallel upper confidence bound acquisition function, the framework autonomously proposes candidate structures with progressively lower energies. Thus, instead of a relaxation via interatomic forces, an acquisition function is guiding the relaxation.

MM 13.3 Tue 10:45 SCH/A251

A Python-based workflow for phase identification and mapping via Raman spectroscopy — •Felix Drechsler[1], Mahnaz Mehdizadehlima[2], Cameliu Himcinschi[1], David Rafaja[2], and Jens Kortus[1] — [1]TU Bergakademie Freiberg, Institute of Theoretical Physics, Freiberg, Germany — [2]TU Bergakademie Freiberg, Institute of Materials Science, Freiberg, Germany

Raman spectroscopy is a powerful tool for identifying phases and compounds. It is highly sensitive to both chemical and structural variations and is particularly attractive due to its minimal sample preparation requirements. This makes it well suited for fast phase identification and the determination of spatial phase distributions, complementing established techniques such as X-ray diffraction, element mapping via X-ray spectroscopy, and phase mapping using electron backscatter diffraction. However, phase-resolved analysis of Raman mappings remains challenging, as it involves processing high-dimensional data matrices and robust identification relies on comparing the complete spectrum with references.

In this talk, we present a Python-based workflow developed to address this challenge. The approach employs multivariate analysis methods and integrates mathematical similarity metrics with reference datasets to enable robust and reproducible phase identification. The proposed workflow provides an efficient way to construct Raman phase maps and offers a valuable tool for material characterization.

MM 13.4 Tue 11:00 SCH/A251

Automated Prediction of Phase Stability with ab-initio Accuracy — •Prabhath Chilakalapudi, Marvin Poul, Jan Janssen, and Jörg Neugebauer — Computational Materials Design, Max-Planck-Institute for Sustainable Materials, Düsseldorf

Developing sustainable metallic alloys-free of toxic elements and compatible with circular synthesis-requires novel and efficient ways to explore large composition spaces. A key bottleneck is the automated, ab-initio-accurate prediction of temperature-composition phase diagrams, where experimental phase data is limited or difficult to obtain.

We present a reproducible, automated workflow that uses Machine-Learned Interatomic Potentials (MLIPs) such as Atomic Cluster Expansion (ACE)[1] and non-equilibrium thermodynamic integration (Calphy[2]) to compute free energies and phase stabilities. By analysing key approximations including point-defect models, different entropic contributions, and free-energy interpolation schemes, we quantify the reliability of the calculated phase boundaries and provide meaningful "error bars" on the diagram. The workflow is demonstrated for representative binary alloys and is structured for gradual scaling to multicomponent systems. We leverage the pyiron[3] workflow framework for reproducible and efficient automation, to accelerate the discovery of sustainable materials.

[1] R. Drautz, Phys. Rev. B 100, 249901 (2019).
[2] S. Menon et al., npj Comput. Mater. 10, 261 (2024).
[3] J. Janssen et al., Comput. Mater. Sci. 163, 24-36 (2019).

15 min. break

MM 13.5 Tue 11:30 SCH/A251

Towards Disorder-Aware Materials Discovery - Recognizing and Modeling Crystallographic Disorder — •Konstantin S. Jakob[1], Aron Walsh[2], Karsten Reuter[1], and Johannes T. Margraf[1,3] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Imperial College London — [3]Universität Bayreuth

Recent computational materials discovery efforts have led to an enormous number of predictions of previously unknown, potentially stable inorganic, crystalline materials. However, these efforts are currently limited to predicting perfectly crystalline materials. As a consequence, many of these predictions cannot be verified in experiments, where kinetic effects, defects, and crystallographic disorder can be crucial. Here, we discuss disorder as a current frontier in materials discovery. To this end, we show that machine learning classification models can reliably recognize disordered materials and demonstrate that a significant fraction of computationally predicted materials are likely disordered [1]. On the example of compositionally complex transition metal ferrite spinels, we then demonstrate how machine learning interatomic potentials and Monte Carlo sampling can be used to tackle such disordered systems efficiently.

[1] K.S. Jakob, A. Walsh, K. Reuter, J.T. Margraf, Adv. Mater. e14226 (2025).

MM 13.6 Tue 11:45 SCH/A251

Efficient Exploration of the Unknown: Distance-Based Active Learning with SISSO Descriptors and Mendeleev Similarities for Materials Discovery — •Sreejani Karmakar[1], Akhil S. Nair[1,2], Lucas Foppa[1], and Matthias Scheffler[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Freie Universität Berlin, Berlin, Germany

The performance of AI models depends strongly on the distribution of their training data, which ideally should be independent and identically distributed. Materials-science datasets often violate this condition, containing redundancy and bias that hinder the discovery of statistically rare high-performance materials. Active learning (AL) helps by building concise, diverse training sets, introducing underrepresented materials classes. Commonly, AL relies on uncertainty estimates derived from the variance of model ensembles[1], but these are frequently overconfident and limit AL efficiency. We introduce an alternative strategy that selects candidate materials based on their distance from the existing training set in a low-dimensional descriptor space[2]. These descriptors, derived via SISSO (sure independence screening and sparsifying operator) symbolic regression approach. This distance-guided approach outperforms ensemble-based uncertainty AL, successfully identifying perovskites with exceptional properties. Adding the Mendeleev similarity metric further improves dataset diversity and supports efficient navigation of unexplored material space.

[1] A. Nair et al., npj Comput. Mater., 11, 150, 2025. [2] D. Wu et al., Inf. Sci., 474, 90, 105, 2019.

MM 13.7 Tue 12:00 SCH/A251

Where Are Large Language Models Actually Useful for Materials Design? — •Hedda Oschinski, Maximilian L. Ach, David Greten, Konstantin S. Jakob, Christian Carbogno, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin

The rapid development of large language models (LLMs) and LLM-based agents has opened new possibilities for accelerating materials discovery and design. In this work, we explore their potential in the context of solar cell materials, a class of systems requiring complex, multi-property optimization across chemistry and materials science. By systematically evaluating a range of tasks for a well-known test set of Elpasolites - from context preparation and descriptor prioritization to design hypothesis generation and autonomous validation within an agent framework - we identify where current LLMs provide genuine utility and where critical limitations remain. Our findings offer a grounded perspective on how these tools can be integrated into materials discovery workflows, and what developments are needed to expand their impact in the future.

MM 13.8 Tue 12:15 SCH/A251

Predictive and interpretable machine learning models for thermodynamics tuning of metal hydrides for hydrogen storage — •Sinan S. Faouri[1], Kai Sellschopp[2,3], Claudio Pistidda[3], and Paul Jerabek[3] — [1]Mechanical and Industrial Engineering Department, Applied Science Private University, Amman, Jordan — [2]Department of Chemical and Process Engineering, University of Canterbury, Christchurch, New Zealand — [3]Institute of Hydrogen Technology, Helmholtz-Centre Hereon, Geesthacht, Germany

Metal hydrides remain among the most promising materials for solid-state hydrogen storage due to their tunable thermodynamic behavior. However, predicting key properties such as equilibrium pressure and hydrogenation enthalpy remains challenging, especially across diverse alloy systems. In this work, we explore feature-based machine learning strategies to model these thermodynamic quantities from elemental descriptors and derived structural features. The study combines experimental and computational data to identify the most relevant predictors governing hydrogen absorption thermodynamics. Particular attention is given to the relationship between atomic-scale size parameters, electronic features, and their collective influence on pressure-enthalpy correlations. The results demonstrate that data-driven approaches can reveal non-obvious structure-property relationships and guide the search for alloys with optimized storage performance. The presented framework offers a step toward integrating machine learning with physical insights for accelerated discovery of functional hydrides.

MM 13.9 Tue 12:30 SCH/A251

Score-based diffusion models for accurate crystal structure inpainting and reconstruction of hydrogen positions — •Timo Reents[1], Arianna Cantarella[2], Marnik Bercx[1], Pietro Bonfà[2,3], and Giovanni Pizzi[1] — [1]PSI Center for Scientific Computing, Theory and Data, CH-5232 Villigen PSI, Switzerland — [2]Department of Physics and Earth Sciences, University of Parma, IT-43124 Parma, Italy — [3]Dipartimento di Scienze Fisiche, Informatiche e Matematiche, University of Modena and Reggio Emilia, IT-41125 Modena, Italy

Generative AI methods are rapidly evolving to speed up and improve materials discovery. Diffusion based models can not only be adopted to generate new materials with desired properties but also to reconstruct crystal structures for which structural information is only partially available. In this work, we use Microsoft's mattergen [1], a diffusion based model originally designed to generate new stable crystal structures, and extend it to reconstruct missing hydrogen sites in crystal structures reported in experimental databases. This is particularly useful as the experimental measurement of hydrogen sites with standard XRD is typically challenging due to weak scattering of hydrogen. We show how to leverage image inpainting approaches known from computer vision, combined with universal machine learning interatomic potentials, to improve the success rate of correctly identifying the missing sites or finding lower energy configurations while significantly lowering the computational cost with respect to a direct DFT approach.

[1] Zeni, C. et al., Nature 639, 624-632 (2025)

MM 14: Liquid and Amorphous Materials I

Time: Tuesday 11:30–12:45 Location: SCH/A315

MM 14.1 Tue 11:30 SCH/A315

Shining Light on Gold-in-Gallium: DFT Insights into Photocatalytic Benzyl Alcohol Oxidation — •Oliver Conquest[1], Chung Nguyen[2], Sarina Sarina[2], and Catherine Stampfl[1] — [1]School of Physics, The University of Sydney, Sydney, Australia — [2]School of Chemical and Biomolecular Engineering, The University of Sydney, Sydney, Australia

Recent experimental results have shown that pure liquid Ga with an oxide later does not perform well as a photocatalyst for Benzyl alcohol conversion to Benzaldehyde. When Au nanoparticles (Au NP) are introduced into the system, it emerges as an excellent Benzyl alcohol conversion photocatalyst. The Au NP develop an ultra-thin amorphous-GaO_x (a-GaO_x) skin when placed in liquid Ga, the a-GaO_x in the presence of Au is expected to play an important role in the photoreaction. Therefore, understanding the reaction mechanism requires atomic level investigation into the a-GaO_x/Au(111), and Au(111)/a-GaO_x/Ga interfaces. We perform molecular dynamics and density functional theory (DFT) calculations to provide insight into the charge and photoexcited properties of the Au(111)/a-GaO_x/Ga heterostructures with a careful emphasis on the a-GaO_x layer. The DFT calculations of the a-GaO_x/Au(111) interface demonstrate the charge transfer characteristics between the Au(111), a-GaO_x Ga-liq layers and provide a new detailed understanding of the photocatalytic mechanisms at play.

MM 14.2 Tue 11:45 SCH/A315

Reactive Edges and Inevitable Adsorption in Carbon Nanomembranes — •Levin Mihlan[1], Filip Vuković[2], Andrei Postnikov[3], Verena Müller[4], and Jürgen Schnack[1] — [1]Universität Bielefeld, Germany — [2]TU Wien, Austria — [3]Université de Lorraine, France — [4]Friedrich-Schiller-Universität, Germany

Carbon nanomembranes (CNMs) are nanometer-thin materials synthesized via electron-induced crosslinking of aromatic self-assembled monolayers. These membranes can be functionalized for various applications, initially serving as molecular filters. In addition to their internal structure, the precise elemental composition is not yet fully understood [1]. Therefore a first-order prediction for ultraviolet photoelectron spectroscopy (UPS) was developed based on DFT-calculated densities of state. Combined with theoretical carbon-only CNM model structures and an analysis of the near-zero binding-energy region, this approach enables statements regarding the saturation of different regions as well as the presence of reactive edges and dangling bonds. Since these regions are highly unstable under ambient conditions, physisorption and chemisorption of elements such as hydrogen and oxygen are to be expected. In this work, various CNM model structures are systematically investigated using this methodology, ultimately supporting the presence of such depositions, provided that other observations are valid.

[1] Dementyev, Petr, et al. "Carbon Nanomembranes from Aromatic Carboxylate Precursors" ChemPhysChem 21.10 (2020): 1006

MM 14.3 Tue 12:00 SCH/A315

Volume increase of silica glass due to water intercalation and silanol group formation — Manuel Enns[1], Wolfgang Körner[1], Christian Elsässer[1,2], and •Daniel F. Urban[1,2] — [1]Fraunhofer Institut für Werkstoffmechanik IWM, Freiburg, Germany — [2]Freiburger Materialforschungszentrum FMF, Albert-Ludwigs-Universität Freiburg, Germany

We present a theoretical study on the change of volume of silica glass due to the intercalation of molecular water and the formation of silanol groups. By a statistical representative set of density functional theory calculations, we obtained a volume increase per mole of molecular water in amorphous SiO_2 of 2.5 cm^3/mol. In comparison, for the reaction of water to silanol groups we found on average a 3.5 times larger volume increase of 8.7 cm^3/mol. Our results show that the exothermic dissolution of H_2O into silanol pairs is not restricted to small rings of size three and four. We find an equal distribution of reaction energies over all ring sizes which we explain by the structural relaxation and the related energy gain of the entire amorphous neighbourhood. Statistically, most exothermic dissolution of H_2O may happen at five-membered rings since they outnumber the three- and four-membered rings in amorphous SiO_2. Our findings shed new light on the underlying mechanisms and the size of the volume change of the water intercalation in silica glass and we discuss our findings with respect to previous experimental and theoretical work.

MM 14.4 Tue 12:15 SCH/A315

Insights into the interplay of relaxation and crystallization of Vit106a glass — •Lukas Musiol[1], Merlin Kempf[2], Lukas Musiol[1], Remi Daudin[2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Université de Grenoble Alpes, CNRS, Grenoble INP, Laboratoire SIMaP, Grenoble, France

Metallic glasses are metastable systems that show relaxation behavior towards a local energy minimum and crystallize when heated sufficiently above their glass transition temperature (Tg). Different modes of relaxation can be accessed by varying the combination of relaxation time and temperature. At temperatures significantly lower than Tg only β-relaxation is expected, corresponding to local rearrangements of few atoms. For temperatures close to Tg and for long times only α-relaxation is observed which corresponds to collective rearrangements in the glass. While these two relaxations are often considered independent, a growing body of evidence shows that they are linked [J. Phys. Chem. Lett., 3 (2012), 735; Intermetallics, 93 (2018), 101]. Additionally few attempts have been made to understand how structural changes during relaxation influence crystallization behavior.

Vit106a as a model system of bulk metallic glasses has been investigated concerning the relaxation dynamics and changes in crystallization behavior using conventional scanning calorimetry correlated to strutural analyses using transmission electron microscopy-based methods.

MM 14.5 Tue 12:30 SCH/A315

Unraveling the Correlation Between Populated Site Energies, Activation Barriers and Saddle Point Energies in Solid Ion Conductors — •Martin Schäfer[1], Mohammad A. Badragheh[2], Michael Vogel[2], and Karl-Michael Weitzel[1] — [1]Universität Marburg, Marburg, Germany — [2]T.U. Darmstadt, Darmstadt, Germany

Transport phenomena in disordered materials are governed by a complex potential energy landscape that includes a distribution of local energy minima (sites),

saddle point energies and local energy barriers. An understanding of the connection of these properties is essential to unravel the transition between local hops and long-range transport.

In this work, the populated site energy distribution (PSED) is experimentally determined by the Charge Attachment Induced Transport (CAIT) technique that yields concentration dependent diffusion coefficients and activation energies by comparison of measured concentration depth profiles to calculated profiles gained by Nernst-Planck-Poisson modeling [1]. The distribution of local barriers is probed through Nuclear Magnetic Resonance (NMR) measurements [2]. For Li3B7O12, the FWHM of the PSED is determined to be 250 meV while the activation energies show a FWHM of about 440 meV suggesting that the apparent energy distribution of saddle points must be significantly broader than the distribution of site energies.

[1] V.H. Gunawan, M. Schäfer, and K.-M. Weitzel, Phys.Chem.Chem.Phys., 26, 14430 (2024)

[2] M.A. Badgragheh, E. Winter, M. Vogel, unpublished results

MM 15: Phase Transformations I

Time: Tuesday 14:00–15:45 Location: SCH/A215

MM 15.1 Tue 14:00 SCH/A215

Quantum Geometric Injection and Shift Optical Forces Drive Coherent Phonons — •Luke Pimlott and Habib Rostami — University of Bath, Bath, United Kingdom

We identify injection and shift rectified Raman forces, which are phononic counterparts of the photogalvanic effect, that drive lattice vibrations and trigger transient emergent properties. These forces are governed by the quantum geometric tensor, a phononic shift vector, and interband asymmetries in the electron-phonon coupling. As a response to pulsed light, the injection force induces displacive atomic motion, while, unlike conventional impulsive mechanisms, the shift force produces impulsive atomic displacement in the resonant interband absorbing regime when time-reversal symmetry is broken. Using the bilayer Haldane model, we quantify the injection and shift forces acting on interlayer shear phonons through both analytical and numerical methods. Strikingly, we reveal strong tunability, both in magnitude and direction, of the rectified forces by varying the driving frequency and magnetic flux, uncovering a distinct quantum geometric mechanism for ultrafast and coherent manipulation of quantum materials.

MM 15.2 Tue 14:15 SCH/A215

Charge Density Wave Transition in $ZrTe_3$ from First Principles — •Josu Diego López and Matteo Calandra Buonaura — University of Trento, Trento, Italy

$ZrTe_3$ is a quasi-one-dimensional compound that undergoes a charge density wave (CDW) transition at 63 K with a propagation vector of $\mathbf{q}_{\mathrm{CDW}}$ =(0.07, 0, 0.33) in reciprocal-lattice units and characterized by a very sharp Kohn anomaly in reciprocal space. Although Fermi surface nesting between the quasi-1D bands has been widely invoked to explain this instability, a complete first-principles characterization of the lattice dynamics is still lacking. In particular, the phonon modes at the CDW wavevector have never been computed, even within the harmonic approximation, leaving open fundamental questions regarding the role of the electron-phonon interaction in this material.

In this work, we analyze from first principles the electronic and vibrational properties of the high-temperature phase of $ZrTe_3$. We show that only the correct characterization of the Fermi surface yields an imaginary harmonic phonon mode consistent with the observed CDW. Having access to the harmonic phonons at the critical wavevector also enables the calculation of the electron-phonon interaction at $\mathbf{q}_{\mathrm{CDW}}$, providing a framework to directly compare the electron-phonon mechanism with the nesting scenario in driving the CDW formation.

Funded/Co-funded by the European Union (ERC, DELIGHT, 101052708).

MM 15.3 Tue 14:30 SCH/A215

Coupled phase transition and valence fluctuations in Fe-doped $BaTiO_3$: a combined DFT and DMFT study — •Zhiyuan Li, Ruiwen Xie, and Hongbin Zhang — Institute of Materials Science, TU Darmstadt, 64287 Darmstadt Germany

Rational control of structural phase transitions in perovskites is a key challenge in materials design. In Fe-doped $BaTiO_3$(BTO), experiments observe a tetragonal-to-hexagonal transition, yet the governing microscopic mechanisms remain unclear. A critical control parameter is the Goldschmidt tolerance factor, which relies intimately on the dopant ionic radius and, consequently, the valence state. However, the valence of Fe in BTO remains a long-standing open question, with conflicting reports necessitating a treatment beyond standard DFT. Here, we employ Density Functional Theory (DFT) combined with Dynamical Mean-Field Theory (DMFT) to investigate this interplay. DMFT reveals that the Fe dopant exhibits strong valence and spin fluctuations, which are significantly suppressed by oxygen vacancies to stabilize a high-spin state. Integrating these electronic insights, our total-energy calculations identify three cooperative mechanisms driving the phase transition: tolerance factor variations, Jahn-Teller distortions, and oxygen vacancy formation. Then a systematic quantitative analysis was performed on these three factors. These findings provide a unified microscopic understanding of defect-mediated phase control.

MM 15.4 Tue 14:45 SCH/A215

Interface structure and migration in phase transformations between Fe_3O_4 and Fe_2O_3 — •Martina Ruffino[1], Baptiste Bienvenu[1], Xuyang Zhou[2], Guangyi Guo[1], Barak Ratzker[1], Dierk Raabe[1], and Yan Ma[3] — [1]Max Planck Institute for Sustainable Materials, Düsseldorf, Germany — [2]Xi'an Jiaotong University, Xi'an, China — [3]TU Delft, The Netherlands

Although redox phase transformations between hematite (Fe_2O_3) and magnetite (Fe_3O_4) entail long-range diffusion, they are known to occur on well-defined $(111)_{\mathrm{mag}}||(0001)_{\mathrm{hem}}$ habit planes, and to maintain the oxygen sublattice fixed up to a change in stacking sequence (fcc and hcp arrangement for Fe_3O_4 and Fe_2O_3, respectively). Moreover, hematite formations during magnetite oxidation, as well as magnetite formations in hematite during reduction, are often observed to be of lenticular shape. In this study, we propose interfacial disconnections (i. e. steps with dislocation character) suitable for the accomplishment of these phase transformations. Using atomistic simulations with an atomic cluster expansion (ACE) potential developed for iron and its oxides, we calculate the equilibrium structures of the disconnections and we study their motion as a means to transform magnetite into hematite and vice-versa. We then validate theoretical calculations experimentally by investigating i) partially oxidised magnetite and ii) partially reduced polycrystalline hematite. Using transmission electron microscopy, we analyse the hematite/magnetite interfaces, characterising them as faceted interfaces containing steps; we observe good agreement with the simulated disconnection structures.

MM 15.5 Tue 15:00 SCH/A215

Grain boundary thermodynamics away from idealized boundaries: How line defects affect stability — •Tobias Brink[1], Swetha Pemma[1,2], Lena Langenohl[1], Saba Saood[1], Yoonji Choi[1], Rebecca Janisch[2], Christian H. Liebscher[2], and Gerhard Dehm[1] — [1]MPI for Sustainable Materials, Düsseldorf, Germany — [2]Ruhr-Universität Bochum, Germany

The concept of grain boundary (GB) phases (or "complexions") was developed to describe how the atomic structure and/or chemistry of GBs depend on external conditions, such as temperature or chemical potential. Analogous to bulk phases, GB phases also affect material properties. Even in the case of pure metals, structural GB transformations impact diffusivity and GB mobility. Simulation studies often concentrate on special, symmetric boundaries, which are easy to describe. It is unlikely, however, that their behavior can be generalized to the variety of imperfect GBs in a real polycrystal.

Here, we use atomistic simulations with empirical potentials to investigate thermodynamics of asymmetric GBs in Cu. Symmetric ⟨111⟩ tilt boundaries exhibit two GB phases. These also exist in asymmetric GBs, but contain multiple line defects (disconnections) that enable the deviation from the symmetric GB plane. We found the same defects in thin film samples using scanning electron transmission microscopy. Most importantly, their presence alters the thermodynamic stability of the two GB phases, even for very small deviations from the symmetric GB. We conclude that defects of defects have to be considered in interface thermodynamics.

MM 15.6 Tue 15:15 SCH/A215

Size effects on phase change: solid-state wetting vs. coherency stress — •Yong Li[1] and Jörg Weissmüller[2,1] — [1]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany

Coherent phase transformations in interstitial solid solutions or intercalation compounds with miscibility gaps are crucial to the behavior of energy storage materials, particularly metal hydride and lithium-ion compounds nanoparticles. Prior studies often attribute size-dependent phase transformation behavior either to solid-state critical-point wetting at particle surfaces or to coherent stresses from solute-saturated surface layers. We introduce a hybrid numerical approach that couples atomistic grand canonical Monte Carlo simulations with continuum mechanics analysis of coherency-stress, allowing wetting and mechanical constraints to be simulated simultaneously or independently, thereby decoupling their respective contributions. For material parameters representative of realis-

tic interstitial solutions, we find that solid-state wetting has only a minor influence, whereas coherency stress dominates the size dependence. Mechanical interactions reduce phase-transformation hysteresis at small sizes and increase solute binding in the solid, thereby lowering the chemical potential 'plateau' at the phase coexistence.

MM 15.7 Tue 15:30 SCH/A215

Critical-point wetting at crystal surfaces: Cahn-Hilliard residuum and occurence of first-order wetting transition — •Marine Bossert[1], Yong Li[2], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany — [2]Institute of Hydrogen Technology, Helmholtz Center Hereon, Geesthacht, Germany

Since its publication in 1958, the work by J.W. Cahn and J.E. Hilliard on the free energy of non-uniform systems [1] has been the basis for numerous studies, such as phase-field simulation of microstructure evolution or solute segregation to lattice defects. Cahn and Hilliard found that the second derivative (Laplacian) of the composition field governs the excess energy of systems with conserved networks of sites - such as crystals. A partial integration of the excess energy gives the gradient-square representation, which has been used in all follow-up works in an approximate form that neglects the partial integration residuum. Inspecting critical-point wetting at the surface of an Ising-type FCC crystal with a miscibility gap, this study shows that the solutions obtained with the (exact) second derivative or with the (approximate) gradient-square expressions for the free energy are in fact qualitatively different: the first-order wetting transition predicted by the gradient-square approach is not confirmed by the second-derivative one. Moreover, atomistic Monte-Carlo simulations confirm the absence of a first-order transition. [1] Cahn, J. W., & Hilliard, J. E. (1958).The Journal of Chemical Physics, 28(2), 258-267.

MM 16: Functional Materials II

Time: Tuesday 14:00–15:45 Location: SCH/A216

MM 16.1 Tue 14:00 SCH/A216

Low and High Dose Gamma Radiation Effect on Germanium-Doped Optical Fibers: Investigation of Color Centers — •Esra Kendir Tekgül — Bilkent University UNAM, Institute of Materials Science and Nanotechnology, Ankara, 06800, TURKEY

Ge-doped optical fibers are widely used in sensing, data transmission, and space technologies, making their radiation resistance crucial. Gamma irradiation creates radiation-induced defects that form color centers, degrading optical transmission. In this study, five Ge-doped fibers and one quartz fiber were exposed to gamma rays of 0.5-50 kGy. RIA values at 550, 600, 680, and 755 nm were measured before and after irradiation, and color centers were identified from the RIA spectra. GeX, Ge-NBOHC, and GeY defects were attributed to Ge contributions, whereas ODC(II), STH1, and STH2 were attributed to the SiO2 matrix. NA and FTIR results showed radiation-induced changes in refractive index and a decrease in NA. Overall, the findings highlight the potential of Ge-doped fibers for radiation-hard applications and dosimetric sensing.

MM 16.2 Tue 14:15 SCH/A216

Switching applications in optical circuits using the electrochromic properties of LiMn2O4 — •Vinit Kumar Agarwalla[1], Yug Joshi[2], Guido Schmitz[1], and Mayank Kedia[3] — [1]Institut für Materialwissenschaft, Universität Stuttgart, Stuttgart Germany — [2]Max Planck Institute for Sustainable Materials, Dusseldorf, Stuttgart — [3]Institut für Photovoltaik, Universität Stuttgart, Stuttgart Germany

Optical communication depends on the accuracy with which the path of light is controlled to minimize signal loss in waveguides. The current method of optimizing the path of light is to maintain the waveguide's refractive index using the thermooptic effect. The waveguide consists of a core in which light travels, surrounded by cladding material to ensure total internal reflection, and a third protective outer layer. Here, I propose using electrochromic lithium manganese oxide(LiMn*O*, LMO) as a waveguide cladding. The primary wave from the core extends into the cladding known as evanescent waves, so changing the cladding*s refractive index changes the evanescent waves' path and thus the entire path of the light. Previous work has shown a change in refractive index in the visible region. Building on that, we measured IR reflectance spectra showing continuous visible-to-IR transitions, 100% reflectance, and resonance shifts with lithiation. Calculations show that a 38 μm waveguide can induce a π phase shift at 1550 nm. We also propose various delithiation methods to alter optical properties without degrading the optical structure.

MM 16.3 Tue 14:30 SCH/A216

In-Situ Activation of a Monolithic SrTiO3 Single Crystal for Room Temperature Hydrogen Sensing — •Karl-Michael Weitzel, Timo Kassubek, and Kevin Rein — Department of Chemistry, Philipps-Universität Marburg, Marburg, Germany

The development of reliable, fast, and cost-effective hydrogen sensors is of increasing importance for the safe implementation of a hydrogen-based economy. This work presents a novel and simple single-step method to convert an insulating strontium titanate (SrTiO3) single crystal into a highly sensitive, monolithic hydrogen sensor that operates at room temperature. The activation is achieved by applying a moderate DC electric field (100 V/cm) across a symmetric Pt/SrTiO3/Pt capacitor structure at 180 ˚C in a pure hydrogen atmosphere (200 mbar). This process causes a drastic and stable reduction in the material's resistance by several orders of magnitude. We propose a model of "field-induced chemical doping" to explain this transformation. The resulting activated crystal exhibits excellent hydrogen sensing properties at room temperature, detecting molecular hydrogen (H2) over an exceptionally wide partial pressure range from 0.0001 mbar to 1000 mbar with an accuracy of a few percent. The sensing mechanism is based on the reaction of hydrogen with the activated SrTiO3 sample, involving the release of electrons back into the conduction band and lowering the device's resistance. This monolithic approach opens a new pathway for designing robust and easy-to-fabricate chemical sensors from wide-bandgap oxides.

MM 16.4 Tue 14:45 SCH/A216

The laser-induced synthesis of Co-MOFs, the investigation of optic, gase sorption, DFT and sensor properties — Saliha MUTLU[1,2], Bülend ORTAÇ[2], Ali KARATUTLU[2,3], Taylan GÖRKAN[2], Engin DURGUN[2], Dilek SÖYLER[4], Saniye SÖYLEMEZ[4], Jelena LILLEPÄG[5], Volkan FILIZ[5], Nergis ARSU[6], and •Sevil SAVAŞKAN YILMAZ[1] — [1]Karadeniz Technical University Chemistry Department, Trabzon, Türkiye — [2]Bilkent University, Institute of Materials Science Nanotechnology and National Nanotechnology Research Center (UNAM), Ankara, 06800 Turkey — [3]Sivas University of Science and Technology, Department of Engineering Basic Sciences, Sivas, 58100 Turkey — [4]Department of Biomedical Engineering, Necmettin Erbakan University, Konya, 42090 Turkey — [5]Helmholtz-Zentrum Geesthacht, Institute of Polymer Research, Max-Planck-Str. 1, 21502 Geesthacht, Germany — [6]Yildiz Technical University, Department of Chemistry, Davutpasa Campus, Istanbul, 34220 Turkey

High-power rapid laser-induced synthesis of MOFs has drawn significant attention due to the rapid and effective preparation conditions for Zn- and Ni-MOFs. In this study, the Co-MOF microcrystals yield visible light photoluminescence with relaxation times on the order of ns, showing controllable properties, including low-temperature paramagnetic state transition, supported by magnetic measurements and DFT calculations. Outstanding performance in gas sorption and electrochemical sensing has been demonstrated with low separation costs and ultra-low LODs for dopamine, respectively.

MM 16.5 Tue 15:00 SCH/A216

First-Principles Study of Electronic and Optical Properties of Mo-Doped $CsPbBr_3$ Perovskites — Said Al Azar[1], Anas Al-Reyahi[2], •Saleh Bashaish[3], and Marwan Mousa[4] — [1]Zarqa University, Zarqa, Jordan — [2]Hashemite University, Zarqa, Jordan — [3]Al-Ahliyya Amman University, Amman, Jordan — [4]Jadara University, Irbid, Jordan

$CsPbBr_3$ perovskites, particularly when doped, show great promise for tandem solar cells and advanced optoelectronics. This study employs density functional theory (DFT) and semi-classical Boltzmann transport theory to comprehensively investigate the structural, electronic, magnetic, thermoelectric, and optical properties of Mo-doped $CsPb_{(1-x)}Mo_xBr_3$ (x = 0, 0.25, 0.5, 0.75). Our calculations confirm the structural stability of all compositions and reveal a transformative electronic behavior: Mo-doping induces a ferromagnetic half-metallic state. Notably, the x = 0.5 composition exhibits an ideal band gap for solar applications (1.872 eV via mBJ) and a high spin-up figure of merit (zT) approaching unity at room temperature. Additionally, enhanced absorption in the infrared region suggests potential for IR photodetectors. These findings establish Mo-doped $CsPbBr_3$ as a compelling multifunctional material for spintronic and high-efficiency optoelectronic devices.

MM 16.6 Tue 15:15 SCH/A216

Optimizing NiTi Interatomic Potentials Through Atomic Cluster Expansion — •Petr Šesták[1,2], Petr Jaroš[1], Miroslav Černý[2], and Petr Sedlák[1] — [1]Institute of Thermomechanics Czech Academy of Sciences, Prague, Czechia — [2]CEITEC, Brno University of Technology, Brno, Czechia

In this work, we present an interatomic potential for NiTi based on the Atomic Cluster Expansion, developed using the Pacemaker software package. We validate this potential by comparing it against the results of simulations using other

interatomic potentials, quantum-mechanical calculations, as well as our own experimental data. Our quantum-mechanical calculations utilize density functional theory (DFT) within the generalized gradient approximation (GGA) to determine the ground-state structural, electronic, thermodynamic, and elastic properties of NiTi in low-temperature (martensitic) phase. The target properties include elastic constants, phonon spectra calculations, and vacancy formation energy. Specifically, the stress-strain method was employed to compute the full tensor of the second-order elastic constants and assess the mechanical stability of the studied phases, ensuring that the results are consistent with those obtained using other established potentials.

MM 16.7 Tue 15:30 SCH/A216

Response of NiTi martensite to mechanical loading — •Miroslav Černý and Petr Šesták — Central European Institute of Technology, CEITEC, Brno University of Technology, Purkyňova 123, Brno, Czechia

Shape-memory alloys are unique materials capable of undergoing large reversible strains and exhibiting the shape-memory effect, which is driven by external changes of temperature. These remarkable properties are based on a martensitic transformation between austenite (high-temperature phase) and martensite (low-temperature phase). The NiTi shape memory alloy has become the most widely used shape memory material in industrial, high-tech, and medical applications due to its unique thermal and mechanical properties.

In this work we aim at fundamental understanding of the behavior of twins in the martensite structure under mechanical loading. For this purpose, we constructed computational supercells representing both the perfect and twinned martensite and studied their responses to shear and tensile loading. Such calculations are computationally very demanding when using ab initio approaches. Therefore, we employed machine learning to develop a new interatomic potential, tailored specifically for the martensite struc-ture. Computationally accessible predictions based on the potential were benchmarked from first principles.

MM 17: Data-driven Materials Science: Big Data and Workflows II

Time: Tuesday 14:00–15:45 Location: SCH/A251

MM 17.1 Tue 14:00 SCH/A251

Modelling Diffusion Kinetics in Refractory High Entropy Alloys Using Graph Neural Network Database Models — •Klemens Lechner[1], Jiyao Zhang[1], Peter Wagatha[2], Wolfram Knabl[2], Helmut Clemens[1], and David Holec[1] — [1]Department of Materials Science, Montanuniversitaet Leoben — [2]Plansee SE

Refractory high-entropy alloys (RHEAs) offer exceptional mechanical and thermal properties, such as high-temperature strength, and may exhibit high-temperature oxidation and corrosion resistance. However, their stability at high temperatures has yet to be confirmed. Nonetheless, even thermodynamically unstable solid solutions can have useful applications if the decomposition is slow. This is inherently connected with the (self-)diffusion kinetics. In this study, we present a workflow for the systematic investigation of diffusion kinetics in RHEAs. The necessary diffusion barriers are predicted using a graph neural network (GNN). We train the GNN using an active learning cycle involving molecular statics simulations with a universal machine-learning interatomic potential (uMLIP). The training data of migration barriers are calculated using the Nudged Elastic Band method. By varying the amount of training data, the GNN can be trained to an accuracy that, in theory, can fully mimic that of the uMLIP but with a more efficient computation. This is crucial for larger-scale modeling applications, e.g., the kinetics of decomposition, ordering or clustering of specific elements. We demonstrate the usage and performance of the GNN to quantify self-diffusion in Mo-Nb-Ta-W alloys using the Kinetic Monte Carlo method.

MM 17.2 Tue 14:15 SCH/A251

Broken neural scaling laws in machine learning for optical properties of metals — •Max Grossmann, Marc Thieme, Malte Grunert, and Erich Runge — Institute of Physics and Institute of Micro- and Nanotechnologies, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Neural scaling laws guide the development of machine-learning models and their training datasets. Here, we investigate them in the context of materials science, where data are inherently costly and scarce, using dielectric functions of metals as an example. We compute dielectric functions for 205,224 intermetallic compounds using high-throughput *ab initio* calculations and train two multi-objective graph neural networks, OptiMetal2B and OptiMetal3B—the latter incorporating three-body interactions—to predict the complex interband dielectric function and the Drude frequency. Systematic variations in the number of training data and model parameters reveal so called "broken" neural scaling laws. Data scaling follows a smoothly broken power law, with steeper slopes occurring above 20,000 materials. In contrast, parameter scaling follows a conventional power law but saturates at around ten million parameters. Including three-body interactions improves accuracy by about 12% but leaves scaling slopes essentially unchanged. These findings suggest that, in the context of spectroscopy, expanding high-quality datasets is a more effective way to improve machine-learning models than optimizing network architectures, increasing body order, or merely increasing network size.

MM 17.3 Tue 14:30 SCH/A251

Simultaneous Learning of Static and Dynamic Charges — Philipp Stärk[1], •Philip Loche[2], Marcel Langer[1], Henrik Stooss[1,3], Michele Ceriotti[2], and Alexander Schlaich[1,3] — [1]Stuttgart Center for Simulation Science, University of Stuttgart, Germany — [2]Laboratory of Computational Science and Modeling, École Polytechnique Fédérale de Lausanne, Switzerland — [3]Institute for Physics of Functional Materials, Hamburg University of Technology, Germany

Long-range interactions and electric response are essential for accurate modeling of condensed-phase systems, yet remain challenging for atomistic machine learning. Static charges modulate Coulomb interactions, while dynamic charges such as atomic polar tensors describe the response to external electric fields. We compare strategies for learning both types of charges: independent models; coupled learning with or without an isotropic dielectric correction; and coupled learning with an environment-dependent screening. While screening corrections are crucial in the coupled case, assuming homogeneous, isotropic screening fails in heterogeneous systems such as water clusters. Learning a local screening restores accuracy for dynamic charges but offers negligible improvement over independent models while increasing computational cost.

MM 17.4 Tue 14:45 SCH/A251

A high-throughput study of heterostructures with polar discontinuities — •Maria Andolfatto[1,2,3], Junfeng Qiao[2,1], Davide Campi[3], and Nicola Marzari[1,2] — [1]PSI - Switzerland — [2]EPFL - Switzerland — [3]Unimib - Italy

Heterostructures composed of two bulk insulating materials with different polarizations can exhibit localized conductive states at the interfaces and could lead to a wide range of technological applications. Currently, most studies focus on perovskite-based materials to engineer such heterostructures, whose number and performance is limited. This project aims to identify new candidate heterostructures exhibiting interface-localized conductive states by leveraging high-throughput computational screening. Starting from thousands of bulk materials, we compute the polarization and we systematically identify thousands of possible interface combinations. Finally, we analyze the resulting localized density of states of thirty-one heterostructures to assess the formation of two-dimensional electron gases (2DEGs).

MM 17.5 Tue 15:00 SCH/A251

Leveraging Koopmans band structure for exciton characterization in materials — •Miki Bonacci[1], Nicola Colonna[1], Edward Linscott[1], and Nicola Marzari[1,2] — [1]PSI Center for Scientific Computing, Theory and Data, 5232 Villigen PSI, Switzerland — [2]Theory and Simulation of Materials (THEOS), Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland

Exciton characterization is crucial for several materials applications, ranging from energy transport and storage technologies to photocatalysis, plasmonic, sensing. The ab initio state-of-the-art approach is many-body perturbation theory (MBPT), in particular the Bethe-Salpeter equation (BSE) [1]. This is usually built on top of computationally demanding G0W0 quasiparticle (QP) band structures (BSE@G0W0 approach). In this work, we demonstrate how it is possible to construct the BSE Hamiltonian starting from Koopmans functionals [2] eigenvalues as the main ingredient for the BSE Hamiltonian (BSE@KI), obtaining optical spectra with comparable accuracy with respect to the BSE@G0W0, at reduced computational cost. Automated workflows to compute BSE@KI are provided within the AiiDA workflow engine [3].

[1] Onida et al., Rev. Mod. Phys., 74(2), 601-659 (2002)
[2] Dabo et al., Phys. Rev. B, 82, 115121 (2010)
[3] Huber et al., Sci. Data, 7(1):300 (2020)

MM 17.6 Tue 15:15 SCH/A251

Many-body perturbation theory vs. density functional theory: A systematic benchmark for band gaps of solids — •Marc Thieme[1,2], Max Grossmann[1], Malte Grunert[1], and Erich Runge[1] — [1]Institute of Physics and Institute of Micro- and Nanotechnologies, Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Institute of Applied Physics, Friedrich Schiller Universität, 07743 Jena, Germany

The band gap is one of the most important material properties for optoelectronic applications. However, predicting band gaps remains a challenging task in materials science. Here, we benchmark many-body perturbation theory against density functional theory, the workhorse of computational materials

science, for predicting the band gaps of solids. We systematically compared four GW variants—G_0W_0 using the plasmon-pole approximation (G_0W_0-PPA), full-frequency quasiparticle G_0W_0 (QPG_0W_0), full-frequency quasiparticle self-consistent GW (QSGW), and QSGW augmented with vertex corrections in W (QS$G\hat{W}$)—against the currently best-performing and popular density functionals. Our results show that the QS$G\hat{W}$ produces band gaps so accurate that they can even flag questionable experimental measurements, albeit at an extremely high computational cost. To balance accuracy and efficiency, we identify lower-cost alternatives, such as the QPG_0W_0 and a rescaled version of the QSGW, which achieve nearly the same accuracy as the QS$G\hat{W}$ while being significantly more efficient, making them promising candidates for generating high-fidelity datasets in machine-learning-driven materials discovery.

MM 17.7 Tue 15:30 SCH/A251

Learning G_0W_0 Self-Energies in Real Space with Equivariant Neural Networks — •Elisabeth Keller, Karsten W. Jacobsen, and Kristian S. Thygesen — CAMD, DTU Physics, Kongens Lyngby, Denmark

Many-body G_0W_0 calculations provide highly accurate quasiparticle energies for semiconductors and insulators beyond standard density-functional theory, but at a much higher computational cost.

To overcome this limitation, we use equivariant neural networks to replace the explicit G_0W_0 self-energy evaluation. The networks are trained on G_0W_0 self-energies from GPAW projected onto an atom-centered LCAO basis. Using this representation, we investigate how the real-space localization of the self-energy enables learning from atomic configurations.

MM 18: Liquid and Amorphous Materials II

Time: Tuesday 14:00–15:30 Location: SCH/A315

MM 18.1 Tue 14:00 SCH/A315

Influence of Phosphorus Content on the Symmetry and Correlation Length of the Medium-Range Order in Pd-Ni-P Bulk Metallic Glasses — •Hongshuai Li, Harald Rösner, and Gerhard Wilde — Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Pd-Ni-P metallic glass is known as an excellent glass former, which enables systematic investigation of how variations in phosphorus (P) content affect its structural characteristics. In this study, we investigate the influence of P concentration on the dominant correlation length and the local symmetries of motifs within Pd-Ni-P metallic glass using fluctuation electron microscopy (FEM) and angular correlation microscopy. In FEM, the relationship between normalized variance and probe size can be used to examine the medium-range order (MRO) in amorphous materials. Our experimental results reveal that, as the composition deviates from the eutectoid composition Pd40Ni40P20, the correlation lengths associated with the dominating motifs undergo significant changes. Moreover, the volume fraction of the medium-range order increases as the P content diverges from the eutectoid composition. Regarding the symmetry analysis, the P content exerts a strong impact on the four-, five-, and six-fold symmetries. Specifically, as the P content moves away from the eutectoid composition, five-fold symmetry becomes prominent relative to the four- and six-fold symmetries.

MM 18.2 Tue 14:15 SCH/A315

Decoupling Structural and Mechanical Behavior in CuZr Metallic Glasses — •Askar Kvaratskheliya[1], Jürgen Eckert[1,2], and Daniel Şopu[1,3] — [1]Erich Schmid Institute of Materials Science, Leoben, Austria — [2]Technical University of Leoben, Leoben, Austria — [3]Technical University of Darmstadt, Darmstadt, Germany

Although lacking of long range order symmetry, metallic glasses (MG) possess a high degree of short- and medium-range order that governs their macroscopic properties. Particularly, in case of CuZr MG, network of five fold symmetry clusters defines the degree of local order. These motifs resist shear, stabilize energy minima, and inhibit strain localization. In this study, we systematically decouple the contributions of distinct motif perturbations by simulating irradiation-induced structural states through targeted atomic dilution. Specifically, we construct post-irradiation analogs of $Cu_{64}Zr_{36}$ MG by systematically removing atoms according to their local motifs. This approach enables decoupling of the influence of local topology from the overall degree of rejuvenation. We investigated how perturbation of specific motifs alters relaxation, stress distribution, and mechanical strength. Recent advances in high-performance computing have enabled a clear shift toward large-scale, high-throughput molecular dynamics workflows. Leveraging this paradigm, we performed an extensive parameter sweep consisting of hundreds of independent molecular dynamics simulations, systematically varying temperature and structural perturbation protocols.

MM 18.3 Tue 14:30 SCH/A315

Influence of Xe swift heavy ions irradiation on the mechanical properties of PdNiP bulk metallic glasses — •Maren Jeromin[1], Marilena Tomut[1,2], and Gerhard Wilde[1] — [1]Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str.10, 48149 Münster — [2]GSI Helmholtzzentrum für Schwerionenforschung, 64291 Darmstadt

Pd40Ni40P20 bulk metallic glass samples that had been subjected to different relaxation states were investigated by nanoindentation and laser scanning microscopy (LSM) for irradiation effects induced by swift heavy ions. The samples were irradiated with 630 MeV Xe-ions at the UNILAC accelerator at GSI in Darmstadt. During irradiation, the samples were partially covered with honeycomb- patterned masks to enable direct comparison between irradiated and non-irradiated areas. LSM revealed a distinct swelling step at the mask boundary, whose height increased with ion fluence and varied systematically with the relaxation state of the material. The observed swelling is attributed to ion track formation, where localized melting and rapid re-solidification generates excess volume due to cooling rates exceeding the initial quenching rate. Nanoindentation measurements demonstrated a fluence-dependent decrease in hardness; however, the hardness of irradiated regions consistently remained higher than that of pristine samples. These findings offer new insight into the structure modification of bulk metallic glasses under medium-mass swift ion irradiation, where elastic collision effects increasingly compete with ion track formation governed by electronic energy-loss processes.

MM 18.4 Tue 14:45 SCH/A315

A ReaxFF study of the covalency-driven cracking-to-shearing transition in metal-metalloid glasses — •Shansi Liao[1], Jürgen Eckert[1,2], and Daniel Şopu[1,3] — [1]Erich Schmid Institute of Materials Science, Leoben, Austria — [2]Technical University of Leoben,Leoben, Austria — [3]Technical University of Darmstadt, Darmstadt, Germany

Revealing the atomistic origins of failure in amorphous solids remains challenging. In metal-metalloid glasses, mechanical response is strongly governed by the breaking and reformation of covalent bonds which cannot be adequately captured by non-reactive interatomic potentials. Here, large-scale reactive molecular dynamics simulations using a ReaxFF potential that includes angular constraints for covalent bonding reveal a composition-dependent transition from cleavage cracking to shear banding in model CuSi glasses. During loading, a highly connected, rigid Si-rich network suppresses strain delocalization, generating mechanically unstable regions characterized by shear-induced reductions in coordination number and severe distortions of Si-Si-Si bond angles. These unstable regions serve as energetically favorable pathways along which the crack advances. As Cu content increases, reduced angular rigidity promotes widespread shear transformation and shear-band-mediated plasticity. In contrast, the modified embedded-atom method potential, which intrinsically overestimates the angular flexibility of the Si-rich networks, fails to reproduce this transition. Our results show that angular rigidity of the interatomic potential is a key descriptor of plasticity in metal-metalloid glasses.

MM 18.5 Tue 15:00 SCH/A315

Macroscopic response of $Pd_{40}Ni_{40}P_{20}$ Bulk Metallic Glasses to GeV ^{238}U Ion irradiation — •Richard von Destinon, Maren Jeromin, Marilena Tomut, and Gerhard Wilde — Institut für Materialphysik, Universität Münster, Münster, Germany

Ion tracks formed by localized heating due to intense electronic excitations of the target atoms offer new pathways to tailor the mechanical properties of bulk metallic glasses. In this work, we investigate the effects of swift heavy ion irradiation on macroscopic behavior such as the hardness, swelling and strain-rate sensitivity on the well-characterized bulk metallic glass $Pd_{40}Ni_{40}P_{20}$. The samples were thermally relaxed at $0.94T_g$ and subsequently irradiated with 1.14 GeV U ions at the UNILAC accelerator at GSI Helmholtzzentrum für Schwerionenforschung, Darmstadt. By using aluminum degraders of different thicknesses, the energy loss of the ions at the sample surface and their corresponding penetration depths were systematically varied. Characterization was carried out using Laser Scanning Microscopy (LSM) as well as nanoindentation with displacement depths up to 0.3 μm. The results show a pronounced increase of swelling as well as a decrease in hardness with increasing irradiation fluences. The strain-rate-sensitivity increases at higher fluences, suggesting that the increased structural heterogeneity within the irradiated metallic glass alters the local stress distribution, affecting the shear band propagation.

MM 18.6 Tue 15:15 SCH/A315

Compositional and Surface Variations in Sasanian Early Islamic Glasses from Gorgan, Ray, and Istakhr — •Farahnaz Bayat Nejad[1], Mohammadamin Emami[2], Rémy Chapoulie[3], and Farzaneh Bayat Nejad[4] — [1]Islamic Azad University, Central Tehran Branch, Tehran, Iran — [2]Art University of Isfahan, Isfahan, Iran — [3]Archéosciences Bordeaux, UMR 6034 CNRS, Université Bordeaux Montaigne, Pessac, France — [4]Islamic Azad University, Central Tehran Branch, Tehran, Iran

This study investigates the compositional and microstructural characteristics of Sasanian*Early Islamic glasses from Gorgan, Ray, and Istakhr. Laser-Induced Breakdown Spectroscopy (LIBS), Scanning Electron Microscopy with Energy-Dispersive X-ray Spectroscopy (SEM-EDX), and Hyperspectral Imaging (HSI) were used to assess elemental composition, surface morphology, and colorant phases. Distinct variations in Ca/K/Na ratios reflect differences in raw materials and production recipes across the three sites. SEM-EDX reveals heterogeneous corrosion layers and localized devitrification, especially in Istakhr samples with silica-rich alteration crusts. HSI spectra identified absorption features of Fe**, Mn, and Cu** chromophores associated with glass coloration. These results provide insight into technological choices and raw material exchange networks in Late Antique Iran, demonstrating the power of non-destructive, multi-analytical methods in archaeometric glass research.

MM 19: Poster Session

Time: Tuesday 18:00–20:00 Location: P5

MM 19.1 Tue 18:00 P5

RuNNer 2.0: A Fast Software Environment forHigh-Dimensional Neural Network Potentials — •Moritz R. Schäfer[1,2], Alexander L. M. Knoll[1,2], J. Richard Springborn[1,2], Henry Wang[1,2], K. Nikolas Lausch[1,2], Moritz Gubler[3], Jonas A. Finkler[4], Gunnar Schmitz[1,2], Alea Miako Tokita[1,2], Emir Kocer[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany — [3]Paul Scherrer Institute PSI, Villigen, Switzerland — [4]Department of Chemistry and Bioscience, Aalborg University, Denmark

Machine learning potentials (MLPs) have emerged as a widely used approach for large-scale atomistic simulations in chemistry and materials science. They offer computationally efficient access to highly accurate potential energy surfaces (PES) derived from ab initio reference data. As techniques in this area continue to grow in complexity and reach greater maturity, the need for robust, efficient, and user-friendly tools becomes increasingly significant. Here, we introduce the second major release of RuNNer, an open-source, stand-alone software package designed for constructing and evaluating second-, third-, and fourth-generation high-dimensional neural network potentials (HDNNPs). RuNNer 2.0 integrates the complete workflow into a fully MPI-parallelized program – from generating atomistic descriptors and training machine learning models to deploying them in molecular dynamics simulations.

MM 19.2 Tue 18:00 P5

Coordination Corrected Enthalpies for the Thermodynamics of Ionic Materials — •Balaram Thakur[1,2] and Rico Friedrich[1,2] — [1]Technische Universität Dresden, 01062 Dresden. — [2]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden.

Accurate formation enthalpies are essential for data-driven materials discovery. Density functional theory (DFT) predictions are accurate for compounds chemically similar to their elemental references (metallic systems like alloys). However, for ionic materials, it shows large deviations from the experimental values (≥ 100 meV/atom), leading to incorrect stability predictions. The coordination-corrected enthalpies (CCE)[1] method addresses this issue by applying corrections based on oxidation state and cation coordination number. This reduces errors to about 25 meV/atom and resolves inconsistencies among polymorphs.

Here, we extend CCE beyond oxides to halides, focusing on fluorides and chlorides, chosen for their diverse bonding environments and technological relevance in the energy sector, electronics, and optics. Using AFLOW [2,3], these corrections broaden the applicability of CCE and improve thermodynamic predictions for halogen-based ionic compounds, thus enabling more reliable design and screening of functional materials.

[1] R. Friedrich, *et al.*, npj Comput. Mater. **5**, 59 (2019).
[2] R. Friedrich, *et al.*, Phys. Rev. Mater. **5**, 043803 (2021).
[3] S. Divilov, *et al.*, High Entropy Alloys and Mater. **3**, 178 (2025).

MM 19.3 Tue 18:00 P5

Experimentally supported machine-learning interaction potential for Pd-Si — •Przemyslaw Dziegielewski[1], Jerzy Antonowicz[1], Zuzanna Kostera[1], Oleksii Liubchenko[2], and Ryszard Sobierajski[2] — [1]Faculty of Physics, Warsaw University of Technology, Warsaw, Poland — [2]Institute of Physics Polish Academy of Sciences, Warsaw, Poland

Classical Molecular Dynamics (MD) simulations were utilised to reproduce the X-ray Free-Electron Laser (XFEL) experiment. Using the pump-probe technique, a Pd-Si alloy with various Si contents was melted and subsequently solidified with a high cooling rate. The EAM (Embedded Atom Method) potentials available for Classical MD allowed us to obtain simulation results showing high consistency with the experiment for pure Pd and the good glass-forming Pd83Si17 alloy.

However, at low Si contents, they become unreliable, generating a structure that is a combination of the hcp and fcc phases, whereas the experimental data clearly indicate the occurrence of the fcc phase only. The two phases differ only slightly in energy, and the occurrence of the hcp phase for alloys with nearly 100% Pd content takes place, for example, under high-pressure conditions. In our presentation, we introduce an alternative approach to simulating metallic alloys using a Machine Learning (ML)-generated potential within the VASP code. Our proposed procedure may constitute a universal approach for the effective and rapid creation of interaction potentials for the purpose of analysing experimental data.

MM 19.4 Tue 18:00 P5

Unveiling Anharmonicity in High-temperature Diffusion Through Transition State Thermodynamic Integration — •Wenchuan Liu[1], Xi Zhang[1], Xu Xiang[1], Sergiy Divinski[2], and Blazej Grabowski[1] — [1]Institute for Materials Science, University of Stuttgart, D-70569 Stuttgart, Germany — [2]Institute of Materials Physics, University of Münster, 48149 Münster, Germany

Accurate modeling of high-temperature atomic diffusion requires a full treatment of thermal effects, particularly anharmonic lattice vibrations, which are often oversimplified in density functional theory (DFT)-based descriptions. We introduce a novel ab initio method, transition state thermodynamic integration (TSTI), that explicitly incorporates anharmonic contributions to vacancy migration Gibbs energies. TSTI combines DFT, molecular dynamics, and machine-learning interatomic potentials within a unified ab initio framework. Applied first to BCC tungsten, the method quantitatively captures non-Arrhenius diffusivities arising from anharmonicity. We further demonstrate its general applicability to metastable HCP aluminum, enabling high-fidelity input for CALPHAD-type mobility modeling. TSTI provides a general route to computing high-temperature diffusivities with DFT accuracy.

MM 19.5 Tue 18:00 P5

Every configuration counts: An Exact Approach to Doping Effects in AlN — •Oliver Heymer and Jens Kortus — Institute of Theoretical Physics, Freiberg, Germany

We present a new method to study doping effects within Kohn Sham density functional theory. Unlike Zungers Special quasirandom structures [1], our approach generates a complete and irreducible set of crystal structures, capturing all possible atomic configurations and making the description exact. Because we preserve full structural information, we can evaluate configurational entropies and identify the temperatures at which disordered doped AlN structures become energetically favored over the undoped material. Finally, we highlight how doping modifies the band structure and the density of states at the Fermi level.

[1] Zunger A, Wei S, Ferreira LG, Bernard JE. Special quasirandom structures. Phys Rev Lett. 1990 Jul 16;65(3):353-356. doi: 10.1103/PhysRevLett.65.353.

MM 19.6 Tue 18:00 P5

OpenCPMD: Plane-wave-based ab initio molecular dynamics code for large-scale HPC facilities — Tobias Klöffel[1,2], Christian L. Ritterhoff[1], Sagarmoy Mandal[1,2,3], Ritama Kar[3], Nisanth N. Nair[3], and •Bernd Meyer[1,2] — [1]ICMM/CCC, FAU Erlangen-Nürnberg — [2]National High Performance Computing Center, FAU Erlangen-Nürnberg — [3]Department of Chemistry, Indian Institute of Technology Kanpur (IITK), India

We present our recent advances in enabling fast and scalable *ab initio* molecular dynamics simulations on massively parallel HPC architectures with OpenCPMD (www.cpmd.org), an open source, plane-wave-based DFT code [1]. Code changes include new algorithms for hybrid functionals (localization of the orbitals, factorization of the Fock operator, multiple time-stepping [2]), revision of data distribution and communication patterns to reduce inter-node communication, introduction of overlapping computation and communication, partitioning the workload by auto-tuning algorithms, and porting to GPUs. The enhanced performance and scalability of the code is demonstrated on simulations of liquid water with up to 2048 molecules in the unit cell. We show that simulations with many hundred of water molecules for several 100 ps can be done now rou-

tinely within a few days, allowing systematic free energy calculations of chemical processes in liquids.

[1] T. Klöffel, G. Mathias, B. Meyer, Comput. Phys. Commun. **260** (2021) 107745
[2] R. Kar, S. Mandal, V. Thakkur, B. Meyer, N.N. Nair, J. Chem. Theory Comput. **19** (2023), 8351–8364

MM 19.7 Tue 18:00 P5

A Hartree-Fock Analysis of the Finite Jellium Model — •Michael Píro and Jaroslav Hamrle — Czech Technical University, Prague, Czech Republic

A Hartree-Fock analysis of the ground-state electronic structure of the finite spherical jellium model is carried out for systems containing up to 520 electrons in a positive background field with densities ranging from 10^{-3} to 1. The study focuses on resolving the energy-level ordering, accurately characterizing the total energy contributions, and evaluating the performance of local exchange and kinetic-energy approximations. All calculations are performed on a high-resolution real-space grid. Significant discrepancies are observed between the exchange energy obtained from the Hartree-Fock approximation and that predicted by the local density approximation (LDA) evaluated at the computed electron densities, both in the inner region and near the surface of the system. To reconcile these differences, a refined expression for the local one-electron exchange energy density is proposed. In addition, the breakdown of the Thomas-Fermi kinetic-energy model near the surface is addressed by introducing an improved expression for the one-electron kinetic-energy density.

MM 19.8 Tue 18:00 P5

Benchmarking Local Geometry Optimization Algorithms for Realistic Potential Energy Surfaces of Solids — •David Greten[1], Konstantin Jakob[1], Karsten Reuter[1], and Johannes T. Margraf[1,2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Universität Bayreuth

Efficient and robust local structure relaxations are central to computational materials discovery. We benchmark several widely used local optimizers (based on the BFGS, FIRE and conjugate gradient approaches) for relaxing inorganic crystal structures on complex many-body potential energy surfaces obtained from a universal machine-learned interatomic potential. From relaxations of over 170,000 trial structures generated via element substitution, we quantify convergence rates, relaxation efficiency, and the stability and diversity of obtained minima. Some algorithms (e.g. BFGS with line-search and SciPy's conjugate gradient) show substantially higher convergence rates and consistently yield low energy minima. Meanwhile, the computational effort of the tested algorithms is broadly comparable. Based on these insights we discuss how to optimally combine algorithms to obtain a good trade-off between robustness and diversity of explored minima.

MM 19.9 Tue 18:00 P5

Acquisition strategies in multi-objective Bayesian optimization — •Tatu Linnala[1,2], Matthias Stosiek[1], Joakim Löfgren[2], and Patrick Rinke[1,2] — [1]Department of Physics, Technical University of Munich, Garching, Germany — [2]Department of Applied Physics, Aalto University, Espoo, Finland

Bayesian optimization (BO) is a machine learning technique for optimizing expensive black-box functions, and it is increasingly used in computational and experimental materials optimization. Many BO applications involve multiple competing objectives, requiring multi-objective BO (MOBO) to approximate the Pareto front. We extended the Bayesian Optimization Structure Search (BOSS) code to support advanced MOBO methods, focusing on acquisition strategies. Specifically, we implemented three variants of the expected hypervolume improvement acquisition function: an exact form for bi-objective problems and Monte Carlo approximations for higher dimensions. Additionally, we included scalarization-based methods for greater computational efficiency. These methods were benchmarked on six test cases, including synthetic functions and a real-world lignin extraction problem. Results show that hypervolume-based methods yield the most accurate predictions at high computational cost, although scalarization methods may sometimes be sufficient. This highlights the trade-off between accuracy and computational cost, and the application specificity of the optimal strategy. We provide guidelines for selecting appropriate MOBO settings, and the extended BOSS code provides a flexible toolkit for multi-objective optimization.

MM 19.10 Tue 18:00 P5

Transfer Learning Pipeline for GRACE Foundation Models for Complex Materials — •Christian L. Ritterhoff[1], Yury Lysogorskiy[2], Anton Bochkarev[2], Bernd Meyer[1], and Ralf Drautz[2] — [1]Interdisciplinary Center for Molecular Materials (ICMM) and Computer Chemistry Center (CCC), FAU Erlangen-Nürnberg — [2]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum (RUB)

Foundation models of machine-learned interatomic potentials (MLIPs) offer overall good accuracy for a wide range of configurational and chemical spaces. However, achieving high fidelity and high efficiency for dedicated applications often requires further refinement of the model. This is commonly achieved by fine-tuning the foundation model on minimal specialized training data followed by distillation of the acquired knowledge into smaller models. We benchmark different strategies for the example of carbon with its demanding diverse chemistry and structure by fine-tuning the GRACE-1L-OMAT foundation model using the dataset by Qamar *et al.* [1]. Data efficiency is analyzed by training only on randomly chosen subsets of the complete dataset. Advantages of fine-tuning are demonstrated by comparing the obtained models against their randomly initialized counterparts. Finally, the resulting high-fidelity GRACE potential is used for knowledge distillation into a fast, local ACE model. This work validates the transfer learning and distillation paradigm as a robust and efficient pathway for creating deployable potentials for complex materials.

[1] M. Qamar, *et al.*, J. Chem. Theo. Comput. **19** (2023) 5151–5167

MM 19.11 Tue 18:00 P5

LLZO grain boundaries with doped amorphous domains by adaptively fine-tuned machine-learning interatomic potentials — •yuandong wang, yute chan, karsten reuter, and christoph scheurer — Fritz-Haber-Institut der MPG, Berlin, Germany

Garnet $Li_7La_3Zr_2O_{12}$ (LLZO) is a highly promising solid-state electrolyte (SSE) for lithium batteries. However, its application faces challenges, primarily arising from Li dendrite formation, the impact of grain boundaries (GBs) on Li transport and stability. Introducing amorphous intergranular domains can mitigate dendrite propagation while enhancing Li-ion mobility in GBs. Moreover, aliovalent cation doping (e.g., Al^{3+}, Ga^{3+}, Nb^{5+}, Ta^{5+}) in both cubic and amorphous LLZO offers additional levers to further enhance key properties. Rationally engineering the morphology of amorphous GBs offers an intriguing approach for tuning electrolyte performance.

In this study, we investigate strategies for generating structural motifs covering Li diffusion, GBs, and amorphous LLZO, which are diversified to include ion hopping transition states, large defects, amorphous motifs, etc. An adaptively fine-tuned MACE machine-learning interatomic potential (MLIP) is trained to accurately model large-scale and realistic nanoscale structures of LLZO with doped amorphous GBs. With the fine-tuned MLIP, the morphology, dopant effects and crystalline-amorphous interactions governing Li-ion diffusion pathways and activation barriers in LLZO can be studied in detail.

MM 19.12 Tue 18:00 P5

SEI-ntific Discoveries: A DFTB Journey with Constant Potential — •Anton Beiersdorfer[1], Tobias Melson[2], Felix Riccius[1], Chiara Panosetti[1], Christoph Scheurer[1], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Max Planck Computing and Data Facility, Garching

Lithium-ion batteries excel in short-term power grid balancing, yet their performance and longevity are strongly impacted by the solid electrolyte interphase (SEI) formed at the anode-electrolyte interface. Accurate SEI-formation modeling demands a simulation framework that can explore timescales inaccessible to *ab initio* molecular dynamics (MD) and is simultaneously capable of accounting for explicit electron transfer – a capability lacking in standard machine-learning interatomic potentials.

To this end, we introduce a novel approach that combines the thermopotentiostat [1] simulation scheme with density functional tight binding (DFTB) electronic structure calculations. This enables MD simulations of the anode-electrolyte interface at constant potential and up to the timescale of initial decomposition reactions on the anode surface. We assess the capabilities and limitations of this approach in providing valuable insights into SEI formation and its impact on battery performance and degradation.

[1] F. Deißenbeck *et al.*, Phys. Rev. Lett. **126**, 136803 (2021).

MM 19.13 Tue 18:00 P5

Separating light and heat effects in the electrochemical performance ofilluminated V_2O_5 lithium-ion battery cells — •Pavel Rozov[1], Tom Wickenhäuser[1], Luca Bischof[1], Ewa Mijowska[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]Faculty of Chemical Technology and Engineering, West Pomeranian University of Technology, Szczecin, Poland

Recent studies have demonstrated that lithium-ion batteries can exhibit enhanced electrochemical performance under optical light illumination. However, light exposure also may cause local heating, making it challenging to separate bare photonic and photo-thermal effects. Here, the effects of light illumination on V_2O_5-based electrodes as photoactive cathode material are studied in lithium metal half-cells in which photo-thermal effects are monitored by means of an in-situ Pt1000 thermometer. Our studies allow us to disentangle photonic and temperature effects. We find slightly enhanced Li+ diffusion under illumination but do not confirm significant light-induced enhancement of the battery performance beyond temperature effects which is reported in the literature.

MM 19.14 Tue 18:00 P5

Shining a Light on Stored Charges: Linking Excitation Spectra to Polaron Dynamics in Solar Battery Materials — •Leon Müller, Matthias Kick, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin

Solar battery materials integrate light harvesting and charge storage within a single component, offering a pathway toward simplified systems that could serve as

key elements in future nanoscale energy devices. First experimental findings suggest that charge storage involves the formation of long-lived polaronic states. However, the underlying processes of exciton generation, subsequent charge separation and trapping that enable stable charge storage remain elusive.

Experimentally, charging is accompanied by a reversible color change from white or yellow to blue, indicating a potentially more dynamic process in which charges can jump between multiple trapping sites. This photochromism has been observed in many of the solar battery materials discovered so far, hinting at a mechanism that may be universal to this class of systems.

To explore the processes of charge generation and trapping, we study $LiNbWO_6$ using time-dependent density-functional theory to model the optical response of polaronic states. By connecting the excitation spectra to the underlying dynamics of the stored charges, we aim to clarify the mechanisms that govern charge localization and stability, thereby establishing a microscopic framework for charge storage in solar battery materials.

MM 19.15 Tue 18:00 P5

Anisotropic Thermoelectric Energy Converters Based on Bi Microwires and Films. — •Leonid Konopko[1], Albina Nikolaeva[1], Tito Huber[2], and Denis Shiversky[1] — [1]Technical University of Moldova, Chisinau, Moldova — [2]Howard University, Washington, DC, USA

We demonstrate an innovative method for thermoelectric energy conversion utilizing a single-element device made from an anisotropic material. In such materials, heat flow generates a transverse thermoelectric electric field perpendicular to the direction of the heat transfer. For our experiments, we produced a sample using a 10-meter-long, glass-insulated, single-crystal tin-doped bismuth microwire (outer diameter - 20 μm; core diameter - 4 μm). A crucial aspect of this process was the successful growth of the microwire as a single crystal, achieved through laser-assisted recrystallization under a strong electric field. The microwire was coiled into a flat spiral and mounted onto a thin copper disk. This sample demonstrated high sensitivity to heat flow, reaching up to 10^{-2} V/W, with a time constant of approximately 0.2 seconds. Bismuth films with thicknesses ranging from 2 to 5 μm were deposited onto mica substrates. Experimental samples of heat flux sensors were then fabricated by recrystallizing these films under laser heating in a strong electric field. The observed voltage dynamics at the output of all sensors, in response to modulated heat fluxes, align well with theoretical predictions for anisotropic thermoelectric elements.

The study was supported by the State Project "ReBRAIN" #25.80013.5007. 07RE, 2025-2026.

MM 19.16 Tue 18:00 P5

Structure and transport properties of Li-Zr-Cl-O oxychloride solid electrolytes — •Ziyan Zhang[1,2], Shuai Chen[3], Peter Müller-Buschbaum[1], and Anatoliy Senyshyn[2] — [1]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany — [2]MLZ, TUM, Garching, Germany — [3]TUM School of Natural Sciences, Chair for Physics of Energy Conversion and Storage, Garching, Germany

All-solid-state batteries using halide-based electrolytes have attracted attention due to their promising combination of room-temperature ionic transport, formability, and interfacial compatibility. Within this class, oxychloride compositions offer an additional degree of freedom via anion chemistry while retaining the beneficial processing of chlorides. The current study systematically characterizes mechanochemically prepared Li-Zr-Cl-O oxychlorides. A targeted Li2+yZrCl6-yOy series was established under standardized processing conditions. Laboratory powder X-ray diffraction was used to quantify the structural response to changes in oxygen content and processing conditions, using Rietveld analysis to determine lattice parameters. Electrochemical impedance spectroscopy yielded ionic conductivities and activation energies at ambient temperature. The resulting dataset provides a detailed composition-processing-structure- transport map for Li-Zr-Cl-O and delineates a practical recipe window for maximizing room-temperature conductivity under a purely mechanochemical synthesis route, thereby laying a robust laboratory baseline for subsequent interfacial and operando investigations.

MM 19.17 Tue 18:00 P5

Segregation of H in planar defects of BCC Fe — •Rohan Kumar, Mariano Forti, Rebecca Janisch, Thomas Hammerschmidt, and Ralf Drautz — Ruhr university Bochum, Universitatstr 150, 44801, Bochum Germany

The transition to a hydrogen-based economy in Europe is well underway, but challenges remain in the development of suitable infrastructure, as well as in migrating the existing facilities. Among other dificulties hydrogen embrittlement of steels hinders the applicability of known and new materials for hydrogen technologies.

This study focuses on the atomistic simulation assessment of hydrogen embrittlement in body-centered cubic (BCC) Fe using advanced computational methods. Density Functional Theory (DFT) is a standard tool for studying segregation phenomena, providing high accuracy but limited to small systems and short time ranges. In the other hand, the recent emergence of universal machine learning interatomic potentials (MLIPs) pose them as a powerful tool to study atomistic systems at larger scales with DFT precision.

In this work, we utilize GRACE MLIP to study tilt and twist grain boundaries (GBs) in ferritic Fe, finding GB energies in agreement with DFT results. The GBs were analyzed using DBSCAN and Voronoi analysis to identify hydrogen segregation sites. We study H segregating of in both tilt and twist GBs and analyze site preference trends.

MM 19.18 Tue 18:00 P5

Experimental Determination of Site Energy Spectrum of Hydrogen in Metal Thin Films — •Magdalena Seiler, Stefan Wagner, and Astrid Pundt — Karlsruhe Institute of Technology (KIT), Institute of Applied Materials (IAM-WK), Engelbert- Arnold-Straße 4, 76131 Karlsruhe, Germany

Metal-hydrogen interactions affect the mechanical properties of structural materials and the performance of solid-state hydrogen storage. Hydrogen occupies the metal lattices interstitial sites or different defects, whose site energy distribution characterizes the metal-hydrogen interaction. The site energy can be affected by the stress state, as suggested by theoretical calculations [1]. In this presentation, the constraints of a thin film adhered to a rigid substrate serve as a model 2D stress state. We experimentally determine the chemical potential of hydrogen in respective metal thin films during electrochemical hydrogen loading, and simultaneously measure the stress resulting in the hydrogen-absorbing, 1D expanding thin film. The result is compared to a Distribution of Site Energies (DOSE) model [2], in which Fermi-Dirac statistics are used to describe the hydrogen occupancy of the density of sites. Thereby, we obtain a site energy spectrum and quantify defect fractions.

[1] A. Dyck, T. Böhlke, A. Pundt, S. Wagner, Scripta Materialia 247 (2024) 116117.

[2] S. Wagner, A. Pundt, AIMS Materials Science 7 (2020) 399-419.

MM 19.19 Tue 18:00 P5

In-Situ Electrochemical Micromechanics of Hydrogen-Charged Palladium — •Hou Zhang[1], Henry Ovri[1], and Shan Shi[1,2] — [1]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany — [2]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, Hamburg, Germany

The substantial lattice parameter mismatch between the hydrogen-diluted and hydrogen-rich phase, coupled with the embrittlement effect in metal hydrides, are critical factors limiting the long-term structural integrity and performance reliability of hydrogen-related functional materials used in actuation, sensing, transportation, and energy storage. Palladium, due to its high hydrogen solubility, rapid hydrogen diffusion at room temperature, and its ability to reversibly absorb and desorb hydrogen through electrochemical control, serves as a model material for studying the underlying chemo-mechanical coupling. However, the local mechanical response and microstructural evolution of Pd during electrochemical hydrogen absorption are not yet fully understood. In this study, we employ an in-situ electrochemical nanoindentation setup to conduct compression tests on Pd micropillars subjected to varying hydrogen concentrations. Electron backscatter diffraction (EBSD) analysis will be used to characterize grain orientation, enabling us to further investigate the influence of crystallographic orientation. The insights gained from this study will deepen the understanding of chemo-mechanical coupling in metal-hydrogen systems and contribute to the advancement of hydrogen-related technologies.

MM 19.20 Tue 18:00 P5

In-depth Study of Hydrogen Permeation through Zinc Coated Steel — •Tatjana Ott[1,2], Elahe Akbari[1], Christoph Cobet[2], Jiri Duchoslav[2], Heiko Groiss[2], Andreas Muhr[3], Reza Sharif[3], Thomas Steck[3], Laura Mears[1], and Markus Valtiner[1] — [1]Institute of Applied Physics, Vienna University of Technology, 1040 Vienna, Austria — [2]Johannes Kepler University Linz, Altenberger Straße 69, 4040 Linz, Austria — [3]voestalpine Stahl GmbH, 4020 Linz, Austria

Objectives: Hydrogen permeation measurements are used to obtain information such as diffusion coefficients and trap sites, as well as to investigate corrosion processes. Studying the hydrogen permeation through zinc coated steel sheets provides insights into the mechanisms of cathodic hydrogen generation and the protective capabilities of different zinc coatings. Utilizing samples prepared with an optimized sample preparation protocol, hydrogen permeation through zinc coated ultra-high-strength steel (UHSS) was investigated.

Results and Conclusions: The electrochemical process for the palladium deposition on steel was optimized, resulting in an increased sensitivity for hydrogen permeation. Different zinc coatings were compared to determine the protective abilities of the coating as well as different types of entry side reactions. Results showed that the zinc coatings provided significant protection against hydrogen permeation. Overall, hydrogen permeation measurements provided valuable insights regarding both the reactions taking place at different coating types and their protective abilities.

MM 19.21 Tue 18:00 P5

Hydrogen-induced resistance response in nanoporous Pd-Cu thin film — •Yushen Huang[1] and Shan Shi[2,1] — [1]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany — [2]Research Group of Integrated Metallic Nanomaterials Systems, Hamburg University of Technology, Hamburg, Germany

The large-scale utilization of hydrogen energy requires high-performance sensing technologies for real-time hydrogen monitoring and leakage prevention. Pd-based hydrogen sensors are considered among the most promising candidates and are widely used in commercial devices due to palladium's strong affinity for hydrogen. However, during cyclic hydrogen absorption and desorption, Pd undergoes repeated phase transition, which can lead to accumulation of local misfit strains and defects. This results in signal hysteresis, prolonged response times, and poor reproducibility particularly in dense Pd films. Inspired by the excellent microstructural stability and actuation performance durability observed in nanoporous Pd bulk samples after over 1500 cycles of phase transition, this work investigates the potential of nanoporous Pd-Cu thin films for hydrogen sensing. In this work, a nanoporous Pd-Cu thin film (~100 nm thick) was prepared via electrochemical dealloying, and its electrical resistance response during electrochemical hydrogen charging was measured using a four-point probe method. Additionally, the pore size of nanoporous Pd-Cu will be tuned by adjusting the preparation conditions and post thermal treatment, enabling the sensors with enhanced stability, long-term reliability, and high-precision hydrogen monitoring.

MM 19.22 Tue 18:00 P5

Crystallization kinetics of supercooled liquid palladium — •Zuzanna Kostera[1], Przemyslaw Dziegielewski[1], Ryszard Sobierajski[2], and Jerzy Antonowicz[1] — [1]Warsaw University of Technology, Faculty of Physics, Warsaw, Poland — [2]Polish Academy of Science, Institute of Physics, Warsaw, Poland

In this work we use large-scale molecular dynamics to study crystallization kinetics of supercooled liquid palladium over 0.3-0.6 T_m (T_m = 1828K). The crystallization temperature strongly affects the final polycrystalline morphology, reflecting temperature-dependent nucleation and growth kinetics. From the evolving grain structure we extract homogeneous nucleation and growth rates and construct a time*temperature*transformation (TTT) diagram. The TTT diagram yields a critical cooling rate of 10^{13} K/s, consistent with Pd's poor glass-forming ability. Homogeneous nucleation peaks at 10^{35} $m^{-3}s^{-1}$ near 0.5 T_m and its temperature dependence agrees with classical nucleation theory.

MM 19.23 Tue 18:00 P5

DFT study of the optical and electronic properties of N-Acyl-N'-Aryl thiourea derivatives — •amani zaghdoudi — University of Carthage, Faculty of Sciences of Bizerte, Laboratory of Materials Physics: Structure and Properties (LR01ES15), Physics of Nanometric Components and Devices Group, Jarzouna 7021, Bizerte, Tunisia

We report a DFT-based theoretical study of novel N-acyl-N'-aryl thiourea derivatives as potential selective fluoride sensors. Molecular structures were optimized at the B3LYP/LANL2DZ level with GAUSSIAN 09.

IR, Raman, and UV-Vis spectra were simulated to probe their vibrational and electronic responses. UV-Vis analysis reveals π-π^* and n-π^* transitions influenced by aryl substituents and fluoride binding. IR and Raman results show characteristic C=O and C=S stretches, with frequency shifts upon complexation, indicating interaction at the thiourea core.

Mulliken and NBO analyses reveal charge redistribution and donor*acceptor interactions. Frontier molecular orbital analysis indicates a reduced HOMO-LUMO gap upon fluoride binding, suggesting enhanced reactivity. These findings support the application of these compounds as promising molecular fluoride sensors.

MM 19.24 Tue 18:00 P5

Electronic properties of Carbon nanoscrolls — •Tzu-Ching Hsu[1], Jhih-Shih You[1], Hsiu-Chuan Hsu[2], and Ion Cosma Fulga[3] — [1]Department of Physics, National Taiwan Normal University, Taipei, Taiwan, — [2]Graduate Institute of Applied Physics, National Chengchi University, Taipei, Taiwan — [3]Institute for Theoretical Solid State Physics, IFW Dresden, Dresden, Germany

Carbon nanoscrolls (CNS), rolled-up structures formed from single-layer graphene, have recently attracted significant attention owing to their distinctive geometry. In this work, we theoretically investigate the topological properties of a series of ABC-stacked CNS with various chiral vectors that break mirror symmetry, within the small-curvature approximation. As the chiral vector is varied, we find that the Dirac cones in the fictitious Brillouin zone shift away from half of the magnetic flux quantum. Furthermore, we show that the combined C_2T symmetry, the composition of a 180° rotation and spinless time-reversal symmetry, protects the Dirac cones even when chiral symmetry is broken. Our results provide a foundation for further studies of the fundamental physics and potential applications of CNS and other two-dimensional materials with similar geometries.

MM 19.25 Tue 18:00 P5

Correlating Atomic Structure and Grain Boundary Energy in the 5D Space of Degrees of Freedom — •Mahkam Madadi[1], Timo Schmalofski[1], Martin Kroll[2], Holger Dette[3], and Rebecca Janisch[1] — [1]ICAMS, Ruhr-University Bochum, Germany — [2]Chair of Stochastics and Machine Learning, University of Bayreuth, Germany — [3]Chair of Stochastics, Ruhr-University Bochum, Germany

In materials design, it is essential to develop grain boundary (GB) models that effectively relate the atomic structure to the macroscopic properties of grain boundaries. Grain boundaries are categorized by five degrees of freedom (DOF), which include grain boundary plane orientation, rotation axis, and the misorientation angles between adjacent grains. On the other hand, the energy associated with these boundaries is governed by microscopic state, including atomic positions and structural units . This study seeks to investigate the correlation between the microscopic structure and the energy of grain boundaries. Previous studies often explored only a subset of these DOFs, typically by varying one or two while keeping the others fixed. In contrast, this study employs molecular statics in combination with a statistical approach [1] to assess the complete 5D space of DOFs and to model and analyze the microstructure-energy relationship.

[1] T. Schmalofski, M. Kroll, H. Dette, and R. Janisch. Towards active learning: A stopping criterion for the sequential sampling of grain boundary degrees of freedom. Materialia, 31:101865, 2023. https://doi.org/10.1016/j.mtla.2023.101865

MM 19.26 Tue 18:00 P5

Machine-learned interatomic potentials for hydrogen-affected fracture in silica minerals — •Valentína Berecová[1,2], Martin Friák[1], and Jana Pavlů[2] — [1]Inst. Phys. Mater., Czech Acad. Sci., Brno, Czech Republic — [2]Dept. Chem., Masaryk Uni., Brno, Czech Republic

Flint, a cryptocrystalline form of silica, is known for its ability to fracture into curved surfaces through conchoidal flaking. Although this behaviour has been used for millennia to produce cutting tools, the atomistic mechanisms that enable such edges remain poorly understood. To clarify these processes, we develop a machine-learned Si-O-H interatomic potential trained on high-accuracy quantum-mechanical data, providing near ab initio resolution at computational costs suitable for simulations. Particular attention is given to hydrogen-related interactions: natural flint contains hydration and hydroxylation that can influence fracture pathways and crack propagation. The training dataset includes hydrogen-containing species, surface terminations, strained configurations, amorphous structures and defect environments. The resulting potential is applied to atomistic simulations of fracture in defect-rich silica, offering new insight into conchoidal fracture at the atomic scale and supporting the design of brittle materials with controlled failure behaviour. Financial support from the Czech Academy of Sciences (Praemium Academiae of M.F. and the Strategy AV21 project "The power of objects: Materiality between past and future") is gratefully acknowledged. Computational resources were provided by e-INFRA CZ and IT4Innovations National Supercomputing Center.

MM 19.27 Tue 18:00 P5

Silica-Supported Nano Metal Complexes Derived from a Schiff Base Ligand: Structural, Theoretical, and Catalytic Investigations — •Tarek El-Dabea — Chemistry Department, Faculty of Science, King Salman International University, Ras Sudr, Sinai 46612, Egypt

Silica-based nanomaterials were prepared from natural silica sand and used as supports for nano metal complexes containing Ru(III), Fe(III), VO(II), and Ag(I) ions. The SiO2 support, obtained via a grinding and paste-based technique, provided a stable high-surface matrix for immobilization. Complexes derived from a bidentate Schiff base ligand were characterized by spectroscopic and analytical methods, confirming their geometry and stoichiometry. Solution studies showed stable metal-ligand coordination, while DFT and TD-DFT analyses gave insights into the optimized structures and electronic transitions consistent with experiment. Among the investigated systems, the Ru(III)/SiO2 composite exhibited distinctive electronic and catalytic properties, efficiently promoting multicomponent reactions under microwave irradiation. Optimized eco-friendly conditions (H2O/EtOH) gave high yields, and the catalyst

MM 19.28 Tue 18:00 P5

synchrotron XAFS Study of Fe3O4/Au core–shell nanoparticles for magnetic–plasmonic applications — •Mai El-Masry[1], Giuliana Aquilanti[2], Messaoud Harfouche[3], Neama Imam[4], and Jan Ingo FLEGE[4] — [1]Thebes Higher Engineering Institute, Cairo, Egypt — [2]Elettra Sincrotrone Trieste, Italy — [3]SESAME Synchrotron, Aman, Jordan — [4]Brandenburg University of Technology Cottbus-Senftenberg, Germany

Magneto-plasmonic nanostructures enable multifunctional biomedical applications, including imaging, sensing, and targeted diagnostics. We synthesized Fe3O4/Au core–shell nanoparticles via a seed-mediated method and characterized them using synchrotron X-ray Absorption Fine Structure (XAFS) at the Fe K and Au L3 edges. XAFS analysis provided element-specific information on oxidation state, coordination, and local structure, confirming core–shell in-

tegrity and strong interfacial coupling. XRD and high-resolution TEM verified a crystalline Fe3O4 core and FCC Au shell, while VSM measurements demonstrated superparamagnetic behavior with high saturation magnetization. EXAFS and XANES results revealed metallic Au and Fe–O coordination consistent with magnetite, confirming successful shell formation. These results establish the structure-property relationship in magnetic–plasmonic nanostructures and demonstrate the importance of SESAME synchrotron techniques for advancing nanomaterials for sensing, imaging, and biomedical technologies.

MM 19.29 Tue 18:00 P5

Relaxation and crystallization behavior of the metallic glass former PdNiP near the glass transition temperature — •Noah Colell — Universität Münster, Institut für Materialphysik, Wihelm-Klemm Str. 10, 48149 Münster

Analysis of $Pd_{40}Ni_{40}P_{20}$ metallic glass is conducted with Flash DSC measurements, realizing high heating and cooling rates. Relaxation is realized through systematically varying temperatures and durations of annealing by cycling to investigate the effects on glass transition and crystallization. Different relaxation modes (α and β) are targeted and their response to the heat treatment is analyzed. Due to the high rates available in Chip calorimetry, the range of temperatures available for relaxation experiments avoiding crystallization can be extended. As one results, it is observed that the relaxation enthalpy does not show a linear trend even with logarithmic scaling. This might be due to the combining effects of α and β relaxation. Through different annealing times different relaxation modes seem to be activated. The so-called shadow glass transition (β) can be seen with smaller duration and converges into a stronger enthalpy recovery with larger ones. This indicates a connection between the two relaxation modes.

MM 19.30 Tue 18:00 P5

Molecular micro-heterogeneity: Structure formation and phase behavior in aqueous alkylamine mixtures — •Lena Friedrich[1], Martina Požar[2], Aurélien Perera[3], Michael Paulus[1], Nicola Thiering[1], Jaqueline Savelkouls[1], Eric Schneider[1], Bernada Lovrinčević[2], Dirk Lützenkirchen-Hecht[4], and Christian Sternemann[1] — [1]Fakultät Physik / DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]University of Split, Faculty of Science, 21000 Split, Croatia — [3]Sorbonne Université, Laboratoire de Physique Théorique de la Matière Condensée, F75252 Paris, France — [4]Fakultät für Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, 42097 Wuppertal, Germany

Aqueous alkylamines exhibit an unusual phase behavior [1] and an intruiging form of self-assembly [2]. X-ray diffraction experiments at BL8 and BL9 (DELTA, TU Dortmund) reveal intense structur factor pre-peaks that vary with composition and chain length, indicating peculiar micro-heterogeneity. Diffraction intensities calculated from MD simulations resemble the measured intensities and show bilayer-like arrangements in which amine headgroups saturate and stabilize water domains, forming transient clusters that prevent macroscopic phase separation, explaining the remarkable miscibility of aqueous amines compared to other associating liquids such as alcohols [3]. Supported by BMBF via DAAD in PROCOPE (57704875 & 50951YA). [1] J. Glinski et al., J. Colloid. Interface Sci. 162, 129-134 (1994); [2] L. Almasy et al., PCCP 21, 9317 (2019); [3] A. Perera et al., arXiv:2510.02146

MM 19.31 Tue 18:00 P5

Effects of physical properties on the solidification kinetics of undercooled Zr-Cu-Ni alloy under reduced gravity — •Chu Yu, Yindong Fang, and Stephanie Lippmann — IAP, FSU Jena, Albert-Einstein-Straße 15, 07745, Jena, Germany

In our previous work, we investigated the solidification kinetics of glass forming alloy Zr50Cu35Ni15 using electromagnetic levitation facilities (EML) under different gravity conditions to compare with the electrostatic levitation facility (ESL). Using both methods, crystal growth velocities increased with increasing undercooling below 260 K. Within the undercooling range 260-320K, velocities plateaued. Compared to ESL, EML on the ground generated stronger convective flow in the undercooled melt. Slight differences in velocities were observed within the undercooling range 50-175K. However, the primary phase is not changed by the magnetic convection. To investigate the differences in the low undercooling region and the physical properties of the melt, we measured the conductivity and viscosity of the melt under reduced gravity during parabolic flight campaign 2023 and 2025. The relationship between viscosity and crystal growth velocities at the low undercooling region is discussed.

MM 19.32 Tue 18:00 P5

Exploring Molecular Fragmentation and Structure in PVP Thin Films via Atom Probe Tomography — •Parisha Diwan — University of stuttgart

In this work, spin coating was used to create thin films of polyvinylpyrrolidone (PVP), which were then analysed using atom probe tomography (APT). APT measurements were performed to investigate the polymer at the nanoscale after lift-outs were created and shaped into sharp edges. The mass spectrum identified the primary molecular fragments generated during analysis, and the 3D reconstruction demonstrated the arrangement of various PVP molecule components in the film. These findings show that APT can help us better understand the structure of polymer thin films by providing specific chemical information. This study supports the future application of APT in polymer research and thin-film characterisation by highlighting its potential as a helpful tool for organic material analysis.

MM 19.33 Tue 18:00 P5

Electronic property analysis of structure and bonding at oxidized aluminium surfaces — •Lütfi Çağlar Ege[1], Nebahat Bulut[1], Zhengqing Wei[1], Inna Plyushchay[2], and Sibylle Gemming[1] — [1]Institute of Physics, TU Chemnitz, Germany — [2]Institute of Physics, National Taras Shevchenko University of Kyiv, Ukraine

The crystal structure has a large influence on material properties that are important for many applications, especially in the case of aluminium oxide (AlO_x), which forms a protective layer on aluminium. Understanding the structure and bonding during the oxidation mechanism of the low-energy aluminium surfaces Al(001), Al(110), and Al(111) is the main interest of this study, which highlights the surface reactivity. We attempted to analyse the interaction of the electronic states and forces of the oxygen and aluminum atoms to observe the relaxed bonding positions. First principles calculations were employed as the theoretical approach to investigate the electronic properties with respect to the position of oxygen within the irreducible wedge of the surfaces.

MM 19.34 Tue 18:00 P5

The vacancy effect to the mechanical properties of high entropy borides — •Nebahat Bulut[1], Inna Plyushchay[2], Anna Pliushchai[1], and Sibylle Gemming[1] — [1]Institute of Physics, TU Chemnitz — [2]Institute of Physics, National Taras Shevchenko University of Kyiv, Ukraine

High entropy transition metal diborides ($HETMB_2$) present complex lattice distortions that strongly influence their mechanical properties. These distortions are the result of atomic mismatch, metal-boron site vacancies, and strong covalent/ionic bonding. The randomly disordered structures of $HETMB_2$ are constructed with equimolar metal atom ratios to obtain the elastic stiffness tensors. Small strains are applied to the equilibrium unit cell to calculate the elastic response by performing first principles calculations using Quantum Espresso. Understanding the influence of lattice distortion on mechanical properties, we introduce distortion parameters which show the vacancy effect of different transition metal atoms. The distortion parameters were quantified based on the interatomic distances of nearest neighbor bond lengths. Mechanical stability and elastic anisotropy of $HETMB_2$ were analyzed as function of configurational disorder. It is discussed how the lattice distortions modify the Peierls barrier for dislocation motion.

MM 19.35 Tue 18:00 P5

Band geometric transverse current driven by inhomogeneous AC electric field — •M Maneesh Kumar, Sanjay Sarkar, and Amit Agarwal — Indian Institute of Technology Kanpur, Kanpur, India

We develop a semiclassical theory for electron wavepacket dynamics in the presence of an inhomogeneous AC electric field. While static electric-field gradients are known to generate charge transport governed by the quantum metric, we show that AC field gradients induce an additional geometric current that vanishes in the DC limit. This response originates from a novel band-geometric quantity, the higher-order connection (HOC) tensor, constructed from cubic products of interband Berry connections. We derive explicit expressions for the AC field-limit and identify the symmetry conditions under which it arises. Remarkably, inhomogeneous AC fields can generate an anomalous Hall-like response even in nonmagnetic systems. Applying the theory to Bernal-stacked bilayer graphene, we demonstrate that the HOC-induced response produces a measurable Hall current peaking at band edges. These results establish inhomogeneous AC fields as a powerful probe of higher-order band geometric quantities beyond Berry curvature and the quantum metric.

MM 19.36 Tue 18:00 P5

Modelling heat transport in BTBT and its derivatives using non-equilibrium molecular dynamics (NEMD) simulations — •Simon Jamnik, Florian Lindner, Florian Unterkofler, and Egbert Zojer — Graz University of Technology

Benzothieno[3,2-b]benzothiophene (BTBT) is a high-performance organic semiconductor whose derivatives C8-BTBT (with an octyl side chain) and Ph-BTBT (with a phenyl side chain) are widely used in OFETs due to their high mobilities, environmental stability and solution processability. Side-chain engineering strongly influences their physicochemical and thermal properties: experiments show that alkyl chains improve solubility while suppressing heat transport, whereas phenyl chains enhance along-chain conductivity and reduce interchain transport.

To analyse these effects, we employ non-equilibrium molecular dynamics (NEMD), which provides a complementary real-space perspective through spatially resolved temperature profiles and enables the direct identification of thermal-transport bottlenecks. Accurate forces for large-scale NEMD were ob-

tained using moment tensor potentials (MTPs) trained on ab initio data generated via VASPs on-the-fly machine-learning force-field (MLFF) framework, allowing near first-principles accuracy at greatly reduced computational cost.

MM 19.37 Tue 18:00 P5

Neural Network Potentials for Molecular Dynamics Simulations of NASICON Solid Electrolytes — •Insa F. de Vries and Nikos L. Doltsinis — Institute of Solid State Theory, University of Münster, Wilhelm-Klemm-Straße 10,48149 Münster

Solid-state electrolytes are by now well-established components for the development of safe and efficient batteries. Among them, the sodium superionic conductor (NASICON) family offers an appealing degree of tunability. Their open framework allows for the substitution of lattice sites and the adjustment of diffusing ion concentration, making them an attractive choice for material design. Accurately modeling and predicting ion and thermal transport properties in these systems by *ab initio* molecular dynamics (AIMD) simulations poses a challenge due to the large supercells and time scales required. In this study, we therefore train neural network (NN) potentials for various members of the $Na_{1+x}Zr_2Si_xP_{3-x}O_{12}$ (x = 0, 1, 2, 3) family using training data obtained by accelerated AIMD [1]. The NN potentials are then employed to calculate the sodium ion diffusion coefficient – a key transport property. The performance and results obtained with the NN potential are validated against those obtained from *ab initio* trajectories. In addition, both the NN potential and the *ab initio* results are then compared to corresponding data generated with a previously developed force field [2].

[1] D.Hamelberg et. al, J. Chem. Phys. 2004, 120, 11919
[2] P. Kumar & S. Yashonath, J. Am. Chem. Soc. 2002, 124, 3828

MM 19.38 Tue 18:00 P5

An extended two-temperature model for copper — •Simon Kümmel and Johannes Roth — FMQ, University of Stuttgart, Germany

The two-temperature model (TTM) describes a set of coupled heat conduction equations of an electronic and lattice subsystem that allows the study of materials under strong electronic excitation following laser irradiation.

Here, we present recent advances in the development of an implementation coupled to a molecular dynamics code. In particular, this implementation allows the study of effects that emerge from the change of the bond strength at high degrees of excitation. For that, we recently developed an electron temperature-dependent interaction potential for copper [1] that is capable of reproducing bond-hardening at high degrees of excitation. We discuss the importance of energy conservation when using such interactions and propose an implementation strategy.

Furthermore, we discuss the importance of taking ballistic electron motion into account before the establishment of an electron temperature within such TTM simulations. We compare two approaches and discuss the differences.

[1] S. Kümmel, J. Roth, J. Phys. D: Appl. Phys. 58, 415302 (2025)

MM 19.39 Tue 18:00 P5

Ballistic transport effects on the thermal conduction in nanowires — Ralf Meyer[1], Graham W. Gibson[2], and •Alexander N. Robillard[1] — [1]Laurentian University, Sudbury, Ontario, Canada — [2]University of Alberta, Edmonton, Alberta, Canada

The effect of ballistic transport on the thermal conduction in nanowires is studied with molecular dynamics and phonon Monte Carlo simulations. Simulations of nanowires between a heat source and a heat sink show — in agreement with previous results by other groups — the occurrence of a non-linear temperature profile with steep temperature gradients near the source and the sink combined with a reduced temperature gradient in the middle of the wire. The reduced gradients in the centre are then compared to a simple radiator model. This model predicts linear temperature profiles with a reduced gradient and discreet jumps at the wire ends. The comparison shows that if the wires are longer than the typical mean free path of the phonons, the radiator model is able to describe the reduction of the temperature gradient in the middle of the wires as well as their thermal resistances. The steep gradients at the wire ends can then be seen as the realization of the radiator model's discreet jumps in the more complex computer simulations.

MM 19.40 Tue 18:00 P5

Many-body localization for fermions and bosons - similarities and differences — •Krystian Jablonowski — University of Warsaw, Poland

In this talk, I will present a study that employs energy-level statistics as a robust diagnostic of localization phenomena across different quantum statistics. Using energy-level statistics, I analyze how Hubbard-type interactions shape the transition between localized and delocalized regimes in disordered many-body systems. Particular attention is given to how the strength of interactions influences spectral properties and dynamical behavior. A central theme of the talk is the contrast between fermionic and bosonic systems. By examining how particle statistics modify level-spacing distributions and the stability of localized phases, the study highlights both shared mechanisms and fundamental differences in their localization dynamics. Beyond mapping out the transition, I discuss how disorder and interaction-induced correlations jointly determine the structure of the many-body spectrum, offering insight into when and why localization persists or breaks down. Overall, the talk aims to provide a unified yet discriminating perspective on how fermions and bosons experience many-body localization, clarifying the similarities and distinctions that arise from their quantum statistical nature.

MM 19.41 Tue 18:00 P5

Perturbation theory for light-induced frequency shifts of thin quartz acoustic resonators — •Marinus Lehmann, Marek Bekir, and Carsten Henkel — Universität Potsdam, Institut für Physik und Astronomie, Germany

Quartz microbalance devices (QCM) are widely used for high precision mass measurements and the characterisation of liquid overlayers. In addition, QCMs are sensitive to various environmental changes like heating due to light irradiation. A light-induced shift of the acoustic resonance frequency has been shown by various groups [1,2]. Its explanation requires a combination of acoustic theory [3] with calculations for heat conduction [4] to model the cross-coupling between static thermal strain and the acoustic resonance. We try to clarify the mechanism by focussing on the time constants of the frequency shift transients.

[1] L. H. Goodman, E. S. Bililign, B. W. Keller, S. G. Kenny, and J. Krim, J. Appl. Phys. 124 (2018) 024502
[2] Ph. Ortner, M. Umlandt, N. Lomadze, S. Santer, and M. Bekir, Analyt. Chem. 95 (2023) 15645
[3] H. F. Tiersten, J. Acoust. Soc. Am. 59 (1976) 879
[4] J. P. Valentin, J. Appl. Phys. 57 (1985) 492

MM 19.42 Tue 18:00 P5

Anomalous resistance behavior of NiTi alloys at high temperatures — •Tianyi Xu[1], Leo Pies[1], Oluwaseyi Oluwabi[2], Sven Graus[1], Andreas Kreyssig[1], Jan Frenzel[2], and Anna E. Böhmer[1] — [1]Experimental Physics IV, Ruhr-University Bochum, Bochum, Germany — [2]Institute for Materials, Ruhr-University Bochum, Bochum, Germany

NiTi-based shape-memory alloys, widely used in actuators, biomedical devices, and high-precision components, are well known for their thermally driven phase transformations and associated functional properties. While their structural behavior has been extensively characterized, the electrical transport properties—particularly at elevated temperatures—remain comparatively unexplored, despite their relevance for high-temperature functional applications. In this work, the electrical resistance of $Ni_{1+x}Ti_{1-x}$ was determined up to temperatures of more than 700 °C. The resistive signature of the established martensite-austenite transition was clearly detected. Remarkably, the resistance exhibits a reproducible exponential increase as the temperature exceeds 500 °C.

This high-temperature behavior has not been reported previously and suggests that additional mechanisms—beyond the known phase transitions—govern charge transport in NiTi at elevated temperatures. These findings highlight the need for deeper investigation of high-temperature electronic behavior in shape-memory alloys. We will discuss the possible mechanisms resulting in this behavior, including the formation of precipitate phases.

MM 19.43 Tue 18:00 P5

Correlated-electron metallic systems at extremely high temperature — •Zuzanna Helena Filipiak[1,2] and Andrew P. Mackenzie[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]School of Physics and Astronomy, University of St Andrews, Scotland, UK

Although the low-temperature regime is the most established experimental phase space to study correlated-electron systems, a unique physical insight can be won from study at much higher temperatures as well. In particular, the unresolved mystery of the Planckian dissipation - with its linear-in-temperature electrical resistivity sometimes persisting over a few orders of magnitude in temperature with an unchanged slope - is worth studying across wide ranges of temperature. We have developed two setups in which resistivity of a metallic sample is measured as a function of temperature (ranging from 2 to 1000 K), magnetic field (up to 14 T) and the chemical reactivity of the exchange gas (oxygen, argon, vacuum). In this contribution we report on our current understanding of the observed presence and lack of resistivity saturation in different compounds from the groups of the weakly-interacting delafossites ($PdCrO_2$ and $PdCoO_2$) and the more strongly-interacting ruthenates (Sr_2RuO_4, $Sr_3Ru_2O_7$ and $Ca_3Ru_2O_7$).

MM 19.44 Tue 18:00 P5

Thermal Conductivity Measurements Using Laser Flash Analysis in $Mg_3(Sb,Bi)_2$ and Related Compounds — •Thomas Terörde[1], Benjamin Bornmann[1], Christian Hess[1], Ran He[2], Vishak Sivasubramaniyan Sudandiradevi[2], and Kornelius Nielsch[2] — [1]Fakultät für Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, Wuppertal, Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, D-01171 Dresden, Germany

This work presents temperature-dependent thermal conductivity measurements of $Mg_3(Sb,Bi)_2$-based thermoelectric compounds obtained using laser flash analysis down to 150 K. Maximizing thermoelectric performance requires high electrical conductivity while simultaneously minimizing thermal conductivity,

which is achieved by reducing the lattice contribution and thereby weakening the Wiedemann-Franz relation. The Sb/Bi ratio of $Sb_{0.6}Bi_{1.4}$ yield favorable band convergence and minimal lattice thermal conductivity. Modification of the transport behavior is sought through additional codoping with Te and Nb. Our systematic measurements as a function of Mg, Te, and Nb contents yield intrinsically reduced thermal conductivity, where an increase in the Te and Nb contents leads to a rise in the thermal conductivity at elevated temperatures, consistent with previous reports.

MM 19.45 Tue 18:00 P5

Li transport in V2O5 quantified by optical microscopy — •Vidula Angane-Ambure, Monica Mead, and Guido Schmitz — Institute of Materials Science, University of Stuttgart, Heisenbergstraße 3, 70569 Stuttgart, Germany

Vanadium pentoxide (V2O5) is an interesting cathode material due to its layered structure and high theoretical capacity; however, its electrochemical performance is strongly limited by lithium-ion transport and the evolution of phase boundaries during (de)intercalation. To measure lithium-ion transport in V2O5 and clarify transport mechanisms we apply a novel method that uses the optical response upon ion intercalation in in-situ optical microscopy. In this setup a clear diffusion geometry is established and therefore weaknesses of conventional electrochemical methods for quantification of diffusion in battery electrode materials can be circumvented. By evaluating the measured RGB values, the diffusion front is determined. Diffusional transport can then be separated from linear transport across a kinetic interface (such as phase boundaries) and the temperature dependence of the ion transport is quantified, yielding an activation energy for transport in V2O5. Additionally, the concentration-dependence of Li transport in V2O5 is studied in lithiation and delithiation experiments, showing faster delithiation than lithiation.

MM 19.46 Tue 18:00 P5

Beyond arsenopyrite's monoclinic model: new insights on triclinic symmetry and local, chemically driven disorder in $FeAs_{1-x}S_{1+x}$ — •Esteban Zuñiga-Puelles[1,2], Ayberk Özden[2], Nebahat Bulut[2], Raul Cardoso-Gil[3], Christoph Hennig[4,5], Gerhard Heide[2], Cameliu Himcinschi[2], Jens Kortus[2], and Roman Gumeniuk[2] — [1]Leibniz Institute for Solid State and Materials Research Dresden, Germany — [2]TU Bergakademie Freiberg, Germany — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [4]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [5]European Synchrotron Radiation Facility, Grenoble, France

In this work, we revisit the structural description of different natural $FeAs_{1-x}S_{1+x}$ specimens. High-resolution synchrotron PXRD reveals additional reflections incompatible with the commonly assumed monoclinic $P2_1/c$ model but fairly consistent with triclinic $P\bar{1}$ symmetry. Raman spectroscopy displays vibrational features deviating from monoclinic simulations, while Mössbauer spectra show multiple inequivalent Fe-sites linked to distinct local crystal electric fields. All samples show weak paramagnetism, and the magnetic moments decrease with increasing As-content, indicating that only a small portion of Fe-atoms resides in environments sufficiently distorted to cause deviations from the expected diamagnetism of low-spin Fe^{2+}. Altogether, the structural, vibrational, and magnetic responses support a revised view of arsenopyrite as a complex Fe-based semiconductor, where local As/S symmetry disruptions and chemically driven disorder govern its physical properties.

MM 19.47 Tue 18:00 P5

Heat-treatment dependent hydrogen embrittlement behaviour of additively manufactured 316L — •Kai Lagemann, Gabriele Palazzo, Stefan Wagner, and Astrid Pundt — Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany

This study investigates the mechanical behaviour of additively manufactured austenitic stainless steel 316L (AM316L) for different post-processing heat treatments and its susceptibility to hydrogen embrittlement. Specimens were produced in the as-built (AB) condition and after heat treatments at 400 °C, 650 °C, 900 °C, and 1050 °C. Comprehensive microstructural characterization and tensile testing were performed to evaluate the correlation between heat-treatment-induced microstructural changes and mechanical properties. Particular this study focuses on assessing the influence of hydrogen on the fracture behaviour and embrittlement sensitivity of the differently heat-treated AM316L conditions. The findings provide an improved understanding of the interplay between additive manufacturing, microstructural evolution during heat treatment, and diffusion-based hydrogen-induced degradation mechanisms in AM316L [1]. [1] Kai Stefan Lagemann, Gabriele Palazzo, Tim Lucas Haag, Svetlana Korneychuk, Stefan Wagner, Christian Kübel and Astrid Pundt. Influence of Microstructure and Heat Treatment on Hydrogen Diffusion in Additively Manufactured 316L Stainless Steel. manuscript submitted, 2026.

MM 19.48 Tue 18:00 P5

In Situ Investigation of Phase Evolution During Oxidation and Reduction of Powder Bed Fusion Copper Powders — •Eric Schneider[1], Lena Friedrich[1], Jaqueline Savelkouls[1], Fabienne Hellwig[2], Milli Suchita Kujur[2], Nick Hantke[3], Arne Röttger[2], Jan T. Sehrt[3], and Christian Sternemann[1] — [1]Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44227 Dortmund — [2]Bergische Universität Wuppertal, Bahnhofstraße 15, D-42651Solingen — [3]Ruhr-Universität Bochum, Universitätsstraße 150, D-44801 Bochum

The additive manufacturing (AM) process of laser-based powder bed fusion of metals (PBF-LB/M) enables the efficient production of complex components with internal cavities. Fabricating dense structures from pure copper remains challenging due to copper's high thermal conductivity and its low absorption of infrared laser radiation. Targeted surface modification, such as oxidation or nickel coating, can enhance the processability and reusability of copper powders. This study examines the oxidation behavior of copper powder in air and its controlled reduction in an $Ar/2\%H_2$ atmosphere at temperatures up to 350 °C. X-ray diffraction measurements were conducted at the BL9 beamline of the DELTA synchrotron radiation source. The findings provide key insights into the evolution of copper powder surfaces under PBF-LB/M-relevant atmospheres and offer practical guidance for industrial copper powder processing. This research is funded by the DFG through projects 508745195, RO 4523/9-1, SE 2935/6-1, and STE 1079/9-1.

MM 19.49 Tue 18:00 P5

Transferable Hamiltonian-learning model for large-scale finite temperature electronic-structure calculations — •Kaiwen Chen, Martin Schwade, and David Egger — Physics Department, TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany

Exploring the optoelectronic properties of large-scale systems across various temperatures and structures using conventional density functional theory (DFT) often encounters significant computational challenges. Recent advancements in machine learning (ML) Hamiltonians and the wide availability of DFT-databases have made it possible to train models, capable of predicting accurate Hamiltonians and electronic structure across the chemical space. However, creating a model that can determine temperature-dependent electronic structure with such transferability remains a difficult task. Building on our earlier work involving a physics-informed temperature-transferable Hamiltonian-learning model [1], we introduce an extension of this method that enables it to be trained on a wider field of compositions and thus be able to predict accurate effective Hamiltonians for different chemical compositions.

[1] M. Schwade, S. Zhang, F. Vonhoff, F. P. Delgado, D. A. Egger, *Physics-informed Hamiltonian learning for large-scale optoelectronic property prediction,* arXiv:2508.20536 (2025).

MM 20: Topical Talk: Shigenobu Ogata

Time: Wednesday 9:30–10:00 Location: SCH/A251

Topical Talk MM 20.1 Wed 9:30 SCH/A251

Neural Network Atomistic Modeling of Dislocation Plasticity in Ceramics — •Shigenobu Ogata and Shihao Zhang — The University of Osaka, Osaka, Japan

Dislocations in ceramics are increasingly recognized as levers for toughening intrinsically brittle materials and for tailoring functional responses. Yet atomistic simulation of their plasticity remains difficult because ceramic bonding combines ionic and covalent character, dislocation cores are often nonstoichiometric and charged, and core structures can be highly extended in complex lattices - features that exceed the fidelity of empirical interatomic potentials. Here, we develop neural network potentials (NNPs) for dislocation plasticity in three representative functional ceramics - ZnO, GaN, and SrTiO3. The NNPs accurately reproduce charged and nonstoichiometric core structures, slip barriers, and the long-range electrostatic interactions between charged dislocations. Leveraging these models, we examine plasticity via nano-pillar compression and nano-indentation, finding excellent agreement with experimental observations. The results establish a practical workflow for constructing NNPs that enable detailed, large-scale atomistic modeling of dislocation behavior in ceramics and open new avenues for predictive exploration of plastic deformation and property tuning in functional ceramic systems.

MM 21: Phase Transformations II

Time: Wednesday 10:15–13:00 Location: SCH/A215

MM 21.1 Wed 10:15 SCH/A215

On the nature of solutal melting in Cu-Pd — •Nagarjuna Remalli[1], Huai Zhang[1,2], Nisha Singh[1], Nuria Navarrete[1], Julien Zollinger[3], and Florian Kargl[1,4] — [1]Institute for Frontier Materials on Earth and in Space, German Aerospace Center (DLR), 51147 Cologne, Germany — [2]Department of Mechanical Engineering, University of Alberta, AB T6G 2G8 Alberta, Canada — [3]Université de Lorraine, Institut Jean Lamour, 54000 Nancy, France — [4]Foundry Institute, Fundamentals of Solidification, RWTH Aachen University, 52072 Aachen, Germany

We report on the kinetics of the solid-liquid (s-l) interface during solutal melting of isomorphous Cu-Pd melting couples. Using X-ray radiography (XRR) with sub-second time resolution the solutal melting dynamics along with the evolution of solute concentration fields was investigated. To this end circular melting couples of different thicknesses (220 μm and 460 μm) were in-situ monitored in an isothermal field at 1090°C slightly above the melting point of copper (1085°C) and well below the one of palladium (1555°C).

Sample thickness dependent differences in dissolution speed were observed which are suggested to be related with buoyancy-driven convective flow. By comparing SEM analysis results of the re-solidified Cu-Pd alloys with the in-situ results good agreement was found. Persistent non-equilibrium conditions were found at the s-l interface at the end of melting, independent of sample thickness or melting mechanism.

MM 21.2 Wed 10:30 SCH/A215

Chemoelastic effects, phase equilibria, and uphill diffusion in Cu-Pd nanoparticles — •Idan Klein, Feitao Li, and Eugen Rabkin — Department of Materials Science and Engineering, Technion - Israel Institute of Technology, Haifa 3200003, Israel

We fabricated nanoparticles (NPs) of Cu-40 at.% Pd alloy via solid state dewetting and subsequent slow-cooling of Cu-Pd bilayers deposited on a sapphire substrate. We observed that some nanoparticles which experienced partial transformation from a disordered A1 FCC phase to the ordered B2 β-CuPd exhibited compositional discontinuity, with the ordered phase being richer in Pd. This compositional discontinuity was associated with fully or partially coherent interphase boundary. At the same time the FCC particles that did not experience any transformation, the fully transformed β-CuPd particles, and partially transformed particles with incoherent interphase boundary exhibited homogeneous distribution of the components. We developed a thermodynamic model which demonstrated that misfit-strain from the coherent interface influences the thermodynamics of the system, depressing the transformation temperature. Redistribution of the components causes changes to the lattice parameter of each of the phases, mitigating the misfit between them, reducing free energy and encouraging the phase transformation.

MM 21.3 Wed 10:45 SCH/A215

Mechanism of structure formation during electrochemical dealloying — •Gideon Henkelmann[1] and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Germany — [2]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany

During electrochemical dealloying of a solid solution, atoms of the more noble species rearrange by surface diffusion to form a connected nanoporous structure with a characteristic length scale. Details of the underlying nanoscale self-organization process, specifically the criteria that select this characteristic length scale, remain to be understood. Here, we study this issue by kinetic Monte Carlo simulations. While previous studies started out with corroding a planar single-crystal surface, our approach starts by forming an internal cavity and follows the evolution of the surface of the growing void. This allows us to focus on passivation or bifurcation of the corrosion front in a realistic scenario with curved and rough surfaces. We find that passivation is governed by simple geometric criteria related to the enrichment of the more noble species on the pore surface. Furthermore, the variation of the resulting structure size with the overpotential may be rationalized by a Gibbs-Thomson-type scaling law.

MM 21.4 Wed 11:00 SCH/A215

ab-initio investigation of short-range order in Fe-Si-Al alloys — •Daniil Khodachenko[1], Franco Moitzi[1,2], Andrei Ruban[2], Oleg Peil[2], and Vsevolod Razumovskiy[1,2] — [1]Christian Doppler Laboratory for digital materials design guidelines for mitigation of alloy embrittlement, Leoben Austria — [2]Materials Center Leoben Forschung GmbH, Leoben Austria

Unique electromagnetic properties of steels with silicon and aluminum make them an excellent choice for the production of transformers and electric motors. These so-called electrical steels have enhanced energy efficiency due to reduced core losses and enhanced magnetic permeability. However, increasing the concentration of silicon and aluminum beyond a critical amount leads to significantly reduced ductility, which makes production very challenging.

The theoretical origin of these embrittlement effects is still not fully understood, as ab initio modeling based on Density Functional Theory (DFT) is rather challenging, due to requiring large supercells and complex magnetic interactions. Such first-principles simulations frequently use approximations that assume a fully random distribution of the alloying elements. However, real systems are not perfectly random, due to atomic interactions, which result in short-range ordering (SRO) of the atomic sites. We investigate atomic SRO phenomena using accurate DFT- and Green's function-based methods to study effective cluster interactions and their magnetic state dependence. Finally, we perform Monte-Carlo simulations to investigate phase transitions and the effect of SRO in these materials.

MM 21.5 Wed 11:15 SCH/A215

Ordering in Mo-Cr-Ti-Al refractory high-entropy alloys via machine learned interatomic potential — •Jiyao Zhang[1], Klemens Lechner[1], Markus Masswohl[2], Petra Spörk-Erdely[2], and David Holec[1] — [1]Department of Materials Science, Montanuniversität Leoben, Franz-Josef-Strasse 18, 8700 Leoben, Austria — [2]Institute of Materials Science, Joining and Forming, Graz University of Technology, Kopernikusgasse 24/I, 8010 Graz, Austria

Refractory high-entropy alloys (RHEAs) offer exceptional mechanical and thermal properties, such as excellent high-temperature strength, making them favorable competitors to nickel-based superalloys. Origin of the superior high-temperature performance of the Mo-Cr-Ti-Al RHEA can be tracked to its two-phase microstructure of disordered BCC and ordered B2 phases. Modeling RHEAs poses significant challenges, as accurate density functional theory (DFT) calculations are extremely time-consuming, a difficulty worsened by the alloys' complex compositions. Universal machine learning interatomic potentials (UMLIPs) have recently emerged as a promising solution. Trained on vast DFT datasets, UMLIPs enable near-DFT accuracy for large-scale simulations of thousands of atoms. In this work, we utilize UMLIPs in mixed Monte Carlo/Molecular Dynamics simulations to evaluate the thermal stability of ordered versus disordered states in Mo-Cr-Ti-Al system as a function of the Al contents. Furthermore, we analyze the impact of composition on order/disorder transition temperature and elastic properties. We validate our findings against experimental data.

15 min. break

MM 21.6 Wed 11:45 SCH/A215

Shear-stress dependent formation of Si-polymorphs during saw dicing analyzed by raman spectroscopy — •Zainab Zainab[1,2], Jörg Debus[2], and Hannes Kurtze[1] — [1]Bernburger street 55, 06366 Köthen (Anhalt) — [2]August-Schmidt-Str. 4, 44227 Dortmund

Raman spectroscopic analysis of diced silicon wafers reveals that the saw cutting process generates considerable amounts of metastable silicon polymorphs (BC8/R8) along with the original diamond-cubic structure (DC-Si). We demonstrate that the formation of these phases exhibits a distinct spatial distribution that correlates with the shear stress profile imposed by the rotating blade. The DC-Si signal is strongest near the bottom of the cut (wafer tape side), while BC8 and R8 phases are most concentrated near the top surface at the blade entry point. This gradient arises from differences in the mechanical stress state: at the top, the steeper blade angle generates substantial shear stress in addition to normal compressive stress, facilitating shear-induced phase transformation at locally applied pressures. At the bottom, the nearly parallel blade trajectory produces predominantly normal stress with minimal shear, suppressing the formation of metastable phases. Additionally, we find that specific feed rates enhance phase transformations and intensify the spatial gradient. These findings confirm that shear stress is the critical enabling factor for polymorph formation during mechanical processing of silicon, consistent with recent studies showing dramatic reduction in transformation pressures under non-hydrostatic conditions.

MM 21.7 Wed 12:00 SCH/A215

Investigating the temperature-driven structural phase transition in α-In2Se3: A Raman study — •Saswata Talukdar, Mitanshi Gupta, Devesh Negi, Suvodeep Paul, Shalini Badola, Shivani Tripathi, Ravi Shankar Singh, and Surajit Saha — Indian Institute of Science Education and Research Bhopal, Bhopal, 462066, India

In recent years, the complex characteristics and polymorphic nature of indium selenide (In2Se3) have distinguished it as a prominent candidate among 2D semiconductors for memory and nano-electronic applications. Despite comprehensive research on its thermal, electrical, and optical properties, the structural dynamics, especially the phase transitions over temperature, remain elusive. In this work, temperature-dependent Raman spectroscopy of bulk α-In2Se3 reveals well-defined spectral signatures corresponding to its multiple polymor-

phic phases, providing direct evidence of its structural transitions. Our results also show that the phase transition is governed not solely by temperature, but it is further influenced by the local strain, which forms wrinkles on the surface of the material, playing a crucial role in directing the transition pathway. Moreover, comparative Raman measurements on exfoliated flakes highlight a pronounced thickness-dependent modulation of the transition behavior, underscoring the critical role of dimensionality in governing phase stability and evolution. Altogether, this work presents a comprehensive picture of the phase transitions in In2Se3, offering valuable insights for its integration into future high-performance phase-change memory applications.

MM 21.8 Wed 12:15 SCH/A215

Transforming martensite in Ni-Mn-Ga within picoseconds — •Klara Lünser[1,2], Yuru Ge[3,4], Fabian Ganss[3], Daniel Schmidt[5,6], Daniel Hensel[5], Mike J. Bruckhoff[7], Bruno Neumann[3,4], Mariana Brede[5], Sakshath Sadashivaiah[8,9], Markus E. Gruner[7], Peter Gaal[5,6], and Sebastian Fähler[3] — [1]University Duisburg-Essen — [2]RCFEMS, Bochum — [3]HZDR, Dresden — [4]TU Dresden — [5]Leibniz IKZ, Berlin — [6]TXproducts, Hamburg — [7]CENIDE, University of Duisburg-Essen — [8]Helmholtz-Institut Jena — [9]GSI Darmstadt

Martensitic transformations are driving a wide range of emerging applications, including high-stroke actuation, mechanocaloric refrigeration, and thermoelastic energy harvesting. However, systematic investigations of the fast dynamics and fundamental speed limits of martensitic transformations are scarce. In this study, we employed a synchrotron-based time-resolved diffraction technique to investigate the martensitic transformation induced by 200 fs laser pulses. Our results show that the transformation from martensite to austenite occurs within 100 ps, limited by the synchrotron probe pulse duration. We also demonstrated that an appropriate laser fluence and undercooling can complete a full transformation cycle within 5 ns, the fastest value reported for martensitic transformation. Our study highlights the importance of analyzing the lattice temperature during martensitic transformations and discusses the need for and limits of this approach. Furthermore, we found that stress must be considered as a competing influence on the martensitic transformation, in addition to temperature.

MM 21.9 Wed 12:30 SCH/A215

In-situ view on contact and solutal melting of Al-Cu — •Florian Kargl[1,2], Matthias Kolbe[1], and Nagarjuna Remalli[1] — [1]Institute for Frontier Materials on Earth and in Space, German Aerospace Center, Cologne, Germany — [2]Foundry Institute, Fundamentals of Solidification, RWTH Aachen University, Aachen, Germany

Melting plays an important role in many technical processes such as casting, additive manufacturing, etc. but is far less understood than solidification. We report on the kinetics of the solid-liquid interface during contact and solutal melting of Al-Cu melting couples. Al-Cu melting couples consisting of an Al-annulus and a Cu-disc in close contact were processed in an isothermal temperature field. The melting process was in-situ monitored with X-radiography with a sub-second time resolution determining interface kinetics and liquid composition changes. For contact melting a temperature below the melting points of Al and Cu but above the eutectic temperature was chosen. For solutal melting the sample was processed above the melting point of Al. We observed contact melting to be initiated along Cu-grain boundaries with intermetallic layers representing the entire phase diagram forming between the liquid and the still solid Cu. The layer structure has been verified post-mortem by optical imaging and quantified by SEM-EDX. Solutal melting was found to be dependent on sample thickness with buoyancy convection increasing the reaction speed in thicker samples. Further, asymmetric reaction patterns were observed to arise due to Al2O3-layer build-up and/or initial Al2O3-presence at the Al-Cu interface and/or partial Al-detachment during melting.

MM 21.10 Wed 12:45 SCH/A215

Forming bicontinuous microstructures by distributed internal melting at the Ni3Sn4 peritectic — •Zhongyang Li[1], Lukas Lührs[1], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg — [2]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany

A recent study on peritectic melting of TiAg suggests that a bicontinuous structure can be obtained through liquid film migration (LFM) during annealing. Without the requirement of mass exchange with the environment, peritectic melting is free of the restrictions on sample size. To date, application of this method is limited to TiAg. In this work, the intermetallic compound Ni3Sn4 is selected as the new parent system for peritectic melting. After annealing and quenching, spherical clusters are obtained, consisting of crystallographically aligned Ni3Sn2 ligaments and interpenetrating Sn phase. The phase decomposition proceeds via the LFM mechanism, i.e. complete melting of Ni3Sn4 and growth of Ni3Sn2 across the melt layer. Constitutional supercooling, induced by a composition gradient within the melt, promotes cellular growth of Ni3Sn2 nuclei, resulting in a ligament structure. Based on previous studies on peritectic and partial melting, we propose the concept of distributed internal melting, which utilizes the internal pre-melting sites (vacancies, dislocations and grain boundaries) to initiate LFM and generates bicontinuous structures through heat treatment.

MM 22: Data-driven Materials Science: Big Data and Workflows III

Time: Wednesday 10:15–12:45 Location: SCH/A216

MM 22.1 Wed 10:15 SCH/A216

Hashing It Out: Overcoming the Duplicate Structure Filtering Bottleneck for Large Data Sets — •Julian Holland, Juan Manuel Lombardi, Chiara Panosetti, and Karsten Reuter — Fritz Haber Institute, Berlin, Germany

With the increasingly data-rich landscape of computational chemistry research, new bottlenecks to material property elucidation have emerged stemming from data processing. Duplicate detection is often an essential data processing step for active learning, global optimization, and general PES exploration algorithms to ensure efficiency and functionality. Such duplication checks typically scale unfavorably with the number of structures, potentially taking longer to perform than the data generation. Hashing-based methods, which have decoupled scaling with dataset size, circumvent this but are conventionally too rigid to reliably find duplicates. In this talk, we present a democratic hashing duplicate detection algorithm that is flexible enough to detect duplicate structures with arbitrarily similar, but distinct, global descriptors nearly instantly. The uniqueness of the structure can be determined by an ensemble of hash functions associated with a set of randomly perturbed global descriptors. We compare the performance of our duplicate detection algorithm against conventional distance-matrix-based methods and introduce a standardized suite of duplicate detection benchmarks. Our algorithm is not only faster but often significantly more robust at detecting known duplicates.

MM 22.2 Wed 10:30 SCH/A216

MC3D: The Materials Cloud FAIR and full-provenance materials database — •Michail Minotakis — PSI Center for Scientific Computing, Theory and Data, 5232 Villigen PSI, Switzerland

Carefully curated databases of materials and their properties have become invaluable resources for a range of applications, from property prediction using machine learning techniques to materials discovery. Here, we introduce MC3D, the Materials Cloud three-dimensional database, in which more than 95% of the available materials are, to date, classified as experimentally known. This database is derived from structures sourced from three major databases: the Pauling File, the Inorganic Crystal Structure Database, and the Crystallography Open Database. After careful curation, the final collection of 72,609 unique stoichiometric compounds is refined using density-functional theory calculations at the PBEsol level, executed in Quantum ESPRESSO and leveraging the SIRIUS library for optimized GPU performance. The AiiDA materials informatics infrastructure (http://aiida.net) manages each workflow stage, ensuring full traceability and preserving simulation provenance. The results are freely accessible in the MC3D section of Materials Cloud (https://mc3d.materialscloud.org) and are already being used as a starting point for materials discovery projects, such as novel thermoelectrics, electrides, superconductors, or materials displaying a large nonlinear Hall effect.

MM 22.3 Wed 10:45 SCH/A216

Building a FAIR Community around Parsing — •Nathan Daelman[1], Alvin N. Ladines[1], Esma Boydas[1], Martin Kuban[1], Bernadette Mohr[1], Sascha Klawohn[1], Rubel Mozumber[1], Christina Ertural[2], Silvana Botti[3], Joseph F. Rudzinski[1], Lauri Himanen[1], and FAIRmat Team[1] — [1]Inst. für Physik, Humboldt-Universität zu Berlin — [2]Department of Materials Chemistry, Federal Institute for Materials Research and Testing, Berlin — [3]RC-FEMS and Faculty of Physics, Ruhr University Bochum

NOMAD [nomad-lab.eu][1, 2] is an open-source data infrastructure for materials science data. One of its most praised features is how NOMAD allows for direct ingestion of various software output formats. This gives data producers access with minimal effort to the whole toolkit infrastructure system regardless of their choice of simulation code. As the NOMAD community extends into related scientific disciplines, parsing procedures should grow alongside and empower casual users to contribute too. To this end, I will be presenting two new parsing frameworks: (i) Mapping Annotation which connects code-specific formats to the NOMAD interoperable schema, while gracefully handling syntatic concerns; (ii) an agentic LLM interface for hooking up third-party parsers via the

Model Context Protocol (MCP). Finally, I will highlight how both approaches fit into NOMAD Plugins and NOMAD Actions.

[1] Scheidgen, M. *et al.*, JOSS **8**, 5388 (2023).
[2] Scheffler, M. *et al.*, Nature **604**, 635-642 (2022).

MM 22.4 Wed 11:00 SCH/A216

Uncertainty Propagation in Machine-learned Interatomic Potentials — •Haitham Gaafer, Jan Janssen, and Jörg Neugebauer — Computational Materials Design, Max-Planck-Institute for Sustainable Materials, Düsseldorf

Accurate multiscale materials modeling requires that uncertainties be quantified and propagated consistently from the electronic-structure level to macroscopic property predictions. Machine-learned interatomic potentials (MLIPs), trained on density-functional theory (DFT) reference data, now routinely reach near-DFT accuracy at dramatically reduced computational cost. Yet the connection between fitting errors in an MLIP and uncertainties in derived physical properties, such as bulk moduli or phase stabilities, remains insufficiently understood. We present a data-driven pyiron workflow designed to analyze how uncertainties originating in MLIP training propagate into thermomechanical property predictions. As a case study, we construct diverse DFT training sets for Cu, Ag, and Au using the Automated Small SYmmetric Structure Training (ASSYST) workflow, and fit computationally efficient atomic cluster expansion (ACE) potentials employing a minimal basis optimized to reach a target root-mean-square error. These potentials are subsequently used to determine equations of state and to quantify uncertainties in key properties, including the equilibrium lattice constant, bulk modulus, and its pressure derivative. Our results provide a transparent link between MLIP fitting quality and property reliability, offering a systematic route for uncertainty-aware atomistic modeling.

MM 22.5 Wed 11:15 SCH/A216

Accurately predicting thermal conductivity using non-equilibrium molecular dynamics simulations and machine-learned force fields — •Florian Unterkofler[1], Lukas Legenstein[1], Sandro Wieser[2], and Egbert Zojer[1] — [1]Graz University of Technology, Austria — [2]TU Wien, Austria

With the rise of machine-learned interatomic potentials, simulations have become an even more crucial tool for predicting material properties. We previously achieved accurate predictions of experimentally observed thermal conductivity of acenes, using system-specific, machine-learned Moment Tensor Potentials (MTPs) within a lattice dynamics approach.[1] To obtain a complementary real-space perspective, we now investigate whether comparable accuracy can be achieved using non-equilibrium molecular dynamics (NEMD).

Here, we present the workflow required to obtain accurate and reliable predictions when applying MTPs in NEMD simulations. We show that, due to the inherently stochastic nature of both MD and MTP training, a thorough statistical analysis of multiple simulations with different initial conditions and different realizations of the MTP is necessary. Furthermore, we highlight the importance of selecting appropriate training data to generate robust MTPs. When these considerations are taken into account, we achieve an excellent agreement between experiments, lattice-dynamics, and NEMD results, with NEMD simulations providing tools to investigate heat-transport bottlenecks in real space.

[1] L. Legenstein et al., *npj Comput Mater* 11, 29 (2025)

15 min. break

MM 22.6 Wed 11:45 SCH/A216

Data-efficient training of interatomic potentials using finite-temperature DFT structures — •Martin Schlipf[1], Sudarshan Vijay[1,2], and Georg Kresse[1,3] — [1]VASP Software GmbH, Berggasse 21/14, 1090 Vienna, Austria — [2]Department of Chemical Engineering, Indian Institute of Technology Bombay, Powai, Mumbai, Maharashtra 400076 India — [3]Faculty of Physics and Center for Computational Materials Science, University of Vienna, Kolingasse 14-16, A-1090 Vienna, Austria

We successfully generated a database of 150,000 unique finite-temperature structures using VASP and a "one-shot" DFT method to systematically sample atomic environments across the periodic table. Despite the small size of our training set compared to the millions typically used for foundation models, our resulting interatomic potentials achieve a force prediction error of 72 meV/Å. This performance is of the same magnitude as current state-of-the-art foundation models when tested against the same high-quality dataset. This result demonstrates that focusing on data quality and chemical diversity at finite temperatures is as impactful as massive data quantity. Furthermore, we showcase the computational infrastructure that made it possible to integrate interatomic potentials into an ab-initio software and discuss necessary enhancements to electronic optimization methods to compute magnetic materials more reliably.

MM 22.7 Wed 12:00 SCH/A216

MACE-based Machine Learning Interatomic Potentials for Iron-Nickel Alloys: Validation Across Composition and Pressure Ranges — •Kushal Ramakrishna[1], Mani Lokamani[1], and Attila Cangi[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), D-01328 Dresden, Germany — [2]Center for Advanced Systems Understanding (CASUS), D-02826 Görlitz, Germany

Machine-learned interatomic potentials have emerged as powerful tools bridging quantum-level accuracy with mesoscale simulations in computational materials science. We present a comprehensive evaluation of MACE models for iron-nickel alloys across a wide range of compositions and pressures, with direct relevance to Earth's core modeling and industrial applications. We construct special quasirandom structures (SQS) to simulate random iron-nickel alloy configurations and train MACE models on density functional theory datasets combined with experimental validation data. Extensive short-range order analysis confirms improved chemical randomness for larger supercells, critical for faithful property sampling. Multiple MACE flavors are systematically compared against experimental measurements for structural and elastic properties in both body-centered cubic and face-centered cubic phases. Our results demonstrate that fine-tuned MACE models achieve remarkable predictive accuracy for equation-of-state behavior and elastic properties across all compositions. This approach successfully bridges computational predictions with experimental observations, enabling accelerated materials discovery for technologically relevant transition metal alloys.

MM 22.8 Wed 12:15 SCH/A216

Benchmarking the MACE Foundation Model for Solid-State Ion Conductors — •Takeru Miyagawa, Yufeng Xu, Levon Satzger, Waldemar Kaiser, and David A. Egger — Physics Department, TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany

Recent progress in foundation model machine learning potentials (MLPs) has demonstrated promising transferability and accuracy across diverse material classes [1, 2]. Instead of being trained from scratch for each new system, these large pretrained models aim to provide broadly accurate force and energy predictions that can be refined for new chemistries with comparatively small datasets. This offers a complementary route to traditional system-specific MLPs and may reduce the cost of studying complex ionic materials.

Here, we benchmark the MACE foundation model [2] on representative solid-state ion conductors (SSICs) through direct comparison with first-principles calculations. We assess its accuracy for phonons and vibrational properties, characterize temperature-driven structural and phase transitions, and analyze ion transport across different phases. We then explore data-efficient DFT-based fine-tuning strategies to improve the foundation model's accuracy for SSICs and clarify the limits and strengths of pretrained representations in the context of ionic transport. References [1] Batatia, I. et al., Adv. Neural Inf. Process. Syst. 35, 11423-11436, 2022, [2] Batatia, I. et al., J. Chem. Phys. 163, 184110, 2025

MM 22.9 Wed 12:30 SCH/A216

MACE-μ-α: A Foundation Model for Molecular Dipole Moments and Polarizabilities — •Nils Gönnheimer[1,2], Venkat Kapil[3], Karsten Reuter[2], and Johannes T. Margraf[1,2] — [1]Universität Bayreuth — [2]Fritz-Haber-Institut der MPG — [3]University College London

Machine-learning interatomic potentials (MLIPs) have had a strong impact on computational chemistry, physics, and materials science in recent years by filling the accuracy gap between first-principles methods and classical force fields, at a fraction of the computational cost of the former. MLIPs are so far typically limited to predicting energies and forces, however, while other properties traditionally obtained from first-principles calculations have remained less accessible. Here, equivariant neural network architectures have led to enormous progress, as they allow the prediction of vectorial and tensorial properties on the same footing as energies and forces.

Here, we present the MACE-μ-α architecture for predicting dielectric properties based on the MACE MLIP framework. Trained on over 1.6 million organic systems, the corresponding foundation model allows the accurate prediction of molecular dipole moments and polarizabilities, as well as Raman and IR spectra (when combined with an MLIP). Notably, despite being trained on gas-phase molecules and clusters, the model also shows transferability to condensed systems such as molecular crystals.

MM 23: Topical Session: Dislocations in Functional Materials I (joint session MM/FM)

Time: Wednesday 10:15–11:30 Location: SCH/A251

MM 23.1 Wed 10:15 SCH/A251

Mechanical seeding of dislocations for room-temperature plasticity in ceramics — •Wenjun Lu[1], Jiawen Zhang[1], and Xufei Fang[2] — [1]Department of Mechanical and Energy Engineering, Southern University of Science and Technology, Shenzhen, 518055, China — [2]Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe,76131, Germany

The pursuit of room-temperature ductile ceramics has long been hindered by their inherent brittleness. Here, we demonstrate a simple strategy to seed mobile dislocations at room temperature with densities up to 1014 m-2, enabling ceramics to sustain plastic compressive strains exceeding 30%. These dislocations multiply through cross-slip and motion, effectively suppressing brittle fracture without high-temperature processing. Using in situ nano-/micromechanical deformation and ex situ bulk tests, we bridge the length scales of plasticity and reveal a strong dependence of yield strength and flow behavior on dislocation density. Specifically, SrTiO3 micropillars transition from brittle fracture (dislocation-free) to plastic yield when mechanically seeded dislocations are present. Yield strength first decreases then rises with increasing dislocation density, reflecting complex structural evolution observed via transmission electron microscopy. These findings highlight dislocation engineering as a viable pathway toward ductile ceramics and open avenues for tuning their mechanical and functional properties through room-temperature dislocation plasticity.

Contribution: Wenjun Lu is the Speaker.

MM 23.2 Wed 10:30 SCH/A251

Impact of mechanically seeded dislocations on the mechanical properties of perovskite ceramics — •Jiawen Zhang[1], Xufei Fang[2], and Wenjun Lu[1] — [1]Southern University of Science and Technology, Shenzhen, China — [2]Karlsruhe Institute of Technology, Karlsruhe, Germany

The inherent brittleness of functional ceramics severely hinders their engineering application. The strong ionic and covalent bonds in ceramics make dislocation nucleation, motion, and multiplication difficult at room temperature. Recent research challenges the conventional perception of ceramics as inherently brittle materials, with dislocations emerging as a promising avenue for enhancing their mechanical properties. By using a Brinell ball indenter to perform surface scratching, crack-free plastic deformation zones with tunable dislocation density can be generated on the ceramic surface. The dislocation generation mechanism and dislocation-dominated plastic deformation mechanism were investigated by introducing dislocations into perovskite SrTiO3 and KTaO3. Room temperature micropillar compression tests then revealed that as the mechanical seeded dislocation density increased,SrTiO3 exhibited a *brittle* to *ductile* transition as the dislocation density increased from ~1010 m-2 to ~1014 m-2. However, the (001) KTaO3 single crystal exhibits a *brittle* to *ductile* then to *brittle* transition as the dislocation density increased from ~1010 m-2 to ~1015 m-2. Additionally, the yield strength displayed a complex trend, initially decreasing and then increasing in these two perovskite oxide ceramics.

MM 23.3 Wed 10:45 SCH/A251

Dislocation interaction with a tilt low angle grain boundary in bi-crystal SrTiO3 — •Kuan Ding[1,2], Atsutomo Nakamura[3], Patrick Cordier[4,5], and Xufei Fang[3,6] — [1]Department of Materials and Earth Sciences, Technical University of Darmstadt, 64287 Darmstadt, Germany — [2]Max Planck Institute for Sustainable Materials, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [3]Department of Mechanical Science and Bioengineering, Osaka University, 1-3 Machikaneyama-chou, Toyonaka, Osaka, 560-8531, Japan — [4]Unité Matériaux et Transformations, Université de Lille, 59655 Villeneuve d'Ascq Cedex, France — [5]Institut universitaire de France (IUF), 75005 Paris, France — [6]Institute for Applied Materials, Karlsruhe Institute of Technology, Kaiserstr. 12, 76131 Karlsruhe, Germany

For applications of ceramics with dislocation-tuned mechanical and functional properties, it is pertinent to achieve dislocation engineering in polycrystalline ceramics. However, grain boundaries (GBs) are effective barriers for dislocation glide at room temperature. It is critical to understand the fundamental processes for dislocation-GB interaction. We investigated a bi-crystal SrTiO3 with a 4° tilt GB. Brinell indentation was used to generate a plastic zone at the mesoscale without cracking, allowing for direct assessment of GB-dislocation interaction. Together with dislocation etch pits imaging and transmission electron microscopy analysis, we observe dislocation pileup, storage, and transmission across the LAGB. Our observations reveal new insights into dislocation-GB interaction at room temperature at mesoscale.

MM 23.4 Wed 11:00 SCH/A251

Dislocation-Mediated Extraordinary Room-Temperature Plasticity in Inorganic Semiconductors — •Xiaocui Li[1] and Yang Lu[2] — [1]Department of Materials Science and Engineering, City University of Hong Kong, Kowloon, Hong Kong SAR, China — [2]Department of Mechanical Engineering, The University of Hong Kong, Pokfulam, Hong Kong SAR, China

Inorganic semiconductors, with their ionic or covalent bonds, are typically brittle at room temperature, restricting their use in flexible electronics. Our recent study reveals that all-inorganic perovskite (CsPbX3, X=Cl, Br, I) single-crystal micropillars can achieve extraordinary room-temperature plasticity with average plastic strain of ~64% (Nat. Mater. 2023, 22, 1175). They can be morphed into distinct geometries without cracks or cleavage. The deformation is mediated by partial dislocations on {011}<0-11> slip system, featuring four equivalent variants that address the lack of deformation pathways in ionic crystals. Sequential activation of variants prevents strain hardening and crack formation caused by dislocation reactions. First-principles calculations attribute this plasticity to low slip barriers enabling sustained deformability and strong Pb-X bonds preserving crystal integrity. Leveraging this deformability, we developed shape-customizable optoelectronic devices that maintain stable functional properties and bandgap energies post-deformation. This discovery overturns the notion of brittleness in inorganic semiconductors, and provides a foundation for advanced applications in flexible electronics and deformable sensors.

MM 23.5 Wed 11:15 SCH/A251

Dislocations as Key Enablers on the Road to Functional and Resilient Oxide Ceramics — •Oliver Preuss[1], Enrico Bruder[2], Zhangtao Li[3], Yinan Cui[3], Jinxue Ding[1], Philippe Carrez[4], and Xufei Fang[1] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Division Physical Metallurgy, Department of Materials and Earth Sciences, Technical University of Darmstadt, Darmstadt, Germany — [3]Department of Engineering Mechanics, Tsinghua University, PR China — [4]Materials and Transformations Unit, Université Lille, Lille, France

Designing oxide ceramics that unite high mechanical resilience with strong functional performance is challenging. We show that introducing ultra-high dislocation densities ($\approx 10^{15}$ m^{-2}) into materials such as MgO and $SrTiO_3$ provides a direct route to enhance both damage tolerance and functional properties. Cyclic Brinell ball scratching at room temperature generates near-surface, dislocation-rich zones of arbitrary size and shape. These regions markedly alter fracture behaviour, arresting propagating cracks and suppressing crack initiation, as demonstrated by Vickers indentation and quasi-in situ DCDC tests. Crystal-plasticity phase-field simulations reproduce the observed toughening mechanism. The dislocation networks also improve transport properties, increasing electrical conductivity while reducing thermal conductivity by nearly half: an advantageous combination for thermoelectric performance. This work establishes a practical strategy for dislocation engineering to achieve oxide ceramics with combined mechanical robustness and enhanced functionality.

MM 24: Invited Talk: Andrea Bachmaier

Time: Wednesday 15:00–15:30 Location: SCH/A251

Invited Talk MM 24.1 Wed 15:00 SCH/A251

Recent advances in processing of rare-earth free MnBi magnets by severe plastic deformation — •Andrea Bachmaier[1], Lukas Weissitsch-Reiner[1], Martin Kraus[1], Michael Meindlhumer[2], and Stefan Wurster[1] — [1]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences — [2]Department of Materials Science, Montanuniversität Leoben

Magnetic materials are key materials needed for Green energy technologies. The research on rare-earth free magnetic materials has increased significantly in recent years, driven by supply chain issues, environmental and social concerns.

Severe plastic deformation processing of magnetic materials and its influence on the magnetic properties have attracted increasing research interest in the last years.

In this contribution, the use of high-pressure torsion deformation to synthesize the rare-earth free α-MnBi phase is in focus. Our recent experimental results of the process-structure-property relationships that link chemistry, synthesis and processing parameters with microstructure evolution and magnetic properties are discussed. An emphasis is put on detailed characterization of the microstructure by backscattered electron imaging, electron backscattered diffraction as well as x-ray diffraction utilizing high energy synchrotron radiation since it strongly influences the magnetic properties.

MM 25: Interface Controlled Properties, Nanomaterials, and Microstructure Design I

Time: Wednesday 15:45–17:00 Location: SCH/A215

MM 25.1 Wed 15:45 SCH/A215

Confined but Active: Atomic-Scale Dynamics of Gallium and Silver Intercalation in Graphene/SiC — •Nadire Nayir[1], Qian Mao[2], Malgorzota Kowalik[2], and Adri van Duin[2] — [1]Paul-Drude-Institut für Festkörperelektronik, Leibniz Institut im Forschungsverbund Berlin e.V., Hausvogteiplatz 5-7, 10117 Berlin, Germany — [2]The Department of Mechanical Engineering, The Pennsylvania State University, PA, US

Metal intercalation at the interface of epitaxial graphene and SiC offers a powerful approach for stabilizing covalently bonded materials in two dimensional form [1-2]. This talk focuses on the atomic-level modeling of 2D metals (i.e. Ga and Ag) grown via confinement heteroepitaxy [2]. The intercalation mechanisms differ notably between metals. Combined photoemission electron microscopy and multiphysics simulatiosn reveal that while metal de-intercalation emerge in all cases, their re-intercalation dynamics vary markedly. For Ag, reversible de- and re-intercalation occurs through defects. In contrast, Ga exhibits irreversible de-intercalation characterized by faster kinetics. Multiphysics simulations integrating ReaxFF and Density functional theory simulations uncover the origin of these distinct behaviors, showing that Ga atoms bind more strongly to graphene than Ag atoms consistent with the faster, irreversible diffusion kinetics observed experimentally. Overall, the findings highlight that both the thermophysical properties of the intercalated metal and its interactions with defective graphene critically determine the intercalation behavior. [1] Nature materials 19 (6), 637-643(2020) [2] Small 20 (11), 2306554(2024)

MM 25.2 Wed 16:00 SCH/A215

Accelerating grain boundary segregation studies in ferritic steels with machine learned interatomic potentials — •Han Lin Mai[1], Tilmann Hickel[2], and Jörg Neugebauer[1] — [1]Max Planck Institute for Sustainable Materials GmbH, Dusseldorf, Germany — [2]BAM Federal Institute for Materials Research and Testing, Berlin, Germany

The segregation of solute and impurities to grain boundaries (GBs) can critically alter the mechanical properties of steels. To predict segregation phenomena, ab-initio methods such as density functional theory (DFT) are frequently used, but their computational expense limits the size of the model GBs viable for computation. This limitation has rendered access to segregation statistics out of reach and therefore has hindered our understanding of segregation phenomena. Here, we present a machine learned interatomic potential (MLIP) for multiple Fe-X binary alloys that predict segregation energies approaching ab-initio accuracy with automated dataset generation techniques. We use these potentials to conduct high-throughput segregation studies to generate segregation energy spectra and compare these to those commonly found in GBs accessible to DFT studies. Commonly purported relationships between GB quantities such as excess volume, site volume and GB energies and the strength of segregation binding of solutes and impurities are re-examined and revised.

MM 25.3 Wed 16:15 SCH/A215

Defect Phase Diagrams for Exploring Chemo-Structural Coupling in Ni Grain Boundaries — •Prince Mathews[1], Ali Tehranchi[1], Jörg Neugebauer[2], and Tilmann Hickel[1,2] — [1]Federal Institute for Materials Research and Testing (BAM), Berlin, Germany — [2]Max Planck Institute for Sustainable Materials, Düsseldorf, Germany

The knowledge-driven framework of defect phase diagrams (DPDs) offers an effective and systematic approach to design materials with tailored properties. Unifying bulk and defect thermodynamics along with the consideration of structural and chemical complexities around defects, DPDs advance the fundamental understanding of defects and can also provide a pathway for guided microstructure design. In this work, we apply the framework of DPDs using ab-initio calculations to evaluate the stability of defect phases and investigate defect phase transformations in Ni grain boundaries. In competition with the nearest intermetallic phase, Nb containing defect phases are stable in Σ5 [001]/(310) whereas Nb containing defect phases are not stable in Σ3 [110]/(111) grain boundaries. Moreover, our findings indicate the preference of solutes to segregate at sites around defects with partial column occupations. Furthermore, with the application of a sub-lattice based model, we present the insights on grain boundary site column coverages as a function of temperature. In addition, we discuss a new approach for determining a characteristic defect width using the solute distribution probability across the defect which facilitates the integration of defects into the CALPHAD methodology.

MM 25.4 Wed 16:30 SCH/A215

Non-Hermitian physics and exceptional points at Z2 Weyl semimetal*ferromagnet junctions — •Tong Wang[1], Robert Amelung[2], and Flore Kunst[1,2] — [1]Max Planck Institute for the Science of Light, Staudtstraße 2, 91058 Erlangen, Germany — [2]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Non-Hermitian systems extend beyond the framework of Hermitian quantum mechanics and allow for the description of open systems with loss and gain. The study of non-Hermitian physics leads to an enrichment of topological phases of matter and practical applications in photonics and sensing. Here we study the junction between a metallic ferromagnet and a Z2 Weyl semimetal [1], where a combined time-reversal symmetry and reflection symmetry leads to degenerate helical Fermi arcs on certain surfaces. The couplings at the material interface give arise to a complex self-energy in the Green's function [2], rendering the effective Hamiltonian of the Fermi arc surface states non-Hermitian. We show that non-Hermiticity can break a degenerate Fermi arc into pairs of exceptional point, and the resulting exceptional phase persists for a wide parameter range regarding the magnetization of the ferromagnet and topological mass term of the semimetal. We also discuss the how the exceptional points may influence physical properties of the Z2 Weyl semimetal. [1] T. Morimoto and A. Furusaki, Phys. Rev. B 89 235127 (2014). [2] E. J. Bergholtz and J. C. Budich, Phys. Rev. Res 1 012003(R) (2019).

MM 25.5 Wed 16:45 SCH/A215

Theory Unravels Electro-Ionic Metal-Support Interactions at Supported Electrocatalyst Nanoparticles — •Yufan Zhang, Tobias Binninger, Jun Huang, and Michael Eikerling — Theory and Computation of Energy Materials, Institute of Energy Technologies, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

Electrochemical energy conversion requires electrocatalysts to accelerate reactions. Most theoretical studies used idealized planar electrodes, whereas real catalysts typically consist of supported nanoparticles (NPs) with heterogeneous compositions and structures that lead to unique electronic and ionic properties.

In this talk, I will present results from our recently published paper [1]. Using density-potential functional theory, we calculate the contact electrification of a Ag NP and a Au support. While traditional view believes that electron redistribution is confined to the NP-support contact interface, we reveal that it also occurs at the NP's external surface, directly influencing the catalytically active sites. The electron redistribution generates an electric field in electrolyte surrounding the supported NP, which further leads to ion separation. The support-induced charge perturbations at the NP's external surface can be no longer described by the classical concept of the potential of zero charge for planar electrode. To address this, we define a global and two local characteristic potentials. It is demonstrated that the electronic and ionic effects are strongly coupled at supported NPs, and are therefore best described as electro-ionic metal-support interactions (EIMSI).

[1] Y. Zhang, et al., Phys. Rev. Lett. 134, 066201 (2025).

MM 26: Transport in Materials: Diffusion, Charge, or Heat Conduction I

Time: Wednesday 15:45–17:00 Location: SCH/A216

MM 26.1 Wed 15:45 SCH/A216

Theoretical investigation of the conductivity of the $LiMnPO_4$ Battery Material — •Franz Winkler and Harald Oberhofer — Chair for Theoretical Physics VII and Bavarian Center for Battery Technologies, University of Bayreuth

Developing better batteries and thus battery materials is a crucial step in humanity's urgent energy transition. Thereby, theory can play an important role in characterizing and understanding the properties of the involved materials. In this contribution we present our work on olivine $LiMnPO_4$ which exhibits some desirable properties such as a high energy density and a high potential and thus operating voltage. However, its adoption is hampered by a bad conductivity. In order to understand the barriers to conductivity and suggest potential remedies we compute electronic and ionic transport properties and how they could be influenced by defects.

The electron and hole band transport mobilities are calculated using Hubbard-corrected electronic density functional theory (DFT+U), both for antiferromagnetic and paramagnetic $LiMnPO_4$ as well as materials derived by substitution. For ionic conductivity we determine the minimal energy path of the Li ions via

the nudged elastic band (NEB) method. To reduce calculational cost and enable larger systems, we use machine learned force fields and refine these models via DFT to transition states. Li ions are transported in $LiMnPO_4$'s 1D channels. However these diffusion paths can be blocked by antisite defects. As those very strongly limit ionic transport we investigate their stability with first-principle DFT, phonon and thermodynamics calculations.

MM 26.2 Wed 16:00 SCH/A216

Multiscale modeling of cooperative defect dynamics in MoS_2 — •Aaron Flötotto[1,2], Erich Runge[1,2], and Christian Dressler[1,2] — [1]Technische Universität Ilmenau, Institut für Physik, Ilmenau, Germany — [2]Technische Universität Ilmenau, Institut für Mikro- und Nanotechnologien, Ilmenau, Germany

Chalcogen vacancies strongly influence the electrical and memristive properties of transition metal dichalcogenides including MoS_2. However, capturing their dynamics at device-relevant time and length scales is challenging due to the high energy barriers associated with individual atomic jumps [1]. We have developed a multiscale framework for MoS_2 that uses *ab-initio* molecular dynamics to generate training data for machine-learning force fields. This step reveals the motifs of cooperative sulfur-vacancy migration and cluster formation [2]: (i) Vacancy migration almost exclusively occurs by vacancy-assisted hopping, implying nonlinearities and suggesting memristive behavior; (ii) An energy barrier comparable to lab temperatures protects long vacancy lines against splitting into smaller vacancy clusters.

These insights are incorporated into a Monte-Carlo model that reproduces several key experimental observations and enables the prediction of device level quantities, such as the vacancy-density-dependence of the diffusion coefficient of sulfur vacancies in MoS_2.

[1] Q. Chen, et al. , ACS Nano 12, 7721-7730 (2018), doi: 10.1021/acsnano.8b01610.

[2] A. Flötotto, et al., arXiv:2508.13790 (2025).

MM 26.3 Wed 16:15 SCH/A216

Coupled Spin–Orbital–Lattice Interactions in FeO: A DFT+U and Heisenberg Analysis — •Hao Chen, Christoph Freysoldt, Mira Todorova, and Jörg Neugebauer — Max-Planck-Institut für Nachhaltige Materialien GmbH, Düsseldorf, Germany

Wüstite (FeO) is a prototypical correlated oxide where spin, orbital, and lattice degrees of freedom are intricately coupled. In addition, significant deviations from stoichiometry can occur via oxygen vacancies and Fe^{2+}/Fe^{3+} mixed valency. Local lattice distortions and orbital reorientations around such defects can modify magnetic exchange pathways and thus the defect formation energies. Using DFT+U, we investigate how the orbital orientation in Fe^{2+} correlates with structural strain and magnetic interactions. Our results reveal a well-defined correlation between the minority-spin t_{2g} occupation and the rhombohedral distortion parameter, giving rise to four distinct symmetry-broken orbital states. By mapping total-energy differences between these orbital configurations onto an effective Heisenberg model, we show that the exchange constants are sensitive to orbital orientation, evidencing strong superexchange–orbital coupling. This framework provides quantitative insight into the competition between Jahn–Teller-like lattice distortions and anisotropic magnetic exchange arising from orbital orientation. Building on this, the study provides a unified DFT+U-based picture of spin–orbital–lattice coupling in FeO and establishes a consistent energetic framework for incorporating spin and orbital effects into defect calculations.

MM 26.4 Wed 16:30 SCH/A216

Quantum interference in higher pseudospin fermions — •Gargee Sharma and Arpan Gupta — Indian Institute of Technology Delhi, Hauz Khas, New Delhi 110016 India

We construct a unified theory of quantum-interference corrections in disordered pseudospin-s fermions described by $k\cdot\mathbf{S}$ Hamiltonians. Employing the rotation-group structure of SU(2), we derive closed-form wavefunctions, scattering and vertex corrections, and Cooperon kernels valid for arbitrary pseudospin s in two and three dimensions. A universal "parity rule" emerges: integer s (orthogonal symmetry, $T^2 = +1$) yields weak localization, half-integer s (symplectic, $T^2 = -1$) yields weak antilocalization, while interband and intervalley scattering renormalize the prefactor via a finite Cooperon-mass matrix. Explicit results for $s = \frac{1}{2}$ and $s = 1$ reproduce graphene and spin-1 Weyl limits and verify the general scaling laws. Our approach resolves the long-standing ambiguity in interband scattering, providing an analytic route for arbitrary s and concrete predictions for multifold-fermion materials.

MM 26.5 Wed 16:45 SCH/A216

Effects of strong electron-electron interactions on the conductivity of free-standing graphene — •Maksim Ulybyshev[1], Adrien Reingruber[1], and Kitinan Pongsangangan[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Würzburg, Germany — [2]Department of Physics, Faculty of Science, Mahidol University, Bangkok, Thailand

Transport in strongly correlated systems is often described using the Boltzmann equation, where correlation effects enter through the collision integral. In practice, the collision integral is usually evaluated with a number of approximations, such as computing scattering amplitudes only up to tree-level diagrams. These approximations become unreliable when interactions are sufficiently strong.

Free-standing graphene provides a representative example, as the effective coupling constant of its low-energy effective field theory exceeds unity. Using unbiased Quantum Monte Carlo (QMC) simulations on lattices with up to 102x102 unit cells and long-range Coulomb interactions, we investigate both the DC and optical conductivity of free-standing graphene. We find that the optical conductivity remains essentially unaffected by interactions, whereas the DC conductivity exhibits a strong dependence on both temperature and interaction strength. We then compare these results with kinetic-theory calculations based on the Boltzmann equation, highlighting how the QMC data can guide improvements in the accuracy of the collision integral.

MM 27: Topical Session: Dislocations in Functional Materials II (joint session MM/FM)

Time: Wednesday 15:45–17:15 Location: SCH/A251

Topical Talk MM 27.1 Wed 15:45 SCH/A251

Dislocations in perovskite oxides: similarities and differences — •Pierre Hirel — Univ. Lille, CNRS, INRAE, Centrale Lille, UMR 8207 - UMET - Unité Matériaux et Transformations, F-59000 Lille, France

The experimental discovery of room-temperature ductility in strontium titanate $SrTiO_3$ in 2001, has revealed the surprising mobility of dislocations in ⟨110⟩{110} slip systems. Atomic-scale simulations have contributed to resolving the core structure of these dislocations, and their role in the ductile-brittle transition. Since then, similar ductile behaviour was found in related perovskite oxides $KNbO_3$ and $KTaO_3$. However, other perovskites like $BaTiO_3$ or $CaSiO_3$ remain essentially brittle at room temperature, despite having the same crystal lattice and similar chemical compositions as ductile perovskites.

MM 27.2 Wed 16:15 SCH/A251

Probing the Known Unknown of the Dislocation Dynamics in Oxides and Semiconductors — •Liming Xiong — NC State University, Raleigh, NC, USA

Dislocation dynamics in oxides and semiconductors are widely aware, but its exact nature and impact on the properties and functionality of these materials are not fully understood yet. One reason is that the well-established knowledge for dislocation dynamics in metals often can't fully explain or even fail when used for oxides and semiconductors. To fill this knowledge gap, here we will present a concurrent atomistic-continuum computational tool for probing the dislocation dynamics in oxides and semiconductors. This tool has a unique feature to accommodate the motion/multiplication of μm-long dislocations together with the atomic-scale core structure evolution along the dislocation within all within one single model. Taking dislocation-seeded SrTiO3 and ZnS as sample materials, we will: (i) map the core structure/stress along a dislocation line to its local charge states and motion mechanism; (ii) measure the dislocation mobility and its dependence on stress, temperature, dopant concentration, charge states, electrical field, light illumination, and dislocation line lengths ranging from nanometers to micrometers; (iii) predict how local internal stress builds up when a mesoscale dislocation slip interacts with an atomically structured grain boundaries, and how such a high local stress may initiate a crack in turn. A consolidation of such simulation data into constitutive rules needed by higher-scale models for interpreting experimental observations will be also discussed.

MM 27.3 Wed 16:30 SCH/A251

Electric Field Effects on Dislocation Motion in SrTiO3 via Mesoscale Indentation — •Alexander Frisch[1], Daniel Isaia[2], Oliver Preuss[2], and Xufei Fang[1] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Department of Materials and Earth Sciences, Technical University of Darmstadt, Darmstadt, Germany

Dislocations in perovskite oxides have the potential of tuning functional properties of electroceramics, however their behavior and stability under externally applied electric fields remain elusive. Therefore, we investigated the effect of high densities of dislocations onto the dielectric breakdown behavior of SrTiO3, a model perovskite material. Lower dielectric breakdown strengths were found in the high-dislocation-density samples, engineered through the Brinell scratching method. Further, the effect of a 2 kV/mm electric field on the introduction and mobility of dislocations in SrTiO3 was investigated. While no changes to the

dislocation plastic zone size, depth, or dislocation distribution were observed, the results suggest the stability of pre-engineered dislocation structures in perovskite oxides under applied electric fields. These results will be interpreted in the context of the dislocation charge state, associated electric field forces, and defect-modified electrical/thermal conductivity.

MM 27.4 Wed 16:45 SCH/A251

Generating a "ferroelectric metal" by preferential reduction of dislocations in $BaTiO_3$ — •Christian Rodenbücher[1], Gustav Bihlmayer[2], Carsten Korte[1], and Kristof Szot[3] — [1]Forschungszentrum Jülich GmbH, Institute of Energy Technologies (IET-4), 52425 Jülich, Germany — [2]Forschungszentrum Jülich GmbH, Peter Grünberg Institut (PGI-1), 52425 Jülich, Germany — [3]University of Silesia, Institute of Physics, 41-500 Chorzów, Poland

Redox processes in transition metal oxides are of high relevance for sensors, information technology, superconductivity, and energy conversion. Perovskites with mixed ionic-electronic conductivity, such as $BaTiO_3$, are of particular interest because oxygen nonstoichiometry controls electronic charge carriers and thus conductivity. Surprisingly, thermal reduction in vacuum can induce metallic behaviour with conductivities far exceeding predictions from point-defect chemistry. To clarify the origin of this metallic state, we investigate the electronic transport, electronic structure, and chemical composition of $BaTiO_3$ single crystals during annealing and cooling under ultrahigh vacuum. Surface-sensitive techniques such as XPS and LC-AFM allow us to correlate electronic structure changes with the insulator-to-metal transition. We find that surface-layer dislocations act as preferential reduction sites, forming conducting filaments that yield macroscopic metallic behaviour despite minimal overall oxygen loss. Metallic behaviour persists into the ferroelectric phase. Nanoscale mapping shows that metallic filaments and piezoelectrically active regions coexist thus explaining how a "ferroelectric metal" can exist.

MM 27.5 Wed 17:00 SCH/A251

Dislocation dynamics in Ni-based superalloys: atomistic simulations and uncertainty quantification — •Geraldine Anis, Thomas Hudson, and Peter Brommer — University of Warwick, Coventry CV4 7AL, UK

Ni-based superalloys exhibit extraordinary strength at high temperatures. This strengthening effect is largely attributed to precipitation strengthening, where dislocations are hindered by precipitates present in their microstructure. In our work, we model dislocation trajectories obtained from Molecular Dynamics (MD) simulations of Ni-Ni_3Al. A reduced model was developed to describe dislocation-interface interactions within this system, which captures important features of the MD dislocation trajectories. The developed model was tested on a representative system and was shown to capture a range of qualitatively different dislocation behaviour. The model parameter distributions were then determined using Differential Evolution Monte Carlo (DE-MC) sampling and a Gaussian process surrogate model. The present approach offers a means of identifying atomistic-scale parameters, which can be used to inform larger length scale simulations of dislocations. Determining parameter distributions using DE-MC means that parameter uncertainties can be propagated through a hierarchy of multiscale models. We illustrate how such uncertainty propagation can be achieved by considering a dislocation mobility law with quantified uncertainties in pure Ni. This work is part of a wider study aiming to model the deformation behaviour of Ni-based superalloys with a focus on quantifying and propagating uncertainties.

MM 28: Members' Assembly

Welcome to this general meeting of the DPG-SKM division MM! All of you, presenters of MM talks or posters and other interested participants of this conference, are cordially invited to this meeting. We will come together in a relaxed atmosphere, supported by drinks and pretzels (at least) for personal exchange. We will award the poster prizes, discuss the current conference, and ask for your suggestions for future Topical Sessions in MM, Symposia, and invited speakers. Take this opportunity to share your ideas regarding our MM program for our next DPG spring meeting.

Time: Wednesday 17:15–18:45 Location: SCH/A251

All members of the Metal and Material Physics Division are invited to participate.

MM 29: Invited Talk: Philipp Pelz

Time: Thursday 9:30–10:00 Location: SCH/A251

Invited Talk MM 29.1 Thu 9:30 SCH/A251

Three dimensional sub-Ångström resolution imaging from 4D-STEM experiments — •Philipp Pelz — Friedrich Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Electron ptychography is rapidly emerging as a way to turn scattered high-energy electron waves into precise three-dimensional atomic maps, effectively solving a challenging inverse problem that links measurement, modeling, and reconstruction. By combining multi-slice physics, joint optimization, and automated data collection, we can now recover sub-Ångström 3D structures even when the experiment violates classical limits in electron microscopy such as depth of focus and tomographic completeness. These methods dramatically expand the range of materials and volumes that can be imaged at true atomic resolution, opening the door to data that is richer, more robust, and more compatible with theory and simulation. I will present several results that bridge experiment and computational modeling through a unified, physics-based reconstruction framework, show applications to nanomaterials and outline our ambitions to scale the method to larger volumes.

MM 30: Interface Controlled Properties, Nanomaterials, and Microstructure Design II

Time: Thursday 10:15–11:45 Location: SCH/A215

MM 30.1 Thu 10:15 SCH/A215

Statistics of Shear-Coupled Grain Growth in Polycrystals — •Marco Salvalaglio[1], Caihao Qiu[2], Jian Han[2], and David J. Srolovitz[3] — [1]Institute of Scientific Computing, TU Dresden, 01062 Dresden, Germany — [2]Department of Materials Science and Engineering, City University of Hong Kong, Hong Kong SAR — [3]Department of Mechanical Engineering, The University of Hong Kong, Pokfulam, Hong Kong SAR

Grain growth in polycrystals, the coarsening of crystalline domains with different orientations, is traditionally viewed as a capillarity-driven process governed by interfacial energy minimization. However, grain-boundary migration can also induce, and in turn couple to, shear deformation, making microstructure evolution sensitive to externally applied stress. At the microscopic level, this behavior arises from the motion of disconnections, steps with dislocation character constrained at grain boundaries. Using a multi-phase-field (PF) framework that incorporates disconnection flow through coarse-graining, we demonstrate that accounting for shear coupling enables realistic grain-growth behavior in single-component polycrystals. Simulations reproduce recent experimental observations of weak correlations between grain boundary velocity and curvature. We then use PF simulations to analyze key aspects of microstructure evolution, including grain-size distributions, grain-shape evolution, and statistical characterization of the evolving network.

MM 30.2 Thu 10:30 SCH/A215

Revealing nanovoids in growth-resistant regions of nanocrystalline Pd–Au using atom probe tomography — •Johannes Wild[1], Fabian Andorfer[4], Svetlana Korneychuk[2,3], Jules M. Dake[4], Dorothée Vinga Szabó[1,2,3], Stefan Wagner[1], Carl E. Krill III[4], and Astrid Pundt[1,2] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology — [2]Institute of Nan-

otechnology, Karlsruhe Institute of Technology — [3]Karlsruhe Nano Micro Facility (KNMFi), Karlsruhe Institute of Technology — [4]Institute of Functional Nanosystems, University of Ulm

Nanocrystalline Pd–Au produced by inert gas condensation (IGC) shows extreme abnormal grain growth (AGG) upon heat treatment. In some cases, narrow regions of residual nanocrystalline material resist coarsening entirely, persisting between abnormally grown grains exceeding 100 μm. We investigate these growth-stagnant regions using site-specific SEM/FIB lift-outs, atom probe tomography (APT) and TEM. FIB cross-sections reveal that these nanocrystalline regions are significantly more porous than the surrounding matrix, and APT reconstructions from them exhibit a strongly elevated density of OH-containing clusters, which are largely absent elsewhere. By analysing local ion-density variations during field evaporation into voids, we show that these OH clusters correspond to nanovoids in the material. Correlating porosity with grain morphology, we find that the most porous regions exhibit the strongest resistance to grain growth, indicating that nanoscale porosity is a key factor in stabilizing the nanocrystalline grain structure in IGC Pd–Au (manuscript submitted).

MM 30.3 Thu 10:45 SCH/A215

Vacancy-mediated extreme abnormal grain growth in inert gas-condensed nanocrystalline Pd–Au: when what's missing runs the show! — Fabian Andorfer[1], Johannes Wild[2], Jürgen Markmann[3,4], Markus Ziehmer[1], Jules M. Dake[1], Torben Boll[2], Dorothée Vinga Szabó[2,5,6], Stefan Wagner[2], Astrid Pundt[2,5], and •Carl E. Krill III[1] — [1]Inst. of Functional Nanosystems, Ulm University — [2]Inst. for Applied Materials, KIT — [3]Inst. of Hydrogen Technology, Helmholtz-Zentrum Hereon — [4]Inst. of Materials Physics and Technology, TUHH — [5]Inst. of Nanotechnology, KIT — [6]Karlsruhe Nano Micro Facility (KNMFi), KIT.

Inert gas-condensed Pd–Au exhibits extreme abnormal grain growth (AGG), marked by a small number of grains growing dendritically through a matrix of nanocrystallites, eventually reaching sizes of 100 μm or more. The triggers for rapid growth of abnormal grains (emergence) and for maintaining this growth advantage (persistence) remain unclear. Annealing under hydrogen accelerates emergence without altering grain morphology, suggesting that the ~ 5 vol% porosity inherent to inert gas condensation not only pins matrix/matrix grain boundaries (GBs) but also governs where and when abnormal grains emerge. In nano-Pd–Au, pores can coarsen by vacancy diffusion along GBs, with larger pores growing at the expense of smaller ones. Small-angle x-ray scattering measurements support such an evolution in pore-size distribution. Vacancy transport, rather than variations in boundary mobility, appears to establish the spatiotemporal conditions for AGG in this system.

MM 30.4 Thu 11:00 SCH/A215

Small-angle x-ray scattering of nanoporous gold - a discussion of the structure factor and its implications for local order — •Celina Passig[1,2], Jürgen Markmann[2,1], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, Germany — [2]Department Hybrid Materials Systems, Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, Geesthacht, Germany

Nanoporous gold (NPG) made by dealloying is a popular model system for studies of size and interface effects as well as microstructure evolution in nanomaterials. Here, we investigate to what extent information on the microstructural geometry may be obtained by Small-Angle X-Ray Scattering (SAXS). It is well established that NPG exhibits a sharp interference peak, indicative of a characteristic wavelength underlying its leveled-wave-like microstructure and, hence, of an exceptional degree of order. Remarkably, our measurements even reveal a secondary peak at larger wave number. We compare the experimental data to simulations for small-angle scattering of NPG generated (1) by kinetic Monte Carlo (KMC) studies of dealloying or (2) as leveled-wave structures. On that basis, we discuss in how far the secondary interference peak is intrinsic to the microstructure of idealized, uniform NPG and what information it provides on the geometry of that microstructure. Since the feature vanishes during coarsening, we inspect how this process affects the order of the ligament network.

MM 30.5 Thu 11:15 SCH/A215

Enhanced Field Emission Current Density in Chemically Engineered Multiwall Carbon Nanotube - Neodymium Oxide Heterostructures — •Anima Mahajan[1], Menaka Jha[2], and Santanu Ghosh[1] — [1]Department of Physics, Indian Institute of Technology, Hauz Khas, New Delhi -110016, India. — [2]Institute of Nano Science & Technology, Knowledge City, Sector-81, Mohali, Punjab- 160062, India.

The MWCNT, neodymium oxide (Nd*O*), and MWCNT-Nd*O* heterostructure were successfully fabricated through a facile three-step synthesis process: the synthesis of MWCNT rods by the chemical vapor deposition technique, the synthesis of the Nd*O* nanoparticles by using the micellar-assisted solid-state route, and the fabrication of the MWCNT-Nd*O* heterostructure. Moreover, the MWCNT-Nd*O* heterostructure exhibits enhanced field emission properties, with a lower turn-on field of 2.4 V/*m compared to pure MWCNT and Nd*O*, which have turn-on fields of 3.6 and 3.8 V/*m, respectively. The emission current stability at a preset value of 6 V/*m over an 8-hour duration is found to be fairly good, characterized by current fluctuations within * 3% of the average value. The enhanced field emission (FE) performance of the MWCNT-Nd*O* heterostructure is attributed to its high enhancement factor (β) of ~3.3*10*.

MM 30.6 Thu 11:30 SCH/A215

Exploring Superconductivity in Misfit Nanodevices — •Sushmita Chandra and Claudia Felser — Nöthnitzer Str. 40, 01187 Dresden

Recently, MISFIT layered compounds (MLCs) have attracted considerable attention in the field of 2D materials due to their unique structure, crystallographic diversity, and chemical tunability. Typically, MLCs can be represented by the general formula [(MX)(1+δ)]m[(TX2)n] with m, n = 1, 2, 3, where M = Sn, Sb, Pb, Bi, rare-earth elements; T = Ta, Nb, Mo, etc., and X = S, Se, Te. The lattice mismatch between the distorted rock salt MX layers and hexagonal TX2 counterparts creates a strained interface in the MLCs which allows a charge transfer from one layer to another, leading to a wealth of fascinating physical phenomena and modulations in the electronic structure. Although MLCs have been extensively studied for their potential applications in thermoelectrics, the fabrication of nanodevices with single- or multilayer MISFIT crystals is a challenging task and has not been explored at all. In this talk, I will present the fabrication of nanodevices based on high-quality MISFIT single crystals. I will also correlate how the misfit strain is associated with the superconducting transition and affects the electronic transport in these natural van der Waals heterostructures.

MM 31: Transport in Materials: Diffusion, Charge, or Heat Conduction II

Time: Thursday 10:15–13:00 Location: SCH/A216

MM 31.1 Thu 10:15 SCH/A216

Thermal Transport through Benzene-1,3,5-Trisamide Fibers — •Eberhard Lukas Flöter and Fabian Pauly — Universität Augsburg, Augsburg, Germany

Benzene-1,3,5-trisamides (BTAs) are a group of chiral and polar molecules which consist of a benzene ring, three amide groups and various side groups. Hydrogen bonding between the amide groups lets the BTAs assemble to columns. These columns pack into hexagonal structures, forming fibers. Since BTAs are chiral and polar, there are multiple configurations that these structures can take. We use nonequilibrium molecular dynamics (NEMD) methods and force fields to model thermal transport through BTA fibers in various configurations. In the presentation we discuss how thermal transport depends on side groups, molecular stacking and defects.

MM 31.2 Thu 10:30 SCH/A216

Phonon Interference in Single-Molecule Junctions — Sai C. Yelishala[1], Yunxuan Zhu[1], •Pablo M. Martinez[2,3], Hongxuan Chen[4], Mohammad Habibi[1], Giacomo Prampolini[5], Juan Carlos Cuevas[3,6], Wei Zhang[4], Guilherme Vilhena[2], and Longji Cui[1,7] — [1]Paul M. Rady Department of Mechanical Engineering, University of Colorado Boulder, USA — [2]Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Spain. — [3]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain. — [4]Department of Chemistry, University of Colorado Boulder, USA — [5]Istituto di Chimica dei Composti Organo Metallici (ICCOM-CNR), Italy. — [6]Condensed Matter Physics Center (IFIMAC), Spain — [7]Materials Science and Engineering Program and Center for Experiments on Quantum Materials, University of Colorado Boulder, USA.

Wave interference opens a new route to control transport properties and has been widely studied in electronic and photonic materials. However, interference of phonons, which govern thermal transport in insulators, has been poorly characterized due to experimental challenges. We report the observation of phonon interference at room temperature in molecular-scale junctions. This is enabled by custom-developed scanning thermal probes which can track heat flowing through a single molecular junction at a time. Using isomers of oligo(phenylene ethynylene)3 with either para- or meta-connected centre rings, we reveal a 40% reduction in thermal conductance for the latter. Quantum-mechanically accurate simulations show this difference arises from the destructive interference of phonons through the molecular backbone.

MM 31.3 Thu 10:45 SCH/A216

Phunky.jl - A Multithreaded Phonon Spectral Function Calculator In Julia — •William L. Wenig and Nakib H. Protik — Humboldt-Universität zu Berlin, Berlin, Germany

The ability to compute the phonon properties of materials is crucial for the understanding of physical phenomena such as transport and spectroscopy. At present, several code packages exist that allow ab initio access to phonon computations. These codes are mostly written in traditional languages such as Python, Fortran, or C++. In this talk we present Phunky.jl, a new tool for computing the harmonic and anharmonic phonon properties of materials. The tool is written in Julia, a language that has been designed specifically for scientific computation. It allows researchers to write software at a high level of abstraction, while generating code that runs at speeds faster or comparable to that of more traditional languages in this domain. Phunky.jl is written in an extensible manner so that one can easily expand and interface it with phonon transport solvers. We will highlight the capabilities of Phunky.jl by calculating the phonon spectral quantities for a selection of materials.

MM 31.4 Thu 11:00 SCH/A216

Understanding How Pressure Enhances Heat Transport in Organic Semiconductors — •Lukas Legenstein[1,2], Sandro Wieser[1,3], Michele Simoncelli[4], and Egbert Zojer[1] — [1]Graz University of Technology, Austria — [2]Montanuniversität Leoben, Austria — [3]TU Vienna, Austria — [4]Columbia University, USA

Understanding how lattice thermal conductivity changes under pressure is increasingly important in materials science, yet difficult to predict because materials exhibit a variety of behaviors, ranging from monotonic increases or decreases to anomalous trends. Molecular crystals, including organic semiconductors, stand out for exhibiting unusually large pressure-induced increases relative to their (ultra-)low thermal conductivities.

Our test system, naphthalene, crystallizes in a herringbone stack, a packing motif common in most π-conjugated organic semiconductors. Measurements up to 2 GPa from previous literature show an isotropic thermal conductivity that is up to four times higher than at ambient conditions. By combining highly accurate machine-learned potentials with the Wigner transport equation, we not only reproduce these findings but also elucidate how compression affects naphthalene's anisotropic thermal conductivity and how phonon tunneling becomes less relevant with increasing pressure. Finally, we trace the pressure-induced enhancement to frequency upshifts and the associated modifications in phonon scattering.

MM 31.5 Thu 11:15 SCH/A216

Building Trust in Ab Initio Machine-Learning Potentials for Extreme Materials – Applications to Strongly Anharmonic Ceramics and Thermal Insulators — •Shuo Zhao[1], Kisung Kang[1,2], and Matthias Scheffler[1] — [1]The NOMAD Laboratory at FHI, Max Planck Society — [2]School of Materials Science and Engineering, Chonnam National University

Thermal insulating ceramics and semiconductors often exhibit significant anharmonicity, particularly associated with rare events such as Frenkel defect creation and rattling phonon modes. These phenomena not only disrupt the phonon picture and the conventional perturbative methods for heat transport, but also pose challenges for the effective and trustful training of machine-learned interatomic potentials (MLIPs). Our contribution describes the implementation of a framework that combines the non-perturbative Green-Kubo formalism with a sequential, uncertainty guided active learning scheme using `AlmoMD`[1] with equivariant neural networks `NequIP`[2] and `So3krates`[3]. The approach is demonstrated by application to possibly ultra-low thermal conductivity materials[4]. Our results not only substantiate reliable predictions of thermal conductivity for strongly anharmonic systems but also pave the way for the accelerated exploration and design of novel thermal insulators.

[1] K. Kang, *et al.*, *Phys. Rev. Mater.* **9**, 063801 (2025). [2] S. Batzner, *et al.*, *Nat. Commun.* **13**, 2453 (2022). [3] J.T. Frank, *et al.*, *Nat. Commun.* **15**, 6539 (2024). [4] T.A.R. Purcell, *et al.*, *Npj Comput. Mater.* **9**, 112 (2023).

15 min. break

MM 31.6 Thu 11:45 SCH/A216

Probing Lattice Anharmonicity and Thermal Transport in Ultralow-κ Materials Using Machine Learning Interatomic Potentials — •Soham Mandal[1], Ashutosh Srivastava[2], Tanmoy Das[1], Abhishek Singh[2], and Prabal Maiti[1] — [1]Centre for Condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore 560012, India — [2]Materials Research Centre, Indian Institute of Science, Bangalore 560012, India

Crystalline solids with ultralow lattice thermal conductivity (κ) are promising candidates for thermoelectric and thermal-barrier applications, yet understanding heat transport in such strongly anharmonic systems remains challenging. Perturbative frameworks such as the Boltzmann transport equation (BTE) are unreliable when anharmonicity is large and higher-order phonon scattering cannot feasibly be computed. Here, we develop machine-learning interatomic potentials (MLIPs) to study heat transport in TlAgSe and $Cs_2PbI_2Cl_2$ and compare three transport formalisms: Green-Kubo (GK), BTE, and the Wigner transport equation (WTE). BTE underestimates κ, while WTE improves agreement but slightly overpredicts due to neglected higher-order scattering. The non-perturbative GK framework captures full anharmonicity and closely matches the experimental κ value. Phonon scattering rates exceeding the Ioffe-Regel limit and the degree of anharmonicity $\sigma^A > 0.5$ confirm the strongly anharmonic nature of both materials. This MLIP-integrated framework advances predictive understanding of ultralow-κ heat transport and supports future materials design.

MM 31.7 Thu 12:00 SCH/A216

Current-voltage curves of transformer oils: Analytical and numerical results — •Markus Bier — Technische Hochschule Würzburg-Schweinfurt, Schweinfurt, Germany

High-voltage transformers contain oil, which should allow for convective heat transport while sustaining electrical insulation. These oils are complex fluids composed of various molecular and colloidal species which, over time, give rise to the formation of charged entities due to numerous, by now not entirely known and fully understood mechanisms. A widely used technique to diagnose transformer oils are current-voltage curves, which can exhibit remarkable and non-trivial transient features upon polarisation of a relaxed oil or repolarisation of an electrically stressed oil. Theoretical modelling provides a bottom-up approach to link current-voltage curves to the underlying charge transport processes. The present contribution reports on analytical and numerical results obtained within theoretical investigations of reaction-drift-diffusion models based on Poisson-Nernst-Planck (PNP) theory. After presenting an analytical solution of the PNP equations for a semi-infinite system in the non-equilibrium steady state as well as analytical cross-over boundaries between different repolarisation regimes, the main features of numerical transient current-voltage curves for polarisation and repolarisation are discussed.

Reference: M. Bier, "Non-equilibrium steady states of electrolyte interfaces", New J. Phys. 26, 013008 (2024).

MM 31.8 Thu 12:15 SCH/A216

Interband effects in the matrix Boltzmann transport equation — •Elena Trukhan and Nakib H. Protik — Department of Physics and CSMB, Humboldt University of Berlin

The current state-of-the-art ab initio method for computing electronic transport properties relies on the Boltzmann transport equation (BTE). However, the BTE fails to capture certain quantum effects, most notably interband coherence. To address this limitation for phonon transport, Simoncelli et al [1]. developed an approach based on the Wigner transport equation, which incorporates these effects by including the off-diagonal terms of the density matrix. This framework was later adapted to electrons by Cepellotti and Kozinsky [2]. Their method, however, involves several critical simplifications; for instance, it ignores kinetic corrections and treats the collision integral within a relaxation time approximation (RTA). Also, modern derivations rely on the assumption of a band-diagonal form of the interaction self-energies, which might not hold generally. In this work, we derive a more general electronic transport equation from a Green's function formalism. Using a modified Kadanoff-Baym Ansatz, we carefully track the terms that survive various standard approximations in the Dyson equations in the band representation, explicitly include electron-impurity and electron-phonon interactions, keeping self-energy in non-diagonal form and present a framework that captures interband coherence while moving beyond the RTA.

[1] M. Simoncelli, et al., Phys. Rev. X 12, 041011 (2022) [2] A. Cepellotti and B. Kozinsky, Mater. Today Phys. 19, 100412 (2021)

MM 31.9 Thu 12:30 SCH/A216

Coulomb and phonon scattering limited transport in doped systems — •Nakib H. Protik and Dwaipayan Paul — Humboldt-Universität zu Berlin, Berlin, Germany

In this talk we present an extension of the elphbolt [1] transport code package that includes the Coulomb interactions among the charge carriers. We perform ab initio calculations to study the effect of these interactions on the transport properties of doped systems over a range of temperatures. Specifically, we probe the charge carrier hydrodynamics in these systems and identify the relative roles of the Coulomb and phonon scattering in the realization these transport regimes. We provide a comparison with recent measurements and comment on the violation of the Wiedemann-Franz law.

[1] N. H. Protik, C. Li, M. Pruneda, D. Broido, and P. Ordejón, The elphbolt ab initio solver for the coupled electron-phonon Boltzmann transport equations, npj Computational Materials 8, 28 (2022).

MM 31.10 Thu 12:45 SCH/A216

Stoichiometric Locking in the High State of Charge in Solid Ion Conductors: A Kinetic Monte Carlo Study — •Roya Ebrahimi Viand, Chiara Panosetti, Christoph Scheurer, Karsten Reuter, and Sebastian Matera — Fritz-Haber-Institut der MPG, Berlin

The advancement of solid-state batteries critically relies on a deep understanding of ion transport in crystalline electrolytes and electrode active materials. We present a kinetic Monte Carlo (kMC) approach with fast update rules for transition propensities that enables efficient simulation of systems with long-range Coulomb interactions. Our study systematically probes the effects of state of

charge (SOC), temperature, and applied external electric field on ionic mobility. We observe a pronounced mobility minimum near 100% SOC, where ions freeze in a low-energy Coulomb superlattice configuration that persists even under applied electric fields. Deviations from stoichiometry dramatically enhance transport by introducing defect pathways, with nearly symmetric behavior for ion and vacancy diffusion. By decomposing the state of charge into a reference and an excess carrier concentration (ΔSOC), we find that the intrinsic mobility per excess carrier remains approximately constant across different SOC values, revealing that transport is fundamentally mediated by the ΔSOC disrupting the reference structure. Analysis of effective activation energies across different SOC values reveals behavior consistent with percolation-controlled transport, where the availability of defect-mediated pathways strongly influences the energy landscape for ion diffusion.

MM 32: Topical Session: Advanced Nanomechanics – Accelerating Materials Physics from the Bottom I

Time: Thursday 10:15–12:45 Location: SCH/A251

Topical Talk MM 32.1 Thu 10:15 SCH/A251

High-Throughput Nanomechanics and Data-Driven Workflows for Mapping Composition-Microstructure-Property Landscapes — •Ruth Schwaiger — Forschungszentrum Juelich, Institute of Energy Materials and Devices, IMD-1: Structure and Function of Materials, Juelich, Germany

Combinatorial and high-throughput (CHT) methods are enabling nanoscale mechanical studies that span broad compositional and microstructural spaces with unprecedented efficiency. This talk presents an integrated perspective on how automated nanoindentation, combinatorial thin-film libraries, and machine-learning analysis jointly accelerate the discovery of composition-microstructure-property relationships.

Combinatorial thin-film libraries provide dense, continuous coverage across multicomponent compositions, enabling systematic mapping of phase formation, defect structures, and mechanical response. For example, CHT workflows applied to Ni-Al coatings captured structural transitions and hardness trends across the phase diagram, enabling development of a mechanistic hardness model that integrates grain-size, solid-solution, and phase-fraction strengthening. To extract intrinsic material properties from such heterogeneous datasets, data-driven analysis methods, ranging from physics-informed regression to unsupervised clustering, allow the identification of mechanically distinct regions, quantification of data sufficiency, and robust separation of compositional, microstructural, and defect-driven effects.

MM 32.2 Thu 10:45 SCH/A251

Reliability of Interatomic Potentials for Surface- and Size-Dependent Mechanical Behavior — •Sriram Anand, Jan Janssen, Jörg Neugebauer, and Erik Bitzek — Computational Materials Design, Max-Planck-Institute for Sustainable Materials, Düsseldorf

Material properties at the nanoscale differ markedly from the bulk, largely due to the increased surface-to-volume ratio. Surface stresses in particular are thought to modify the elastic response and contribute to the anomalous mechanical behavior of nanoobjects. These effects are typically investigated using atomistic simulations; however, the interatomic potentials used in such studies are generally not fitted to surface stresses. As a consequence, both the quantitative values (e.g., Young's modulus) and, to a lesser extent, the deformation mechanism of nanoobjects obtained from simulations may deviate from physical reality.

Here, we present a systematic study of surface stresses, nonlinear elasticity, and stacking-fault energies in FCC metals as predicted by a broad set of classical and machine-learning interatomic potentials. Using first-principles data as reference, we compile a benchmark database of these key quantities and demonstrate - through tensile deformation of nanowires - how the choice of potential can markedly influence simulated mechanical properties and deformation behavior. Our benchmark of surface stresses, higher-order elastic constants, and fault energies provides a robust foundation for the accurate design of reliable next-generation nanoelectromechanical devices.

Topical Talk MM 32.3 Thu 11:00 SCH/A251

Expanding nanoindentation capabilities: Data-driven and novel experimental approaches — •Michael Wurmshuber[1], Matthias Glosemeyer[1], Pouya Hassanzadeh Sarhangi[1], Verena Maier-Kiener[2], Heinz Werner Höppel[1], and Matthias Göken[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Montanuniversität Leoben, Leoben, Austria

As material discovery and manufacturing accelerate through artificial intelligence and additive manufacturing, high-throughput materials characterization is essential to ensure fast-paced material development. Here, nanoindentation with its capability to measure small material volumes and individual microstructural constituents in a quick manner, has the edge over classical slow-paced mechanical testing. Since Oliver and Pharr's groundbreaking work, nanoindentation has developed to extract not only hardness and modulus but numerous other mechanical properties through specialized indentation protocols. This talk presents two approaches to further extend the information space we receive from nanoindentation. First, we introduce a novel spherical indentation technique enabling local mapping of inelastic backstrain via loading-unloading-reloading experiments, allowing for the mapping of underlying geometrically necessary dislocation networks. Second, we demonstrate how artificial neural networks and ensemble methods can accelerate flow curve characterization from standard Berkovich nanoindentation. Together, these advances demonstrate how data-driven and experimental innovations can significantly expand the information accessible from nanoindentation measurements.

15 min. break

Topical Talk MM 32.4 Thu 11:45 SCH/A251

Additive Manufacturing and Nanomechancics - where is the Link? — •Ralph Spolenak — Laboratory for Nanometallurgy, Department of Materials, ETH Zurich, Switzerland

While size effects in mechanical properties of metals created by whisker growth and thin films had been known since the 1950s, the introduction of micro- and nanoscale subtractive manufacturing (also known as focused ion beam milling) became a game changer as it allowed to study size effects practically independent of the material and its microstructure. The contribution will focus on additive micro- and nanoscale manufacturing with voxel sizes down to 30 nm and how both the manufacturing process (with regards to microstructure control and chemistry) as well as the dimension influences mechanical properties. Comparison will be made to sputter deposited materials including self-organized microstructure, such as nanoporosity by dealloying or local pore formation by Kirkendall voiding, as well as nanostructured reactive multilayers. Finally, the potential combination of subtractive and additive processes will be discussed.

MM 32.5 Thu 12:15 SCH/A251

Mechanical Behaviour of Nafion Membranes — •Mateja Jovanović[1,2,3], Matthias Baldofski[2], Nicolas Bernhard[2], Marcin Rybicki[2,4], Miljan Dašić[3], and Igor Stanković[3,5] — [1]Institute of Technical Sciences of the SASA, K. Mihailova 35/IV, 11000 Belgrade, Serbia — [2]Freudenberg Technology Innovation SE&Co. KG, Hoehnerweg 2-4, 69469 Weinheim, Germany — [3]Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Zemun, Serbia — [4]Freudenberg e-Power Systems GmbH, Bayerwaldstrasse 3, 81737 München, Germany — [5]Departamento de Ingeneria Mecanica, Universidad Tecnica Federico Santa Maria, Av. Espana 1680, Valparaiso, Chile

Proton Exchange Membrane Fuel Cells (PEMFCs) utilise polymer membranes like Nafion, valued for their proton conductivity and mechanical integrity. In this work, we examine the stress-strain response of Nafion membranes, focusing on how hydration, crystallinity, and temperature modulate mechanical behavior, using molecular dynamics simulations. Here, we demonstrate that membrane hydration level and structural ordering fundamentally influence mechanical properties under applied stress. Water distribution and polymer chain dynamics are closely connected to the stress-strain response, suggesting that structural organization at the nanoscale is crucial in governing overall mechanical performance across different conditions. By integrating clustering algorithms, structural descriptors, and stress-strain analyses, this study provides a comprehensive view of how membrane architecture and environmental factors govern mechanical performance.

MM 32.6 Thu 12:30 SCH/A251

The Fracture toughness of thin films — •Mathias Göken[1], Benoit Merle[2], and Jun Lou[3] — [1]Department of Materials Science & Engineering I, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Materials Science and Engineering, Universität Kassel, Germany — [3]Department of Materials Science and NanoEngineering, Rice University, Houston, Texas, USA

The mechanical properties of thin films play a pivotal role for applications either as freestanding films or as coatings. So far, the understanding of the fracture toughness of very thin films and especially of their thickness dependence is limited. Bulge testing is a very reliable technique for characterizing the mechanical properties of thin films, where a freestanding film is subjected to a controlled pressure from underneath and the deflection of the film is recorded. Bulge tests

have shown that the fracture toughness of ductile and soft Au drops down to extremely low values of only 2 MPam1/2 if the film thickness is reduced to 100 nm. On the other hand, single layer graphene has shown a fracture toughness of around 4 MPam1/2. In this paper the thickness dependence of the fracture toughness is discussed based on an old and simple basic fracture mechanics concept derived by Bluhm and Knott in the 1960th. It is shown, that based on this model it is easy to predict the fracture toughness of thin films and their thickness dependence. The results agree surprisingly well with the experimental data on graphene and Au thin films.

MM 33: Invited Talk: Stefan Nolte

Time: Thursday 15:00–15:30 Location: SCH/A251

Invited Talk MM 33.1 Thu 15:00 SCH/A251

LPBF with Ultrashort Laser Pulses - Additive Manufacturing Beyond Current Limits — •Stefan Nolte[1,2], Hagen P. Kohl[1], Lisa Matthäus[1], Tobias Ullsperger[1], Dongmei Liu[1], and Stephanie Lippmann[1] — [1]Friedrich Schiller University Jena, Institute of Applied Physics, Jena, Germany — [2]Fraunhofer Institute for Applied Optics and Precision Engineering IOF, Jena, Germany

Ultrashort-pulse lasers introduce additional degrees of freedom to powder bed fusion through the choice of pulse duration, repetition rate, and pulse energy. The short interaction times enable extremely high local temperatures and highly confined melt pools, with heat accumulation tunable through the pulse repetition rate. This allows precise control over melt dynamics, thermal gradients and cooling rates, which remain largely fixed in continuous-wave systems. A key outcome is accelerated solidification and pronounced grain refinement. The confined melt geometry and reduced heat accumulation suppress segregation, cracking, and vaporization-driven compositional shifts, enabling alloys and microstructures that are difficult to achieve with conventional laser melting. These processing characteristics contribute to improved mechanical uniformity, enhanced phase distribution, and greater design flexibility in alloy development. We will introduce the governing mechanisms of ultrashort-pulse interaction in metal additive manufacturing and highlight their impact through material case studies. Demonstrated benefits include grain refinement in Al-Si, dense and crack-free structures in refractory metals, and reduced vaporization with improved composition control in hypereutectic Al-Li.

MM 34: Hydrogen in Materials I

Time: Thursday 15:45–17:30 Location: SCH/A215

MM 34.1 Thu 15:45 SCH/A215

In-situ mechanical characterization of 316Ti hollow specimens in hydrogen environments - from ambient down to 20 K — •Elvina Gaisina, Simeon Eckerle, Camelia Schulz, Zahra Abbasi, Astrid Pundt, and Klaus-Peter Weiss — Karlsruhe Institute of Technology, Germany

The Application of Liquid Hydrogen (AppLHy) project explores the feasibility of a hybrid pipeline system transporting liquid hydrogen while simultaneously using the cold enables superconducting electrical energy transmission. Developing such a system requires a reliable understanding of material behavior under cryogenic conditions and exposure to hydrogen environments. However, conventional test setups that simulate these conditions are often large, complex, and require extensive safety measures to prevent hydrogen leakage. To provide a safer and more efficient testing method, this study presents an in-situ mechanical testing approach using hollow cylindrical specimens pressurized with gas. Austenitic stainless steel 316Ti, a widely applied cryogenic compatible material, was selected for testing. The hollow specimens were filled with hydrogen or helium at pressures up to 200 bar and subjected to tensile loading at temperatures ranging from ambient down to 20 K. The results show that some hydrogen-induced effects become noticeable primarily after substantial plastic deformation. Significant changes in mechanical properties and fracture behavior are observed only at 200 K.

MM 34.2 Thu 16:00 SCH/A215

In situ Micromechanical Investigation of Hydrogen Embrittlement Mechanisms in Fe3%Si — •Maral Sarebanzadeh[1], Svetlana Korneychuk[1,2], Rolf Rolli[1], Hans-Christian Schneider[1], Astrid Punt[1], Xufei Fang[1], and Christoph kirchlechner[1] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Insitute of Nanotechnology, Karlsruhe Institute Technology, Karlsruhe, Germany

Hydrogen embrittlement (HE) remains a critical limitation for the reliable use of hydrogen in structural applications. Among the proposed micromechanisms, hydrogen-enhanced localized plasticity (HELP) is widely discussed, suggesting that hydrogen facilitates dislocation motion and localizes deformation. However, its microstructural manifestation remains insufficiently understood and rarely observed directly. To address this, we investigate HE in Fe3%Si using in-situ micropillar compression combined with tritium charging, leveraging the advantage of probing a few dislocations in a well-defined geometry. Micropillar tests conducted before and after charging with a protium/tritium gas mixture show a strong increase in yield strength, indicating pronounced dislocation blocking rather than enhanced glide. We demonstrate that dislocations can lose mobility, with the activating stress increasing by a factor of 2-3. Transmission electron microscopy (TEM) and electron energy loss spectroscopy (EELS) investigations are being performed to identify hydrogen-containing features around dislocations and to clarify how hydrogen governs dislocation mobility in bcc materials such as Fe3%Si.

MM 34.3 Thu 16:15 SCH/A215

Theoretical study of temperature dependencies in HELP- and HEDE-based damage models on the fatigue behavior of ferritic steel by hydrogen — Alexandra Stark[1,2], Petra Sonnweber-Ribic[1], and •Christian Elsässer[2,3] — [1]Robert Bosch GmbH, CR, 71272 Renningen — [2]Fraunhofer IWM, 79108 Freiburg — [3]University of Freiburg, FMF, 79104 Freiburg

In this theoretical study, the influence of temperature dependencies in hydrogen embrittlement (HE) models on the fatigue damage of ferritic steel is investigated by using a coupled hydrogen-diffusion and crystal-plasticity finite-element simulation framework. We focus on the characteristic "bell-shaped" dependence of HE on temperature and examine its effects by means of HE models based on Hydrogen Enhanced Local Plasticity (HELP) and Hydrogen Enhanced Decohesion (HEDE) mechanisms. Hydrogen-induced fatigue damage is monitored by a fatigue indicator parameter (FIP): maximized damage occurs within a narrow temperature range consistent with experimental results reported in literature. Our results arise from an interplay of plastic strain localization and hydrogen trapping, combined with a sufficiently efficient supply of hydrogen. The findings of this study highlight how the interplay of hydrogen diffusivity, trap filling kinetics, and available diffusible hydrogen plays a critical role for the temperature dependence of HE. In addition, the influence of varying trap binding energies is explored, which has a substantial effect on both temperature behavior and induced fatigue damage.

MM 34.4 Thu 16:30 SCH/A215

Atomistically Informed Grain-Boundary Thermodynamics for Phase-Field Modelling of Hydrogen-Driven Microstructural Evolution in Aluminium — •Bharathi Ganesh Ganesan Sekar[1], Ali Tehranchi[1], Tilmann Hickel[1], and Nils Warnken[2] — [1]Bundesanstalt für Materialforschung und -prüfung, Berlin, Germany — [2]University of Birmingham, Birmingham, United Kingdom

Hydrogen-driven microstructural evolution in polycrystalline aluminium (Al) is strongly influenced by grain-boundary (GB) structure and hydrogen (H) segregation. We aim to develop an atomistically informed phase-field framework to describe these effects, with relevance to hydride formation. Molecular-statics simulations were performed for representative FCC Al symmetric-tilt boundaries $\Sigma5(310)$, $\Sigma5(210)$, and $\Sigma3(111)$ to assess whether H segregation can initiate hydride formation. Instead, H induces defect-mediated structural transitions and shows distinct relaxation pathways during ingress and discharge. At high H content, the GB cleaves and free surfaces form. To generalise these insights, a library of 250 microstates was generated for each GB plane normal within the $\Sigma5$ family by sampling rigid-body translations and boundary-plane atomic fractions. This enables construction of GB energies as a function of plane normal, with temperature dependence introduced through Boltzmann weighting. H effects are included by evaluating segregation energies for the minimum-energy microstate of each plane normal, yielding H-chemical-potential-dependent GB energies. These results provide essential GB energetics for phase-field modelling of H-driven microstructural evolution in Al.

MM 34.5 Thu 16:45 SCH/A215

Understanding of hydrogenation induced planar defects in a proton-based battery material — •Yujun Zhao, Stefan Zaefferer, Yug Joshi, and Dierk Raabe — Max-Planck-Institut für Nachhaltige Materialien, Max-Planck-Straße 1, 40237 Düsseldorf, Deutschland

Research on nickel-metal hydride batteries provides valuable insights for advancing hydrogen storage systems. However, the battery cycle stability is limited by crystalline defects generated during hydrogenation. Therefore, an in-depth understanding of these defects is critical for improving the long-term cyclic performance of electrode materials. In this work, electrochemically charged hydrogen induces the formation of planar defects and dislocation bands in LaNi5 intermetallic compound. The correlations among crystallographic orientations, defect characteristics, and local hydrogen concentration were explored by multiscale characterization techniques, including electron backscattered diffraction (EBSD), electron channeling contrast imaging (ECCI), transmission electron microscopy (TEM), and atom probe tomography (APT). In particular, the atom probe evaporation behavior of LaNi5 along different orientations are revealed, clarifying the local magnification effect and the loss of spatial resolution. The influences of the planar defects on the evaporation behaviors of metallic elements and hydrogen atoms are also discussed.

MM 34.6 Thu 17:00 SCH/A215

Hydrogen Solution Energies at Microstructural Defects in Ferritic Steels — •Onur Can Şen[1,2,3], Santiago Benito[2], Sebastian Weber[2], and Rebecca Janisch[3] — [1]Max Planck Institute for Sustainable Materials, Germany — [2]Institute for Materials, Chair of Materials Technology, Ruhr-University Bochum, Germany — [3]ICAMS, Ruhr-University Bochum, Germany

Hydrogen is essential for sustainable industries but can also cause severe degradation through hydrogen embrittlement (HE). Trapping H at microstructural defects helps mitigate HE, though its efficiency depends on how each defect affects H solution energy.

This study combines experiments and DFT calculations to examine how microstructural defects in ferritic steels influence H trapping, focusing on different grain boundary (GB) types with and without segregants.

DFT was used to calculate solution energies at several special GBs in ferrite, both clean and with alloying elements (Cr, Cu, Ti) or vacancies, and these energies were linked to structural and electronic GB parameters.

Ferritic model alloys with varied compositions were produced and characterised. By optimizing processing, we increased the fraction of special GBs in the microstructure (Şen et al., JMRT (2025)).

The calculated solution energies serve as input for Oriani's model to predict thermal desorption spectra of these alloys.

Overall, this work shows how combining simulations and experiments clarifies the role of microstructural heterogeneities in HE.

MM 34.7 Thu 17:15 SCH/A215

Investigation of phase stability and defects in FeTi for H2 storage application — •Shankha Nag[1], Ali Tehranchi[1], Ruben Bueno Villoro[2], Christian Liebscher[2], Yuanyuan Shang[3], Claudio Pistidda[3], and Tilmann Hickel[1] — [1]Bundesanstalt für Materialforschung und -Prüfung, Berlin, Germany — [2]Fakultät für Physik und Astronomie, Ruhr Universität Bochum, Bochum, Germany — [3]Helmholtz-Zentrum Hereon, Geesthacht, Germany

Safe, durable, and efficient storage remains a central hurdle in hydrogen economy, where metal hydrides offer a promising route, particularly for stationary applications. Among these materials, FeTi stands out as a cost-effective system capable of reversible hydrogen uptake and release under near-ambient conditions. As part of BMBF-funded collaborative project GreenH2Metals, we performed atomistic simulations aimed at elucidating experimentally observed microstructural transformations such as formation of secondary phases and hydrides. We analyzed the thermodynamic stability of competing phases using ab initio calculations and examined chemical segregation as well as heterogeneous precipitation at dislocations and planar defects. Defect phase diagrams, along with the roles of vacancies and antisite defects in bulk diffusion, are explored in detail. The impact of various tramp elements on these processes is assessed through high-throughput calculations enabled by workflow frameworks such as pyiron. Together, these computational insights support a data-driven alloy design strategy for optimizing FeTi-based materials for sustainable hydrogen storage.

MM 35: Additive Manufacturing / Transport in Materials III

Time: Thursday 15:45–17:30 Location: SCH/A216

MM 35.1 Thu 15:45 SCH/A216

Tailoring Microstructure and Mechanical Properties of LPBF Ti-5553 Alloy by STA Heat Treatment — •Yang Lei[1,2], Parthiban Ramasamy[2], and Jürgen Eckert[1,2] — [1]Department of Materials Science, Chair of Materials Physics, Montanuniversität Leoben, Jahnstraße 12, A-8700 Leoben, Austria — [2]Erich Schmid Institute of Materials Science, Austrian Academy of Sciences, Jahnstraße 12, A-8700 Leoben, Austria

Ti-5553 is a metastable β titanium alloy widely used in aerospace gears due to its exceptional strength, toughness, and hardenability. However, Laser Powder Bed Fusion (LPBF) fabrication introduces significant limitations, particularly strong anisotropy and persistent columnar grains.

Solution Treatment and Aging (STA) offers a critical pathway to tailor these properties. This study investigates the microstructural evolution during STA, revealing a competition between nucleation driving force and diffusion kinetics that dictates the initial α-phase morphology. Notably, the columnar β grain size was restricted after heat treatment due to Zener pinning effect exerted by α precipitates, which impedes boundary migration and suppresses recrystallization.

Consequently, the specific microstructural features formed during solution treatment significantly influence subsequent aging behavior. Since β-grain refinement is inhibited, the enhancement in tensile strength is attributed primarily to Orowan strengthening via dispersed precipitates rather than Hall-Petch strengthening.

MM 35.2 Thu 16:00 SCH/A216

Electron Microscopy Investigation of AM316L before and after Heat Treatment: Implications for Hydrogen Diffusion — •Gabriele Palazzo[1,2,3], Kai Stefan Lagemann[1], Svetlana Korneychuk[1,2,3], Stefan Wagner[1], Christian Kübel[2,3], and Astrid Pundt[1] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Karlsruhe Nano Micro Facility, Karlsruhe, Germany

As hydrogen technologies evolve, understanding local hydrogen-metal interactions in structural alloys becomes critical. High-pressure hydrogen storage requires materials resistant to hydrogen embrittlement (HE). Austenitic stainless steels are promising, and selective laser melting (SLM) enables attractive properties but can reduce resistance to hydrogen environmental embrittlement (HEE). We investigate additively manufactured 316L (AM316L) steel and its interaction with dissolved hydrogen, focusing on microstructure evolution under directed heat treatments. SEM and (S)TEM with STEM-EELS/EDX map elemental distributions, while EBSD and STEM-ACOM resolve grain structure and sub-grain dislocation cells (SDC). Comparing as-built and heat-treated states by ex-situ TEM and hydrogen diffusion measurements, we show that heat treatment alters the microstructure, reduces hydrogen diffusivity, and lowers HEE susceptibility [1]. [1] Kai Stefan Lagemann, Gabriele Palazzo, Tim Lucas Haag, Svetlana Korneychuk, Stefan Wagner, Christian Kübel, and Astrid Pundt. Manuscript submitted. 2026.

MM 35.3 Thu 16:15 SCH/A216

Diffusion processes in magnetron sputtered copper-gold thin films: layer design, argon pressure tuning and Kirkendall effect — •Oliver Wipf and Ralph Spolenak — Departement of Materials, ETH Zürich, Vladimir-Prelog-Weg 1-5/10, 8093 Zürich, Switzerland

Controlled Kirkendall voiding is a promising diffusion process to fabricate hollow nano- and micro-structures. This work extends the understanding and use of the Kirkendall effect as a route to fabricate voids in magnetron sputtered copper-gold thin films, a process with a high degree of control over the deposited thin films and a pathway to scalable, novel applications of diffusion self-organized thin film technology.

To study the diffusion in the thin films, double and triple layered samples were fabricated using low and high argon gas pressures during the deposition. Annealing of the samples resulted in large voids located at the wafer to film interface and in the center of the film, depending on the layer structure. Using a comprehensive diffusion study, we demonstrate that diffusion in copper-gold thin film diffusion couples is dominated by vacancies moving, which leads to the growth of Kirkendall voids.

MM 35.4 Thu 16:30 SCH/A216

Visualizing lithium dynamics in battery electrodes by operando optical microscopy — •Monica Mead[1], Shihao Wei[1], Vidula Ambure[1], Nadine Kerner[1], Roham Talei[1], Yug Joshi[2], and Guido Schmitz[1] — [1]Max Planck-Institut für nachhaltige Materialien GmbH, Max-Planck-Straße 1, 40237 Düsseldorf — [2]Universität Stuttgart, Heisenbergstraße 3, 70569 Stuttgart

Typically, chemical diffusion coefficients of Li-ions in battery electrodes are measured by purely electrochemical methods such as potentiostatic or galvanostatic intermittent titration technique (GITT/PITT), cyclic voltammetry (CV) or electrochemical impedance spectroscopy (EIS). Surprisingly, the correspondingly

determined diffusion coefficients vary within up to ten orders of magnitude. This cannot be explained solely by the influence of concentration dependence and microstructure. To clarify the origin and thereby understand which additional factors influence the ion transport, alternative methods have to be developed and applied. Therefore, we apply a method based on optical microscopy and the optical response upon Li intercalation in different Li-ion battery electrodes, such as lithium manganese oxide, lithium titanate, vanadium oxide and silicon. With this method, the transport along several hundreds of micrometres can be measured, which allows differentiation between different transport mechanisms (diffusion/transport across a kinetic barrier). We find that abovementioned electrochemical methods tend to underestimate the diffusion coefficient. We discuss the origin with respect to the transport mechanism.

MM 35.5 Thu 16:45 SCH/A216

Kinetic analysis of lithium transport in silicon anode using operando optical microscopy — •Shihao Wei[1], Monica Mead[1], Yug Joshi[2], and Guido Schmitz[1] — [1]Heisenbergstraße 3, 70569, Stuttgart, Germany — [2]Max-Planck-Straße 1, 40237, Düsseldorf, Germany

Understanding lithium diffusion and phase transformation in silicon(Si) anodes is essential for the advancement of high-capacity lithium(Li)-ion batteries. In this work, Li transport behavior and phase evolution are investigated using an in-situ optical method, which enables direct visualization of phase movement and measure Li migration across phase boundaries, advantages not offered by conventional techniques, such as EIS, SIMS, and NMR. First, it is observed that the lithiation process on a semi-infinite plane is predominantly governed by diffusion-controlled parabolic growth, with minimal evidence of interface-controlled linear growth. The temperature dependence of transport is explored, quantified with an Arrhenius-like model, revealing the activation energy of diffusion and interfacial reaction. In contrast, delithiation exhibits markedly sluggish kinetics and behaves fundamentally differently. To investigate this behavior, smaller circular geometries with limited diffusion depth creating a 2D transport scenario are examined. In these confined structures, lithiation is demonstrated by a Deal-Grove-type model. Remarkably, during delithiation, instead of a distinct moving interface, the lithiated phase gradually fades as lithium ions leave. Such a difference implies that lithiation and delithiation follow distinct reaction pathways.

MM 35.6 Thu 17:00 SCH/A216

W diffusion in Mo-Ta alloys: temperature dependence and vacancy energetics — •Aditya Burla[1], Xiang Xu[2], Felix Kipke[1], Hartmut Bracht[1], Xi Zhang[2], Blazej Grabowski[2], Gerhard Wilde[1], and Sergiy V Divinski[1] — [1]Institut für Materialphysik, Universität Münster, 48149 Münster, Germany — [2]Institut für Materialwissenschaft, Universität Stuttgart, 70569 Stuttgart, Germany

Refractory metals and their alloys have gained renewed attention with the emergence of high-entropy alloy concepts, driven by their exceptional properties at elevated temperatures. However, despite their technological significance, diffusion data for refractory binary systems remain sparse, limiting predictive understanding of defect-mediated transport at high temperatures. This study addresses this gap by investigating tungsten diffusion in the binary Mo-Ta system. Diffusion profiles were measured using secondary ion mass spectrometry after annealing in the temperature range of 1373K to 2273K. A key focus is on correlating the diffusion behavior with the vacancy formation energies. Complementary computational analysis provides atomistic insights, revealing composition-dependent variations in vacancy energetics within the Mo-Ta system. Its influence on W diffusivity and activation energies is discussed. This combined approach provides a comprehensive framework for understanding W diffusion and vacancy-controlled transport in Mo-Ta alloys, offering valuable guidance for the design of advanced refractory materials.

MM 35.7 Thu 17:15 SCH/A216

Hydrogen Diffusion in ß-MoO_3 Thin Films Governed by Structural Changes — •Tim K. Hecker, Martin Becker, and Peter J. Klar — Institute of Experimental Physics I and Center for Materials Research, Justus Liebig University Giessen, Giessen, Germany

Hydrogen incorporation strongly alters the electronic, optical and structural properties of transition-metal oxides. In MoO_3, hydrogen intercalation forms H_xMoO_3 bronzes that exhibit reversible color changes, lattice distortions and notably higher hydrogen diffusion coefficients. Although these effects are central to electrochromic, catalytic, sensing and energy storage applications, the mechanisms of hydrogen transport remain poorly understood, especially in the metastable ß-phase. To address this, we performed electrochemical hydrogen insertion into ß-MoO_3 thin films covered by a PMMA layer, only allowing incorporation in a small, well-defined uncovered stripe. Hydrogen only enters through this gap and then diffuses laterally beneath the PMMA in a semi-infinite space. Using the electrochromic response of MoO_3 in combination with the Beer-Lambert law, we monitored the hydrogen concentration in-situ. These diffusion profiles were then analyzed with a deep-learning algorithm to extract concentration dependent diffusion coefficients. We identify two distinct increases in the diffusion coefficient as hydrogen concentration rises. Complementary Raman measurements during intercalation and deintercalation link these changes to partial structural transformations, each increasing the hydrogen diffusion coefficient by nearly one order of magnitude.

MM 36: Topical Session: Advanced Nanomechanics – Accelerating Materials Physics from the Bottom II

Time: Thursday 15:45–17:15 Location: SCH/A251

Topical Talk MM 36.1 Thu 15:45 SCH/A251

High-temperature micropillar compression for understanding dislocation-precipitates interactions in Ni-Based superalloys — •Subin Lee[1], Sangwon Lee[2], Pyuck-Pa Choi[2], and Christoph Kirchlechner[1] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Department of Materials Science and Engineering, Korea Advanced Institute of Science and Technology (KAIST), Daejeon, South Korea

The mechanical role of plate-like μ phases, topologically close-packed (TCP) precipitates, in Ni-based single-crystal superalloys was investigated using bulk and in situ SEM micropillar compression, supported by electron microscopy and APT. The μ phase showed strong temperature-dependent behavior: it remained rigid at room temperature, enforcing single-slip deformation, but became more compliant at 500 °C through bending and non-basal shearing.

Although acting as local obstacles to slip, μ phases consistently lowered the CRSS of micropillars. This softening resulted from deformation within the μ phase and from microstructural changes in the surrounding γ/γ' matrix. APT revealed Ta enrichment at the μ/γ' interface, enhancing γ' strengthening, while elastic mismatch shifted slip traces away from the interface by tens of nanometers.

Overall, these results highlight the dual role of μ phases. This integrated understanding of μ-phase deformation, interfacial chemistry, and matrix softening provides a fundamental mechanistic understanding for how TCP precipitation shapes the high-temperature mechanical behavior of Ni-based superalloys.

MM 36.2 Thu 16:15 SCH/A251

Nanomechanics of Silicon: Linking Phase Transitions to High-Temperature Plasticity — •Verena Maier-Kiener and Gerald Schaffar — Montanuniversität Leoben, Department materials Science, Leoben, Austria

This presentation focuses on phase transformations in silicon revealed through high-resolution nanoindentation techniques and their interplay with high-temperature deformation behavior. Using a novel unloading contact pressure approach with continuous stiffness measurement (CSM), pressure-induced phase transitions during indentation are investigated with improved precision. The method enables direct calculation of mean contact pressure during unloading and reveals the influence of load-holding segments on transformation onset, aligning well with high-pressure literature data, and was confirmed by Raman spectroscopy. To contextualize these findings, complementary high-temperature nanoindentation studies are discussed. In monocrystalline (100) silicon, a transition from phase transformation to dislocation-controlled plasticity occurs between 300 °C and 400 °C, with further changes above 800 °C. Additionally, spherical nanoindentation on a 1.2μm silicon film at 500 °C and 700 °C extracts stress-strain behavior, confirming thermally activated dislocation glide. Together, these results provide a comprehensive view of silicon's mechanical response, bridging nanoscale phase transformation analysis with bulk high-temperature deformation mechanisms.

MM 36.3 Thu 16:30 SCH/A251

In situ TEM nanomechanics of neutron-irradiated nanocrystalline carbides and the role of amorphous shells in local mechanical response — •Elchin Huseynov — Institute of Radiation Problems of Ministry of Science and Education, 9 B.Vahabzade, Baku AZ 1143, Azerbaijan

Predicting the mechanical reliability of neutron-exposed ceramics remains challenging because classical micromechanical tests average over complex, irradiation-induced defect structures at the nanoscale. In particular, nanocrystalline carbides develop near-surface amorphous layers and defect-rich shells whose role in governing deformation and failure is still poorly quantified. This work introduces an in situ TEM-based nanomechanical workflow for neutron-irradiated nanocrystalline 3C-SiC. Reactor-irradiated nanoparticles at graded fluences serve as a model for plasma-facing and core structural ceramics. Ex situ HRTEM/SAED reveals pronounced agglomeration and a continuous amorphous shell up to 5 nm thick encasing a crystalline core. Building on this microstructural baseline, in situ TEM traction and gentle indentation experiments on nanoparticle films and micro-sized volumes are used to track shell stability and defect evolution under load via ring broadening, lattice-fringe de-coherence and defect coalescence at the shell/core interface. The results reveal a critical amorphous-shell thickness above which deformation concentrates in the disordered layer and promotes early crack initiation, whereas thinner or discontinuous shells favour more homogeneous load transfer across the crystalline core.

MM 36.4 Thu 16:45 SCH/A251

Mechanical Properties of Irradiated Zircaloy Cladding and Their Impact on Structural Integrity During Dry Interim Storage — •Tzu Yen Lin[1], Michel Herm[1], Volker Metz[1], Maria Vrellou[2], and Christoph Kirchlechner[2] — [1]Karlsruhe Institute of Technology, Institute for Nuclear Waste Disposal, P. O. Box 3640, 76021 Karlsruhe, Germany — [2]Karlsruhe Institute of Technology, Institute for Applied Materials, P. O. Box 3640, 76021 Karlsruhe, Germany

In Germany, spent nuclear fuel is planned for disposal in a deep geological repository after 2050. The SNF assemblies are stored in dual-purpose casks, while delays in repository commissioning may extend storage beyond licensed periods. Evaluating the safety of Zircaloy-4 cladding during extended dry storage requires assessing the effects of irradiation damage, hydride formation, and microstructural evolution. This work aims to establish a reliable micromechanical testing methodology for irradiated Zircaloy-4. As a precursor to irradiated samples, Electron Backscatter Diffraction (EBSD) and nanoindentation were performed on non-irradiated cladding in hydrogenated and non-hydrogenated states. EBSD revealed variations in grain size, texture, anisotropy, and dislocation density from manufacturing processes, with further increases from hydrides. Nanoindentation showed higher hardness and reduced modulus in hydride regions compared with the α-Zr matrix. Occasional pop-ins in load-displacement curves indicate dislocations or microstructural discontinuities, consistent with misorientation patterns observed in EBSD.

MM 36.5 Thu 17:00 SCH/A251

Experimental evidence and first-principles verification of deformation of basal twist grain boundaries in Ti — •Biaobiao Yang[1,2], Samuel Hémery[3], Wei Shao[1,2], Victoria Tucker[1,4], Michael S. Titus[1,4], Miguel A. Monclús[1], and Javier LLorca[1,2] — [1]IMDEA Materials Institute, C/Eric Kandel 2, Getafe, 28906 - Madrid, Spain — [2]Department of Materials Science, Polytechnic University of Madrid / Universidad Politécnica de Madrid, E.T.S. de Ingenieros de Caminos, 28040 - Madrid, Spain — [3]Institut Pprime, ISAE-ENSMA, Université de Poitiers, CNRS UPR 3346, Téléport 2, 1 avenue Clément Ader, BP 40109, Futuroscope-Chasseneuil Cedex, 86961, France — [4]School of Materials Engineering, Purdue University, 701 West Stadium Ave., West Lafayette, IN 47907, USA

Recent studies show that Basal Twist Grain Boundaries (BTGBs) are important fatigue-crack nucleation sites in Ti alloys. Micropillar compression combined with high-resolution microscopy revealed extremely easy interfacial shear: one basal grain slides over the other at very low critical resolved shear stresses (45-205 MPa), far below those required for common <a> basal slip. To explain this behavior, first-principles calculations were used to determine the grain boundary energies of BTGBs with different twist angles. The results show that variations in twist angle or in-plane translation produce only negligible changes in grain boundary energy, indicating intrinsically low shear resistance. Together, these experimental and computational findings clarify why BTGBs serve as potent crack-nucleation sites in Ti alloys.

MM 37: Development of Calculation Methods I

Time: Thursday 15:45–17:00 Location: SCH/A315

MM 37.1 Thu 15:45 SCH/A315

The two-particle Green's function in the particle-particle channel: A survey of approximations — •Caja Annweiler[1], Lucia Reining[2], and Claudia Draxl[1] — [1]Humboldt Universität Berlin, Berlin, Germany — [2]École Polytechnique, Palaiseau, France

While in general setting up and solving the Bethe-Salpeter equation (BSE) is out of reach for realistic systems, it provides an ideal starting point for constructing approximations. In the particle-hole channel, this has lead to established approaches such as the GW-level approximation to capture excitonic effects. This framework can be extended to the BSE in the particle-particle channel (pp-BSE), obtained by choosing a different time-ordering in the two-particle Green's function. The result is an equation describing the propagation of two particles (either electrons or holes). While formally similar to the ph-BSE, it is a promising alternative for the calculation of the exchange-correlation energy and yields important information for topics such as pair correlations in superconductors. Despite growing interest in the pp-BSE, systematic investigations of approximations remain scarce.

In the present work we consider a variety of approximations to the pp-BSE. For this purpose, exactly solvable model systems of interacting electrons provide valuable insights into the minimal ingredients needed to capture the key physics. We present approximations from many-body perturbation theory (HF, GW, etc.) at the level of the self-energy Σ and interaction vertex Ξ on small Hubbard models, with the aim of advancing our understanding of approximations in the pp-channel.

MM 37.2 Thu 16:00 SCH/A315

Reliable Super-Resolution for Real-Time Electronic Structure Theory — •Alexander Gorfer, Karsten Reuter, and Matthias Kick — Fritz-Haber-Institut der MPG, Berlin

Calculating excited state spectra of large systems is often prohibitively expensive with standard frequency-domain methods such as the Casida equations, the Bethe-Salpeter Equation (BSE), or Equation-of-Motion Coupled Cluster (EOM-CC). Real-time methods provide an alternative, as all modes are excited simultaneously. However, long simulation times are required to resolve narrow spectral features with traditional Fourier signal analysis, significantly limiting system size. Super-resolution methods such as Compressed Sensing promise high-resolution spectra from much shorter signals but assume the spectrum to be sparse, an assumption which breaks down in larger systems where sharp features are embedded in a quasi-continuum of smaller nearby peaks. To overcome this, we combine newly designed highly noise-tolerant super-resolution techniques with physically motivated filtering. Using approximate frequency information, we identify the brightest transitions and extract only these important modes from the time propagation. By doing so, we effectively precondition the problem for super-resolution, reducing the number of required time steps for signal reconstruction to a minimum. We demonstrate our approach on systems containing several hundred heavy atoms, achieving up to 20-fold speedups while maintaining spectral accuracy even for signals dominated by large continua.

MM 37.3 Thu 16:15 SCH/A315

Electron thermalization in TDDFT and Ehrenfest molecular dynamics — •Tobias Zier, Uday Panta, and David A. Strubbe — University of California, Merced, USA

A non-equilibrium electronic state will in general thermalize toward an equilibrium state due to electron-electron interactions as well as interactions with ions. The description of such processes has remained unclear and controversial in time-dependent density functional theory (TDDFT), given that the occupation numbers remain fixed over time and that adiabatic functionals do not include explicit dissipation. Nevertheless in the literature signs of thermalization to a Fermi-Dirac distribution have been found in effective occupations constructed by projection of the time-dependent wavefunctions onto the ground state. Key issues include whether this process is physical or an artefact, connection to the Eigenstate Thermalization Hypothesis, and the dependence on the density of states, external fields, and xc functionals. To shed light on these phenomena, we study explicit time propagation of graphene after ultrafast laser pulses, with the Octopus real-space code, with and without ionic motion in Ehrenfest molecular dynamics. We study oscillations and the approach to an effective Fermi-Dirac distribution as well as decay of off-diagonal density matrix elements. This work has implications for treatment of statistical mechanics in a TDDFT framework and the nature of time-dependence in xc functionals, as well as for practical calculations of light-matter interactions especially for strong fields as in laser fusion experiments leading to warm dense matter and plasmas

MM 37.4 Thu 16:30 SCH/A315

Bulk plasmons in elemental metals — •Claudia Cardoso[1], Dario Leon[2], and Kristian Berland[2] — [1]S3 Centre, Istituto Nanoscienze, CNR, 41125 Modena, Italy — [2]Department of Mechanical Engineering and Technology Management, Norwegian University of Life Sciences, NO-1432 Ås, Norway

We have developed an effective analytical representation of the main collective excitations of the dielectric response of 26 elemental metals, starting from first principles calculations. Spectral band structures are then constructed , by ex-

tending our earlier model based on multipole-Padé approximants (MPA) [1,2] to incorporate both momentum and frequency dependence (MPA(q)). With this representation, we are able to identify plasmonic quasiparticle dispersions exhibiting complex features, including non-parabolic energy and intensity dispersions, discontinuities due to anisotropy, and overlapping effects that lead to band crossings and anti-crossings. We find good agreement with available experimental data. The results for elemental metals and their effective MPA(q) representation establish a reference point that can guide both fundamental studies and practical applications in plasmonics and spectroscopy.

[1] D. A. Leon, C. Cardoso, T. Chiarotti, D. Varsano, Phys. Rev. B 104, 115157 (2021).

[2] D. A. Leon, A. Ferretti, D. Varsano, E. Molinari, and C. Cardoso, Phys. Rev. B 107, 155130 (2023).

MM 37.5 Thu 16:45 SCH/A315

Probing the influence of core-hole and atomic multiplets in the final states on L2,3 edges for high-throughput studies — •Prathibha Chandrashekhar, Felix Sorgenfrei, Patrik Thunström, Olle Eriksson, and Heike C. Herper — Department of Physics and Astronomy, Uppsala University

Core level spectroscopy like X-ray absorption spectroscopy and the corresponding X-ray magnetic circular dichroic signals are powerful tools to study a wide variety of element specific properties in materials. In this work, we use ab initio density functional theory (as implemented in RSPt[1]) with multiplet ligand field theory to simulate the spectra by constructing and solving the single impurity Anderson model. We simulate the $L_{2,3}$ edges of transition metals in Heusler alloys, aiming to explore the suitability of the method for future high throughput studies, we look at $CoFeMnSi$ and Ni_2MnGa as our initial test cases. These alloys have been extensively studied for their fascinating tunable electronic and magnetic properties which find applications in spin resolved conductance devices, magnetocalorics and spintronics. We test the influence of Slater-Condon parameters on the spectra. We show that the final state effects are crucial in observing the fine structure and the branching ratio between the edges. This work is funded by Horizon Europe MSCA Doctoral Network grant n.101073486, EU-SpecLab, funded by European Union. [1] RSPt, Relativistic Spin Polarized Toolkit (2017).

MM 38: Invited Talk: Manja Krüger

Time: Friday 9:30–10:00 Location: SCH/A251

Invited Talk MM 38.1 Fri 9:30 SCH/A251

Alloy design and deformation behaviour of Mo-based silicide materials — •Manja Krueger — Otto-von-Guericke University Magdeburg

Multi-phase refractory metal-based silicide alloys are attractive candidates for high temperature structural applications. The mechanical behaviour and the oxidation response of this type of materials is significantly affected by the microstructural design, i.e. the chemical composition of the solid solution phase, the volume fraction and homogeneous distribution of the solid solution phase and the silicide phases, the grain size and orientation as well as the concentration of dissolved detrimental impurities and impurity phases. Balancing the ambient and high temperature properties requires to tailor the microstructures, which can be realized by the optimization of the chemical composition using additional alloying elements and the modification of alloying concepts with respect to the manufacturing method. However, processing of refractory metals and alloys is quite challenging due to the ultra-high melting point above 2000°C and their strong tendency to oxidize at intermediate temperatures. This presentation will show the successful processing and tailoring of multi-phase Mo-Si-B alloys by powder metallurgical (PM) routes, directional solidification (DS) processes and laser-based additive manufacturing (AM) techniques. It will be shown that the AM materials are crack-free and the constituents are homogeneously distributed. The microstructure is very fine as can be compared to powder metallurgically processed Mo-Si-B.

MM 39: Hydrogen in Materials II

Time: Friday 10:15–12:45 Location: SCH/A215

MM 39.1 Fri 10:15 SCH/A215

Coulometric and (Magneto-)Optical Methods for Studying Hydrogen Absorption into Metals — •Felix Engelhardt, Karin Leistner, and Markus Gössler — Chemnitz University of Technology, 09107 Chemnitz, Germany

Hydrogen absorption into metals like palladium is a widely studied process with applications in hydrogen sensors, hydrogen storage systems, and recently magneto-ionics[1,2]. A major challenge in this field is to accurately quantify the hydrogen concentration within the metal. Traditionally, complex techniques such as nuclear reaction analysis or neutron scattering are used for this purpose. Alternatively, coulometric and (magneto-)optical methods are possible and offer the advantages of a simpler setup and operation under ambient conditions. We revisit the coulometric quantification of electrochemically absorbed hydrogen in metals and metallic multilayers, as well as the analysis of hydrogen absorption kinetics. Potential- and time-dependent coulometry was performed in a liquid-electrolyte flow cell designed to avoid side reactions. Complementary measurements of (magneto-)optical reflectivity of the metals upon hydrogen absorption were carried out to support findings from electrochemical methods. This presentation highlights common pitfalls in hydrogen absorption analysis and shows that, when these errors are minimized, the coulometry method yields accurate average hydrogen concentrations and reliable kinetic data. These results encourage the use of electrochemical methods in catalysis and hydrogen research. [1]M. Bischoff et al., Adv. Funct. Mater. 2024, 34, 2405323 [2]Huang, M. et al., Nat. Nanotechnol. 2021, 16, 981

MM 39.2 Fri 10:30 SCH/A215

Interfacial kinetics of hydrogen absorption in nanoporous palladium — •Seoyun Sohn[1,2], Nora Brunkhorst[2], Jürgen Markmann[2,1], and Jörg Weissmüller[1,2] — [1]Institute of Materials Physics and Technology, Hamburg University of Technology, 21073 Hamburg, Germany — [2]Institute of Hydrogen Technology, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany

Sorption of hydrogen at metal surfaces is a key process controlling energy-conversion reactions, electrocatalysis, and battery operation. To focus on the interfacial sorption step and minimize bulk-transport contributions, we explore nanoporous (np) Pd as a model system, following the charging/discharging kinetics during electrochemical charging or exposure to H_2 gas at controlled partial pressure. Our observations point towards thermally activated transition across an internal barrier–between adsorbed and absorbed H–as the rate limiting step, and they exhibit anomalous kinetics, where absorption or desorption rates do not monotonously decrease with time. The command critiques the applicability of the Butler-Volmer equation–as a classic approach to the kinetics–and we advertise an alternative kinetic rate law that resolves the problematic issues of the classic approach. We show that the new rate law explains important features of the observations, specifically when admitting for a coherent initiation of the phase change.

MM 39.3 Fri 10:45 SCH/A215

Local hydrogenation of polycrystalline Pd nanodisks studied with in-situ TEM — •Svetlana Korneychuk[1,2], Carl Andersson[3], Stefan Wagner[1], Christoph Langhammer[3], and Astrid Pundt[1] — [1]IAM-WK, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]KNMFi, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]Chalmers University of Technology, Göteborg, Sweden

Hydrogen distribution and concentration in metals is of central importance for many areas of hydrogen technology, such as hydrogen storage, detection, and hydrogen embrittlement. In particular, arrays of Pd nanodisks can serve as optical hydrogen sensors [1] at room temperature owning to fast kinetics of hydrogen absorption and desorption of Pd. Here we demonstrate hydrogen distribution and concentration in polycrystalline Pd nanodisks with the lateral resolution down to 4 nm extending our previous study on the local measurement of hydrogen concentration in Pd nanoparticles with in-situ TEM [2]. By measuring the shift of the Pd bulk plasmon peak with scanning transmission electron microscopy combined with energy electron loss spectroscopy during in-situ hydrogen gas loading and unloading, local detection of the hydrogen concentration is achieved in TEM. The method offers a way to observe hydrogen concentration at different sites: grain boundaries, surface and grains starting from early stages of hydrogenation to compete hydride formation identifying the pathways of hydrogenation of polycrystalline metals. [1] C. Wadell, et al., ACS Nano 2014 8 (12), 11925-11940 [2] S. Korneychuk, et al., Small 2025, 21, 2407092.

MM 39.4 Fri 11:00 SCH/A215

A comparative density functional theory study of hydrogen adsorption in metal organic frameworks — •Ikutaro Hamada — Department of Precision Engineering, Graduate School of Engineering, The University of Osaka , Suita, Osaka 565-0871, Japan

Metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) have attracted considerable attention due to their design and synthesis flexibility, enabling applications in catalysis, gas adsorption, and separation. Among these, hydrogen storage is one of the most extensively studied properties of MOFs. However, their hydrogen storage capacity remains low, particularly at room temperature, which limits industrial and commercial applications. To design MOFs with enhanced hydrogen storage capability, it is essential to understand the microscopic details of hydrogen adsorption and absorption within these frameworks. In this work, we assess the accuracy of dispersion-inclusive exchange-correlation functionals against the coupled cluster method using hydrogen-benzene complexes, and we investigate hydrogen adsorption in UiO-66, UiO-67, and UiO-68 as prototypical MOFs. We will present details of our systematic exploration of the geometric and electronic structures of hydrogen molecules and their stability within UiO-66, UiO-67, and UiO-68.

MM 39.5 Fri 11:15 SCH/A215

Machine Learning Potential Approach to Complex Hydrogen-Surface Interactions: GRACE Applied to the H/Sn/Ru System — •Manuel Enns and Daniel F. Urban — Fraunhofer IWM, Wöhlerstraße 11, 79108 Freiburg, Germany

Understanding hydrogen interactions with contaminated metal surfaces remains a challenging problem in computational materials science, requiring methods that balance accuracy with computational efficiency to capture complex multi-component dynamics. We demonstrate the application of a GRACE machine learning interatomic potential to study hydrogen behavior on tin-contaminated ruthenium surfaces - a system that exemplifies the challenges of modeling reactive adsorbates on multi-element surfaces. Data from density functional theory calculations on hydrogen penetration mechanisms through ruthenium surfaces with varying tin coverages was used to fine-tune the GRACE potential, enabling computationally efficient molecular dynamics (MD) simulations. The resulting MD simulations successfully capture key dynamic processes including hydrogen diffusion and jump mechanisms, tin growth kinetics at a prior hydrogen coverage, and low-energy hydrogen deposition. This case study demonstrates GRACE's capability to handle complex multi-component systems involving reactive species, providing atomic-level insights into how surface contamination affects hydrogen penetration pathways and adsorbate interactions.

15 min. break

MM 39.6 Fri 11:45 SCH/A215

Diffusion of hydrogen in platinum during HER catalysis — Aparna Saksena[1], Bingxin Li[1], Yujun Zhao[1], J. Manoj Prabhakar[1], Mira Todorova[1], Jörg Neugebauer[1], Dierk Raabe[1], Baptiste Gault[1,2], and •Yug Joshi[1] — [1]Max Planck Institute for Sustainable Materials (MPI-SusMat), Max Max-Planck-Straße 1, 40237 Düsseldorf — [2]Univ Rouen Normandie, CNRS, INSA Rouen Normandie, Groupe de Physique des Matériaux, UMR 6634, F-76000 Rouen, France

Platinum remains the most common electrocatalyst used for hydrogen evolution reaction (HER) in acidic conditions. It is generally believed to act as a proton-blocking catalyst with adsorption of reaction intermediates limited to its surface. In this study, we thoroughly examine how Pt interacts with hydrogen and deuterium (H/D) within the bulk by monitoring the mass change of a Pt electrode in real-time during galvanostatic heavy/water splitting, using an electrochemical quartz crystal microbalance. Surprisingly, we observe an irreversible mass increase over time along with changes in the overpotential for both HER and DER. Atom probe tomography of the Pt electrode after DER confirms that D diffuses into the bulk. The results are supported by density functional theory, showing the formation of an interstitial solid solution of H in Pt. These results challenge the conventional belief that Pt-proton interactions are only surface-limited. They suggest a need to revisit catalyst design strategies, which currently focus on surface-adsorbed species and the rate-limiting Volmer step, by also considering the bulk diffusion of H/D within the Pt matrix.

MM 39.7 Fri 12:00 SCH/A215

Hydrogen induced small polarons in iron oxides using occupation-matrix control DFT+U calculations — Ahmed Abdelkawy, •Mira Todorova, and Jörg Neugebauer — Max Planck Institute for Sustainable Materials, Max-Planck-Str.1, 40470 Düsseldorf

Over 6% of global CO_2 emissions come from using carbon-based reducing agents in iron production. Replacing these agents with hydrogen would result in water as the sole byproduct, thereby reducing harmful emissions. To understand H-based reduction of iron oxides, we focus on hydrogen interactions with bulk hematite (Fe_2O_3). Modeling transition metal oxides is challenging because conventional DFT-GGA has self-interaction errors and inadequately treats the Coulomb repulsion in partially filled d-orbitals. Corrections such as DFT+U or exchange-correlation functionals, which incorporate a fraction of the exact exchange, further complicate matters because they generate a multitude of metastable configurations that DFT cannot predict. In this study, we use DFT+U with occupation matrix control to map the energy landscape of the small electron polaron generated by H interstitials. We construct the three-dimensional potential energy surface of H interstitials using the resulting ground-state configurations. This enables us to gain detailed insight into hydrogen kinetics and rate-limiting steps.

MM 39.8 Fri 12:15 SCH/A215

An atomic-scale master-equation model study of the mobility of a dislocation core interacting with interstitial hydrogen in a metal — •Daniel Pfalzgraf[1], Daniel F. Urban[1,2], and Christian Elsässer[1,2] — [1]Fraunhofer IWM, Wöhlerstraße 11, 79108 Freiburg, Germany — [2]Freiburg Materials Research Center (FMF), University of Freiburg, Stefan-Meier-Str. 21, 79104 Freiburg, Germany

We examine the influence of interstitial hydrogen in a metal on the motion of a dislocation by means of a master equation model. This model takes as input atomic-scale information, such as material-specific defect-migration energy barriers and interatomic interaction energies, to produce the drift velocity of a mechanically driven dislocation core segment as a function of the local hydrogen concentration around it. Our approach can take detailed correlation effects into account, for example, that the dislocation core acts as a mobile hydrogen trap, resulting in an inhomogeneous distribution of hydrogen around it. The results can be used to estimate in which ranges of temperature or interaction strength the presence of hydrogen increases or decreases the mobility of the dislocation core, which is of interest in the context of hydrogen embrittlement mechanisms.

MM 39.9 Fri 12:30 SCH/A215

Hydrogen induced strain instability in Aluminum — •Ali Tehranchi[1,2], Bharathi Ganesh Ganesan Sekar[1], and Tilmann Hickel[1,2] — [1]Bundesanstalt für Materialforschung und -prüfung (BAM), D-12489, Berlin, Germany — [2]Max Planck Institute for Sustainable Materials, D-40237 Düsseldorf, Germany

Hydrogen embrittlement is a persistent form of metal degradation that arises from the complex interactions between hydrogen atoms and defects within metallic lattices. Environmental nanoindentation has become a standard experimental technique for probing these interactions, particularly the mechanisms underlying hydrogen-assisted deformation. In this work, we employ comprehensive large-scale molecular statics simulations in aluminum, complemented by ab initio calculations, to investigate the influence of hydrogen on homogeneous dislocation nucleation –the primary mechanism responsible for pop-in events observed under low-radius indenters. Our defect phase diagram analysis shows that, at hydrogen chemical potentials relevant to nanoindentation experiments, vacancy formation is significantly enhanced, leading to a substantial increase in the concentration of vacancy–hydrogen complexes. These complexes produce large local misfit strains, which in turn reduce the critical shear stress required for material instability and the onset of homogeneous dislocation nucleation.

MM 40: Transport in Materials: Diffusion, Charge, or Heat Conduction IV

Time: Friday 10:15–12:30 Location: SCH/A216

MM 40.1 Fri 10:15 SCH/A216

Quantum oscillation and tunable charge density wave of kagome metal ScV6Sn6 — •Changjiang Yi, Xiaolong Feng, Chandra Shekhar, and Claudia Felser — Max Planck Institute for Chemcial Physics of Solids

Compounds with kagome lattice structure are known to exhibit Dirac cones, flat-bands, and van Hove singularities, which host versatile quantum phenomena. We investigate the magnetoelectric transports along with the theoretical calculations of, a nonmagnetic charge-density wave (CDW) metal. ScV6Sn6 exhibits Shubnikov de Haas quantum oscillations, which help to shape the Fermi-surface (FS). The Dirac band is demonstrated along with a nonzero Berry phase. In addition, the compound also shows the anomalous Hall-like behavior up to the CDW phase transition. Under Cr substitution and hydrostatic pressure, the CDW is largely suppressed. The suppression of CDW phase under pressure can be well captured by our first-principles calculations, evidenced by the lift of imaginary phonon bands. The MR and Hall resistance behave differently under Cr substi-

tution and pressure. Our study reveals that the anomalous Hall-like behavior arises from the kagome lattice and persists as long as the lattice is maintained.

MM 40.2 Fri 10:30 SCH/A216

Investigating UAHE in layered delafossite by high-energy electron irradiation. — •Elina Zhakina[1,2], Philippa McGuinness[2], Romain Grasset[3], Seunghyun Khim[2], Marcin Konczykowski[3], and Andrew Mackenzie[2,4] — [1]Department of Applied Physics and Quantum-Phase Electronics Center (QPEC), The University of Tokyo, Bunkyo, Tokyo, Japan — [2]Max Planck Institute for Chemical Physics of Solids — [3]Laboratoire des Solides Irradis, CEA/DRF/IRAMIS, Ecole Polytechnique, CNRS, Institut Polytechnique de Paris, Palaiseau, France — [4]Scottish Universities PhysicsAlliance, School of Physics & Astronomy, University of St. Andrews, St. Andrews, United Kingdom

PdCrO2 belongs to the delafossite family of extremely pure triangular lattice metals. While its Pd layers are metallic, the CrO2 layers are Mott insulating and order antiferromagnetically below 37 K. PdCrO2 [1]. It exhibits an unconventional anomalous Hall effect (UAHE), the origin of which has been the focus of substantial critical discussion. To investigate the origin of UAHE, we conducted a systematic study of the influence of point defects on the Hall effect of PdCrO2, the results of which are reported here. We introduced point-like defects into focused ion beam-sculpted microstructures of PdCrO2 by irradiating them with high-energy electrons. Comparing the results of UAHE as a function of disorder, we demonstrate UAHE behaviour attributed to its extrinsic origin.

MM 40.3 Fri 10:45 SCH/A216

Anisotropic anomalous Hall effect in distorted kagome GdTi3Bi4 — •Avdhesh Kumar Sharma[1], Bo Tai[1], Subhajit Roychowdhury[2], Premakumar Yanda[1], Ulrich Burkhardt[1], Xiaolong Feng[1], Claudia Felser[1], and Chandra Shekhar[1] — [1]Max Plank Institute for chemical physics of solids, Dresden, Germany — [2]Indian institute of science education and research, Bhopal, India

GdTi3Bi4 crystallizes in layered Ti-based kagome nets intertwined with zigzag Gd chains along the a-axis and orders antiferromagnetically below 15 K. Here, we present the temperature and field-dependent electrical transport of GdTi3Bi4 in different directions. The material exhibits anomalous Hall conductivity of 410 Ω-1 cm-1 at 2 K for B || c and it is completely absent for B || a, despite the similar magnetization observed in both orientations. This behavior is quite contradictory, as anomalous Hall effect (AHE) typically scales with the magnetization. Through first principles calculations, it is demonstrated that in the presence of time reversal symmetry broken by the Gd 4f sublattice and spin orbit coupling, the magnetization direction controls the orbital mixing in the Ti t_2g bands, relocating Berry curvature hot spots and producing the observed orientation selective anomalous Hall conductivity (AHC). The results establish GdTi3Bi4 as platform for investigating new avenues of AHE, such as directional AHE, and thus shed new light on the intricate coupling between magnetic and electronic structures, paving the way for exploring novel quantum phenomena.

MM 40.4 Fri 11:00 SCH/A216

Nernst effect in superconducting Weyl semimetal t-PtBi2 — Federico Caglieris[3], •Michele Ceccardi[1], Dmitriy Efremov[1], Grigory Shipunov[1], Iryna Kovalchuk[1,4], Saicharan Aswartham[1], Arthur Veyrat[1,5], Joseph Dufouleur[1,7], Daniele Marré[2,3], Bernd Büchner[1,7], and Christian Hess[1,6,7] — [1]IFW Dresden — [2]University of Genoa — [3]CNR SPIN — [4]Kyiv Academic University — [5]LPS Orsay — [6]Wüppertal University — [7]TU Dresden

Topological materials are among the most promising areas of research in Condensed Matter Physics, offering breakthroughs in dissipationless electronics or in error-free quantum computing. The combination of non-trivial topology and superconductivity opens to novel quantum devices. The discovery of intrinsic materials where such properties appear together represent a frontier in modern condensed matter physics. Trigonal PtBi2 has recently emerged as a possible candidate, being the first example of superconducting type-I Weyl semimetal. However, several aspects of this promising compound still need to be unveiled, concerning its complicated band structure, the actual role of Weyl points in determining its electronic properties and the nature of the superconducting transition. In the work, we experimentally investigated t-PtBi2 single crystals and exfoliated flakes by means of the Nernst effect, which has been demonstrated to be a powerful probe for study the fermiology of complex materials.

15 min. break

MM 40.5 Fri 11:30 SCH/A216

Negative quadratic magnetoresistance generated by spin fluctuations in the metamagnetic bilayer strontium ruthenate Sr3Ru2O7 — •Bastien Michon[1,2], Elisa Auffray[1], Amir Meddas[1], Zhiqiang Mao[3], Freek Massee[1], Pascale Senzier[1], Claude Pasquier[1], and Siham Benhabib[1] — [1]Laboratoire de Physique des Solides - University of Paris-Saclay, Orsay, France — [2]SOLEIL synchrotron, Saint Aubin, France — [3]Eberly College of Science, The Pennsylvania State University, University Park, USA

The bilayer strontium ruthenate Sr3Ru2O7 hosts a metamagnetic transition around 8T and was widely studied for its quantum criticality characterized by its linear-in-temperature resistivity. While most prior work has focused on the magnetic field evolution of the resistivity exponent α, the magnetoresistance (MR) has received less attention. Our low-temperature relative MR measurements on high-purity single crystals reveal two key features absent from the literature:

1. a well-defined negative quadratic MR between 30 and 100K, consistent with enhanced spin fluctuations, and 2. a non-monotonic MR evolution at low temperature within the 1.6-12K range.

The metamagnetic MR peak around 8T reaches nearly 90% at the lowest temperatures, broadens with increasing temperature, shifts to lower fields, and completely disappears between 20-30K. At higher temperature, the MR changes sign and follows a perfect negative H* dependence, with maximum amplitude around 30-40K. These measurements provide the first detailed mapping of the MR in Sr3Ru2O7 across a broad temperature range and up to 14T.

MM 40.6 Fri 11:45 SCH/A216

Quantum Transport in Atomic-Sized Contacts Using Break-Junction Experiments — •Guillem Pellicer and Carlos Sabater — Department of Physics, University of Alicante

The study of atomic-sized metallic contacts is fundamental to understanding the limits of electronic transport at the nanoscale. We present a comparative analysis of electronic transport in atomic-sized contacts, contrasting the behavior of noble metals with that of reactive metals under both ambient conditions and inert atmospheres. We examine how environmental interactions influence the formation and stability of these nanocontacts, employing clustering algorithms to analyze these effects.

MM 40.7 Fri 12:00 SCH/A216

Atomic Transistor-Based Implementation of Logic Gates — •Merlin Schieler[1], Florian Schieren[1], Carlotta Buchner[1], Felix Frank[1], Ida Göbel[1], Katja Marschall[1], Fanqing Xie[1], Florian Wertz[1], and Thomas Schimmel[1,2] — [1]Institute of Applied Physics, Karlsruhe Institute of Technologie (KIT), 76131 Karlsruhe, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technologie (KIT), 76344 Eggenstein-Leopoldshafen, Germany

An atomic-scale quantum conductance switch was demonstrated in our group which allows to open and close an electrical circuit by the controlled and reproducible reconfiguration of individual silver atoms within an atomic-scale junction. The only movable parts of the switch are the contacting atoms. The device is fabricated by electrochemical deposition of silver atoms between the source and the drain electrode. It is entirely controlled by an external voltage of a few millivolts applied to an independent gate electrode. Controlled switching was performed between a quantized, electrically conducting "on-state" exhibiting a conductance of $G_0 = \frac{2e^2}{h} \approx \frac{1}{12.9\,\mathrm{k\Omega}}$ or preselectable multiples of this value and an insulating "off-state". The device, which reproducibly operates at room temperature, represents an atomic transistor or relay, opening intriguing perspectives for the emerging fields of quantum electronics and logics on the atomic scale.

Here, we show a first demonstration of logical operations such as NAND and NOR with electrical circuits consisting of two atomic-scale quantum conductance switches.

MM 40.8 Fri 12:15 SCH/A216

Quantum transport in α-Sn atomic-sized contacts tuned by strain — Francisco Guzmán[1], Wynand Dednam[2], Andres Martinez-garcia[1], Enrico Lombardi[2], Carlos Untiedt[1], and •Carlos Sabater[1] — [1]University of Alicante — [2]University of South Africa

Tin (Sn) transitions from metallic β-Sn (above 286 K) to α-Sn (diamond-cubic, zero-gap semiconductor) below this temperature. α-Sn's electronic properties are theoretically tunable under strain, potentially yielding a Dirac semimetal or topological insulator. We experimentally investigated the quantum electronic transport of α-Sn nanocontacts at 4.2 K using a Scanning Tunneling Microscopy break junction (BJ) setup. Conductance measurements revealed three distinct groups via machine-learning clustering. Supported by Molecular Dynamics (MD) simulations and Density Functional Theory (DFT) calculations with Spin-Orbit Coupling (SOC), our findings demonstrate that atomic contact geometry is crucial for quantum transport in α-Sn, providing insights for spintronics applications.

MM 41: Development of Calculation Methods II

Time: Friday 10:15–12:45 Location: SCH/A251

MM 41.1 Fri 10:15 SCH/A251

Atomistic Framework for Glassy Polymer Viscoelasticity Across 20 Frequency Decades — •Ankit Singh[1], Vinay Vaibhav[1,2], Caterina Czibula[3], Timothy W. Sirk[4], and Alessio Zaccone[1] — [1]Department of Physics "A. Pontremoli", University of Milan, Via Celoria 16, 20133 Milan, Italy — [2]Institut für Theoretische Physik, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [3]Institute of Bioproducts and Paper Technology, Graz University of Technology, Inffeldgasse 23, 8010 Graz, Austria — [4]US Army DEVCOM Army Research Laboratory, Aberdeen Proving Ground, Maryland 21005, United States

Glassy polymers are central to engineering applications, yet their viscoelastic response over broad frequency and temperature ranges remains difficult to characterize. We extend non-affine deformation theory by incorporating a time-dependent memory kernel within the Generalized Langevin Equation for atomistic non-affine motions, yielding frequency-dependent mechanical response. Applied to poly(methyl methacrylate) (PMMA), the method captures the shear modulus and relaxation spectrum across more than twenty decades in frequency, from hundreds of terahertz down to the millihertz regime, thus bridging polymer mechanics from ordinary to extreme scales. Our predictions show quantitative consistency with independent estimates from oscillatory-shear molecular dynamics, Brillouin scattering, ultrasonic spectroscopy, Split-Hopkinson testing, and dynamic mechanical analysis (DMA), demonstrating a unified theoretical computational route for multiscale characterization of polymer glasses.

MM 41.2 Fri 10:30 SCH/A251

Clarifying the existence of a miscibility gap in platinum-palladium alloys via compositional fluctuations — •Florian Groll, Sebastian Eich, and Guido Schittz — Institute of Materials Science, Stuttgart, Germany

In materials science, the Gibbs free energy is of central importance for calculating phase diagrams. CALPHAD assessments require extensive experimental measurements and data obtained from well-equilibrated samples. For alloy systems with extremely low diffusion coefficients, achieving such equilibrium can be very time-consuming or practically impossible. Because this approach relies only on nanometer-scale equilibration, it provides a significantly more efficient route to the determination of CALPHAD parameters for systems with extremely slow diffusion. The palladium-platinum system is a well-known example for those kind of systems with unknown miscibility gap. In this study, we determine the Pd*Pt phase diagram by extracting the curvature of the Gibbs free energy from local composition fluctuations in the solid state using fluctuation theory. The experimental data needed for applying the local fluctuation theory are obtained from atom probe tomography, and the phase diagram is subsequently calculated.

MM 41.3 Fri 10:45 SCH/A251

Exploring the magnetic phase behaviour of MnAl with a novel sampling method, beginning from first principles — •Georgia A Marchant[1,2], M Nur Hasan[1], Rafael Vieira[1], Julie B Staunton[2], and Heike Herper[1] — [1]Uppsala University, Uppsala, Sweden — [2]University of Warwick, Coventry, United Kingdom

The demand for powerful magnetic materials is ever-increasing, as they dominate our modern technological landscape. Addressing rare earth (RE) criticality is crucial, so the search for viable permanent magnets that are RE-free and RE-lean continues. MnAl, with around 55% Mn content, has been a popular candidate for research in this regard. It transforms from the paramagnetic epsilon phase to the ferromagnetic tau phase when annealed appropriately, but the transition rate enhances under a surprisingly modest magnetic field. To shed light on this, we have computationally predicted the magnetic properties of MnAl across the transition.

The method uses data from first-principles calculations to build efficient atomic models of the phases' magnetic interactions. Thermodynamic properties are then determined with nested sampling (NS). Recently, NS has proven to be a powerful alternative to Markhov chain Monte Carlo sampling (MCMC). While NS has been used extensively in non-magnetic physical chemistry, this work represents its first application to magnetic materials. We present these results to demonstrate the power of NS; compare its effectiveness to MCMC; and unveil previously-unknown magnetic phases of MnAl.

MM 41.4 Fri 11:00 SCH/A251

A Demonstration of the Finite-Temperature Upside-Down Adiabatic Connection with the Asymmetric Hubbard Dimer — •Vincent Martinetto[1,2,3], Juri Grossi[1], and Aurora Pribram-Jones[1] — [1]University of California, Merced, CA 95343, United States — [2]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [3]Center for Advanced Systems Understanding, 02826 Görlitz, Germany

The finite-temperature upside-down adiabatic connection is an integral expression for the decorrelation free energy, a quantity of interest when considering finite-temperature strictly correlated electrons. This approach smoothly connects a thermal ensemble of strictly correlated electrons to an ensemble with realistic interaction strength while requiring the density of the system to remain fixed across all interaction strengths. As the strictly correlated limit is the natural opposite of the Kohn-Sham limit, it can provide new insights into the difficult regime of strong correlation in finite-temperature systems. An exact demonstration of the upside-down finite-temperature adiabatic connection will be performed with the asymmetric Hubbard dimer, along with a discussion of strong correlation in finite-temperature systems.

MM 41.5 Fri 11:15 SCH/A251

Towards self-consistent electrostatic corrections for charged defects in periodic boundary conditions — •Ermanno Botti[1,2,3], Davide Campi[3], Nicéphore Bonnet[2], and Nicola Marzari[1,2] — [1]PSI, Switzerland — [2]EPFL, Switzerland — [3]UniMiB, Italy

Charged point defects in semiconductors and insulators play a pivotal role in determining a wide range of physical properties, significantly impacting materials behavior and device performance. First principles calculations have become an essential tool to better characterize defects properties and to speed up technological advancements. However, some key defect properties, such as formation energies in the dilute limit, are highly sensitive to finite size effects in periodic boundary conditions DFT simulations. These issues arise from long range Coulomb interactions between periodic replicas and the neutralizing background needed to prevent the divergence of the electrostatic potential. To reduce these effects, corrections are required to remove these spurious electrostatic interactions. In this work we extend an a-posteriori correction scheme to achieve self-consistency in the open access package Quantum Espresso and test it on simple systems.

15 min. break

MM 41.6 Fri 11:45 SCH/A251

Tessellation-free full charge density method for atom-centered basis sets — •Franco Moitzi[1], Andrei V. Ruban[2,3], Vsevolod I. Razumovskiy[1], and Oleg E. Peil[2] — [1]Christian Doppler Laboratory for Digital material design guidelines for mitigation of alloy embrittlement, Materials Center Leoben Forschung GmbH, Vordernberger Straße 12, A-8700 Leoben, Austria — [2]Materials Center Leoben Forschung GmbH, Vordernberger Straße 12, A-8700 Leoben, Austria — [3]Department of Materials Science and Engineering, Royal Institute of Technology, 10044 Stockholm, Sweden

Accurate Poisson solvers are essential for reliable total energies and forces in Density Functional Theory (DFT) calculations. Atom-centered basis methods, such as Korringa-Kohn-Rostoker methods, often rely on Voronoi tessellations to decompose space, which complicate Poisson solutions in the interstitial region due to the high l-cutoffs required for the nearly flat charge there and the boundary discontinuities, leading to numerical instabilities as atoms move. We introduce a tessellation-free method that avoids these issues by decomposing the charge into non-overlapping atomic spheres and an interstitial region.

Following Andersen *et al.*, the interstitial charge is expanded in screened spherical waves—Helmholtz-equation solutions with special boundary conditions—and smoothly extended from the atomic spheres, allowing the Poisson equation to be solved analytically. Their analytical properties allow accurate evaluation of the Hartree potential, electrostatic, and exchange-correlation energies, enabling precise and efficient DFT calculations with atom-centered basis sets.

MM 41.7 Fri 12:00 SCH/A251

Machine-Learning Augmented Electronic Structure Calculations via Adaptive DFTB Parameters — •Yihua Song, Christoph Scheurer, Karsten Reuter, and Chiara Panosetti — Fritz Haber Institut der MPG

As a semi-empirical DFT approximation, Density Functional Tight Binding (DFTB) combines reduced computational cost with accessible electronic structure, providing a compromise between the full physicality of *ab initio* methods and the speed of machine-learning interatomic potentials. Yet, its accuracy in realistic systems remains limited due to intrinsic approximations and dependence on parametrization quality. To this end, we propose that the precalculated Slater-Koster (SK) electronic interaction tables in DFTB should be adapted to local atomic environments and demonstrate proof-of-principle studies showing the improved electronic structure description. Building on the observed smoothness of SK integrals across chemical and spatial environments, we use machine learning based on atomic descriptors to continuously adapt the parametrization beyond discrete atomic types. As a prototype, we introduce the DFTB Orbital Verity Engine (DOVE), a machine-learning framework that learns subtle discrepancies in electronic parameters across diverse local environments from reference electronic structures. We successfully validate it against complicated

systems with multiple coordination states. This machine-learning framework for environment-adaptive tight-binding parameterization enables scalable electronic structure simulations with enhanced fidelity, efficient speed, and physical interpretability.

MM 41.8 Fri 12:15 SCH/A251

Detecting topologically-protected surface states in doped systems using the coherent potential approximation — •Artem Chmeruk, Dylan Jones, and Liviu Chioncel — University of Augsburg, Augsburg, Germany

The signature of the non-trivial electronic band structure is the existence of gapless conducting states at interfaces where the topological invariant changes. This change signals a topological phase transition, which in real systems can be accomplished through doping. Modeling doping effects can be done by combining density functional theory and coherent potential approximation, which gives the possibility to model a continuous range of concentrations, and provides a sensitive probe to detect the emergent electronic states. Here, we analyse the topologically-protected surface states in $Bi_{2-x}Sb_xSe_3$.

MM 41.9 Fri 12:30 SCH/A251

Defect-induced vibrational modes in graphene — •Iskander Mukatayev, Guillaume Radtke, and Michele Lazzeri — Sorbonne Université, CNRS UMR 7590, MNHN, IMPMC, 4 place Jussieu, 75252 Paris, France

We present a general framework for investigation of the vibrational properties of point defects in graphene, motivated by recent advances in vibrational EELS that enable phonon spectroscopy with atomic resolution. Our approach combines DFT and density-functional perturbation theory with a force-matching procedure [1-2], in which interatomic force constants (IFCs) are computed independently for pristine graphene and defect-containing supercells and then merged to dynamical matrices of very large systems(up to 20000 atoms). This strategy enables the modeling of isolated defects without defect-defect interactions while retaining full ab initio accuracy.

We investigate a wide range of point defects including substitutional dopants (B, N, Si, P), single, double vacancies and Stone-Wales reconstruction. Depending on the details of defect-induced bond reconstruction, different behaviours are observed ranging from quasi-localized (or resonant) states falling in the continuum of the bulk to high-frequency fully localised modes. From these examples we draw conclusions of the conditions of occurrence of both types vibrations.

1. M. Lazzeri, P. Thibaudeau, Phys. Rev. B 74, 140301 (2006)

2. G. Radtke, S. Klotz, M. Lazzeri, P. Loubeyre, M. Krisch, A. Bossak, Phys. Rev. Lett. 132, 056102 (2024)

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Overview of Invited Talks and Sessions

(Lecture halls HSZ/AUDI, HSZ/0201, HSZ/0204, HSZ/0401, HSZ/0403, TRE/PHYS, TRE/MATH, and WILL/A317; Poster P2)

Invited Talks

O 2.3	Mon	11:00–11:30	HSZ/0201	**Superconducting Fermi arcs.** — •Andrii Kuibarov, Susmita Changdar, Oleksandr Suvorov, Luminita Harnagea, Bernd Büchner, Sergey Borisenko
O 5.1	Mon	10:30–11:00	HSZ/0403	**Can the mineral-water interface save the world? Mineral carbonation, enhanced weathering and negative emissions** — •Philip Pogge von Strandmann
O 5.4	Mon	11:30–12:00	HSZ/0403	**Machine learning exploration of water binding and ice nucleation at silicate and carbon surfaces** — •Mie Andersen
O 7.1	Mon	10:30–11:00	TRE/MATH	**Magnetic Order in 2D Materials Beyond Bulk Constraints** — •Jeison Fischer
O 8.3	Mon	11:00–11:30	WILL/A317	**Controlling nanostructures on surfaces via intermolecular interactions** — •Yunjun Cao
O 14.1	Mon	15:00–15:30	TRE/MATH	**Spin and time-resolved ARPES and the orbital angular momentum of light** — Pierre Nonnon, Romain Géneaux, Karol Hricovini, Christine Richter, David Bresteau, •Mauro Fanciulli
O 15.1	Mon	15:00–15:30	WILL/A317	**Tuning Spin-1/2 Interactions in Graphene: From Long-Range Coupling to Altermagnetic Order** — •Beatriz Viña-Bausá, Manuel A. García-Blázquez, Antonio T. Costa, Joao C. G. Henriques, Roberto Carrasco, Eva Cortés-del Río, Diego Expósito, Pierre Mallet, Jean-Yves Veuillen, Joaquín Fernandez-Rossier, Juan J. Palacios, Iván Brihuega
O 33.1	Tue	10:30–11:00	HSZ/0201	**During-synthesis functionalization of graphene layers** — •Cristina Africh
O 36.1	Tue	10:30–11:00	HSZ/0403	**Acidity in nanoconfinement from ab initio and NNPs simulations** — Anthony Baldo, Muhammad Saleh, Kevin Leung, •Marialore Sulpizi
O 36.4	Tue	11:30–12:00	HSZ/0403	**Living Interfaces: Dissolution and Precipitation Processes at Mineral-Brine Interfaces Revealed by AFM** — •Igor Siretanu, Vincenzo Alagia, Saravana Kumar, Shilpa Mohanakumar, Max Nederstigt, Chinmay Shukla, Michel Duits, Frieder Mugele
O 37.1	Tue	10:30–11:00	TRE/PHYS	**Calculations of excited electronic states by converging on saddle points on the electronic energy surface** — •Hannes Jonsson
O 37.4	Tue	11:30–12:00	TRE/PHYS	**Many-Body Theory meets Electrochemistry: Electronic Structure of Cathode Materials** — •Silke Biermann
O 39.3	Tue	11:00–11:30	WILL/A317	**Electric double layer of platinum electrodes** — •Marc Koper
O 39.6	Tue	12:00–12:30	WILL/A317	**First-principles modelling of electrochemical interfaces** — •Axel Gross
O 51.1	Tue	14:30–15:00	TRE/MATH	**Ultrafast aqueous electric double-layer dynamics** — •Mischa Bonn
O 51.3	Tue	15:15–15:45	TRE/MATH	**Interface-specific nonlinear THz spectroscopy** — •Chuanshan Tian
O 52.1	Tue	14:30–15:00	WILL/A317	**Dynamics of catalytically active, atomically precise clusters on reducible oxide supports under the (fast) scanning tunneling microscope** — •Friedrich Esch
O 55.3	Wed	11:00–11:30	HSZ/0204	**Cationic Mixing in Ultrathin Oxide Films: How substrate and oxygen conditions control nanoalloying.** — •Jacek Goniakowski
O 57.1	Wed	10:30–11:00	HSZ/0403	**From Plasmonic Near-Fields to Electron Dynamics - A Photoemission Perspective** — •Pascal Dreher
O 60.1	Wed	10:30–11:00	WILL/A317	**Disentangling the origins of spin polarization in (inverse) photoemission from solid surfaces** — •Jürgen Henk

O 64.1	Wed	15:00–15:30	HSZ/0403	**Cantilever based Scanning Force Microscopy: Ultimate Sensitivity and Quantitative Imaging of Nanoscale Spin Textures** — •Hans J. Hug
O 64.6	Wed	16:30–17:00	HSZ/0403	**Single-spin sensing: A molecule-on-tip approach** — •Laurent Limot
O 66.1	Wed	15:00–15:30	TRE/MATH	**Ultrafast exciton dynamics in 2D semiconductors and electric field gated devices** — •Jan Philipp Bange
O 67.1	Wed	15:00–15:30	WILL/A317	**New frontiers of one step model of photoemission for quantum materials** — •Jan Minar
O 78.1	Thu	10:30–11:00	HSZ/0401	**The Wendelstein 7-X plasma vessel vacuum system from a scientific perspective** — •Georg Schlisio, Torsten Bräuer, Stylianos Varoutis, Paul McNeely, Dirk Hartmann, Chandra Prakash Dhard, Dirk Naujoks, Victoria Hak, the W7-X team
O 82.1	Thu	10:30–11:00	WILL/A317	**Low-energy inverse photoelectron spectroscopy (LEIPS): probing unoccupied states and conduction band structure in functional materials** — •Hiroyuki Yoshida
O 82.2	Thu	11:00–11:30	WILL/A317	**Enhanced Sensitivity in Low-Energy Inverse Photoemission Spectroscopy with an Off-Axis Parabolic Mirror for Efficient Light Collection** — •Yongsup Park, Jong-Am Hong, Kyu-Myung Lee, Min-Jae Maeng
O 85.1	Thu	15:00–15:30	HSZ/0401	**From light to pressure: Laser-based quantum technologies for the realization of high-precision pressure and vaccum standards** — •Tom Rubin
O 86.1	Thu	15:00–15:30	HSZ/0403	**Ultrafast Dynamics at Surfaces with Machine Learning Surrogates** — •Reinhard Maurer
O 94.1	Fri	9:30–10:00	HSZ/0204	**Surface Chemistry on Copper Oxides** — •Dario Stacchiola
O 97.1	Fri	9:30–10:00	TRE/PHYS	**Questions of Selectivity in Electrocatalysis** — •Vanessa J. Bukas
O 98.1	Fri	9:30–10:00	TRE/MATH	**Electron-phonon interactions in the time domain: from non-equilibrium phonon dynamics to theoretical spectroscopy** — •Fabio Caruso

Invited Talks of the joint Symposium SKM Dissertation Prize 2026 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	HSZ/0002	**Stochastic-Calculus Approach to Non-equilibrium Statistical Physics** — •Cai Dieball
SYSD 1.2	Mon	10:00–10:30	HSZ/0002	**Nonuniform magnetic spin textures for sensing, storage and computing applications** — •Sabri Koraltan
SYSD 1.3	Mon	10:30–11:00	HSZ/0002	**Anomalous Quantum Oscillations beyond Onsager's Fermi Surface Paradigm** — •Valentin Leeb
SYSD 1.4	Mon	11:00–11:30	HSZ/0002	**Coherent Control Schemes for Semiconductor Quantum Systems** — •Eva Schöll
SYSD 1.5	Mon	11:30–12:00	HSZ/0002	**On stochastic thermodynamics under incomplete information: Thermodynamic inference from Markovian events** — •Jann van der Meer

Invited Talks of the joint Symposium Designing Quantum Materials with Light: From Floquet to Cavity Engineering (SYFC)

See SYFC for the full program of the symposium.

SYFC 1.1	Mon	9:30–10:00	HSZ/AUDI	**Subcycle videography of strong-field controlled band structures** — •Rupert Huber, Manuel Meierhofer, Ulrich Höfer
SYFC 1.2	Mon	10:00–10:30	HSZ/AUDI	**Engineering Quantum Materials through Structured Cavity Vacuum Fluctuations** — •Angel Rubio
SYFC 1.3	Mon	10:30–11:00	HSZ/AUDI	**Floquet engineering of quantum materials: from semiconductors to semimetals** — •Shuyun Zhou
SYFC 1.4	Mon	11:15–11:45	HSZ/AUDI	**(Quantum) Light Control of Materials** — •Dante Kennes
SYFC 1.5	Mon	11:45–12:15	HSZ/AUDI	**Lightwave-driven electrons in a Floquet topological insulator** — Daniel Lesko, Tobias Weitz, Weizhe Li, Selina Nöcker, Celina Hüttner, Tamara Pröbster, Simon Wittigschlager, Christian Heide, Ofer Neufeld, •Peter Hommelhoff

Invited Talks of the joint Symposium AI and Data Challenges behind Emerging Self-Driving Laboratories (SYAI)

See SYAI for the full program of the symposium.

SYAI 1.1	Thu	9:30–10:00	HSZ/AUDI	**Data and Experimental Foundations for Reliable Self-Driving Laboratories** — •Dr. Marcus Tze-Kiat Ng
SYAI 1.2	Thu	10:00–10:30	HSZ/AUDI	**Digital Catalysis - AI for Experiment Planning and Control** — •Christoph Scheurer
SYAI 1.3	Thu	10:30–11:00	HSZ/AUDI	**Autonomous, Data-Driven Workflows for Materials Acceleration Platforms with pyiron** — •Jan Janssen, Joerg Neugebauer
SYAI 1.4	Thu	11:15–11:45	HSZ/AUDI	**Machine Learning for Autonomous Optimization and Discovery of Materials** — •Pascal Friederich
SYAI 1.5	Thu	11:45–12:15	HSZ/AUDI	**Transforming Our View on Transformers in the Sciences** — •Kevin Maik Jablonka

Sessions

O 1.1–1.1	Mon	9:30–10:15	TRE/PHYS	**Topical Talk Wulfhekel (joint session O/TT)**
O 2.1–2.7	Mon	10:30–12:30	HSZ/0201	**Electronic structure of surfaces: Spectroscopy, surface states I**
O 3.1–3.7	Mon	10:30–12:15	HSZ/0204	**Scanning probe techniques: Method development I**
O 4.1–4.7	Mon	10:30–12:15	HSZ/0401	**Metal & Semiconductor substrates: Adsorption and reaction of small molecules I**
O 5.1–5.6	Mon	10:30–12:30	HSZ/0403	**Focus Session: Mineral-water interfaces I**
O 6.1–6.8	Mon	10:30–12:30	TRE/PHYS	**Organic molecules on inorganic substrates: Adsorption and growth I**
O 7.1–7.7	Mon	10:30–12:30	TRE/MATH	**2D Materials: Electronic structure, excitations, etc. I (joint session O/HL/TT)**
O 8.1–8.7	Mon	10:30–12:30	WILL/A317	**Nanostructures at surfaces:1D, 2D, networks I**
O 9.1–9.12	Mon	15:00–18:00	HSZ/0201	**Organic molecules on inorganic substrates: electronic, optical and other properties I**
O 10.1–10.11	Mon	15:00–17:45	HSZ/0204	**2D Materials beyond graphene: Growth, structure and substrate interaction (joint session O/HL/TT)**
O 11.1–11.8	Mon	15:00–17:00	HSZ/0401	**Metal & Semiconductor substrates: Adsorption and reaction of small molecules II**
O 12.1–12.11	Mon	15:00–17:45	HSZ/0403	**Scanning probe microscopy: light matter interaction at atomic scales**
O 13.1–13.12	Mon	15:00–18:00	TRE/PHYS	**Solid-liquid interfaces: Reactions and electrochemistry I**
O 14.1–14.11	Mon	15:00–18:00	TRE/MATH	**Ultrafast electron dynamics at surface and interfaces I**
O 15.1–15.11	Mon	15:00–18:00	WILL/A317	**Spins on surfaces at the atomic scale I**
O 16.1–16.2	Mon	18:00–20:00	P2	**Focus Session: Structure and Dynamics of Solvent at Electrochemical Interfaces – Poster**
O 17.1–17.12	Mon	18:00–20:00	P2	**Spins on surfaces at the atomic scale – Poster**
O 18.1–18.6	Mon	18:00–20:00	P2	**New methods: Theory – Poster**
O 19.1–19.10	Mon	18:00–20:00	P2	**Vacuum Science & Technology: Theory and Applications – Poster**
O 20.1–20.1	Mon	18:00–20:00	P2	**Electronic structure theory – Poster**
O 21.1–21.2	Mon	18:00–20:00	P2	**Surface magnetism – Poster**
O 22.1–22.6	Mon	18:00–20:00	P2	**Surface dynamics – Poster**
O 23.1–23.10	Mon	18:00–20:00	P2	**Catalysis and surface reactions – Poster**
O 24.1–24.7	Mon	18:00–20:00	P2	**Solid-liquid interfaces: Reactions and electrochemistry – Poster**
O 25.1–25.2	Mon	18:00–20:00	P2	**Solid-liquid interfaces: Structure, spectroscopy – Poster**
O 26.1–26.5	Mon	18:00–20:00	P2	**Plasmonics and nanooptics: Fabrication, characterization and applications – Poster**
O 27.1–27.7	Mon	18:00–20:00	P2	**Plasmonics and nanooptics: Light-matter interaction, spectroscopy – Poster**
O 28.1–28.8	Mon	18:00–20:00	P2	**Oxide and insulator surfaces: Structure, epitaxy and growth – Poster**
O 29.1–29.3	Mon	18:00–20:00	P2	**Oxides and insulators: Adsorption and reaction of small molecules – Poster**
O 30.1–30.4	Mon	18:00–20:00	P2	**Metal & Semiconductor substrates: Structure, epitaxy and growth – Poster**
O 31.1–31.6	Mon	18:00–20:00	P2	**Metal & Semiconductor substrates: Adsorption and reaction of small molecules – Poster**
O 32.1–32.1	Tue	9:30–10:15	TRE/PHYS	**Topical Talk Witte**
O 33.1–33.7	Tue	10:30–12:30	HSZ/0201	**Graphene: Growth, structure and substrate interaction (joint session O/HL)**
O 34.1–34.8	Tue	10:30–12:30	HSZ/0204	**Catalysis and surface reactions I**

O 35.1–35.7	Tue	10:30–12:15	HSZ/0401	**Organic molecules on inorganic substrates: Adsorption and growth II**
O 36.1–36.6	Tue	10:30–12:30	HSZ/0403	**Focus Session: Mineral-water interfaces II**
O 37.1–37.6	Tue	10:30–12:30	TRE/PHYS	**Electronic structure theory I**
O 38.1–38.8	Tue	10:30–12:30	TRE/MATH	**Ultrafast electron dynamics at surface and interfaces II**
O 39.1–39.6	Tue	10:30–12:30	WILL/A317	**Focus Session: Structure and Dynamics of Solvent at Electrochemical Interfaces I**
O 40.1–40.21	Tue	14:00–16:00	P2	**Ultrafast electron dynamics at surface and interfaces – Poster (joint session O/TT)**
O 41.1–41.4	Tue	14:00–16:00	P2	**Topology and symmetry protected materials & Topological insulators – Poster (joint session O/TT)**
O 42.1–42.9	Tue	14:00–16:00	P2	**Electronic structure of surfaces: Spectroscopy, surface states – Poster**
O 43.1–43.17	Tue	14:00–16:00	P2	**Scanning probe microscopy: light matter interaction at atomic scales – Poster**
O 44.1–44.17	Tue	14:00–16:00	P2	**Scanning probe techniques: Method development – Poster**
O 45.1–45.11	Tue	14:00–16:00	P2	**Organic molecules on inorganic substrates: Adsorption and growth – Poster**
O 46.1–46.11	Tue	14:00–16:00	P2	**Organic molecules on inorganic substrates: electronic, optical and other properties – Poster**
O 47.1–47.4	Tue	14:30–15:30	HSZ/0201	**New methods: Theory**
O 48.1–48.6	Tue	14:30–16:00	HSZ/0204	**Metal & Semiconductor substrates: Structure, epitaxy and growth**
O 49.1–49.5	Tue	14:30–15:45	HSZ/0403	**Plasmonics and nanooptics: Light-matter interaction, spectroscopy I**
O 50.1–50.7	Tue	14:30–16:15	TRE/PHYS	**Electronic structure theory II**
O 51.1–51.3	Tue	14:30–15:45	TRE/MATH	**Focus Session: Structure and Dynamics of Solvent at Electrochemical Interfaces II**
O 52.1–52.5	Tue	14:30–16:00	WILL/A317	**Oxide and insulator surfaces: Structure, epitaxy and growth I**
O 53.1–53.1	Wed	9:30–10:15	TRE/PHYS	**Topical Talk Parkinson**
O 54.1–54.8	Wed	10:30–12:30	HSZ/0201	**Nanostructured surfaces and thin films**
O 55.1–55.7	Wed	10:30–12:30	HSZ/0204	**Oxide and insulator surfaces: Structure, epitaxy and growth II**
O 56.1–56.7	Wed	10:30–12:15	HSZ/0401	**Scanning probe techniques: Method development II**
O 57.1–57.7	Wed	10:30–12:30	HSZ/0403	**Plasmonics and nanooptics: Light-matter interaction, spectroscopy II**
O 58.1–58.8	Wed	10:30–12:30	TRE/PHYS	**Organic molecules on inorganic substrates: Adsorption and growth III**
O 59.1–59.8	Wed	10:30–12:30	TRE/MATH	**2D Materials: Electronic structure, excitations, etc. II (joint session O/HL/TT)**
O 60.1–60.7	Wed	10:30–12:30	WILL/A317	**Focus Session: Unoccupied States by Inverse Photoemission I**
O 61.1–61.11	Wed	15:00–17:45	HSZ/0201	**Organic molecules on inorganic substrates: electronic, optical and other properties II**
O 62.1–62.11	Wed	15:00–17:45	HSZ/0204	**Graphene: Electronic structure, excitations, etc. (joint session O/TT)**
O 63.1–63.11	Wed	15:00–17:45	HSZ/0401	**Topology and symmetry protected materials & Topological insulators (joint session O/HL/TT)**
O 64.1–64.9	Wed	15:00–17:45	HSZ/0403	**Surface Magnetism**
O 65.1–65.12	Wed	15:00–18:00	TRE/PHYS	**Solid-liquid interfaces: Reactions and electrochemistry II**
O 66.1–66.10	Wed	15:00–17:45	TRE/MATH	**Ultrafast electron dynamics at surface and interfaces III**
O 67.1–67.11	Wed	15:00–18:00	WILL/A317	**Focus Session: Unoccupied States by Inverse Photoemission II**
O 68.1–68.6	Wed	18:00–20:00	P2	**Nanostructured surfaces and thin films – Poster**
O 69.1–69.13	Wed	18:00–20:00	P2	**Nanostructures at surfaces:1D, 2D, networks – Poster**
O 70.1–70.7	Wed	18:00–20:00	P2	**2D materials: Stacking and heterostructures – Poster (joint session O/TT)**
O 71.1–71.23	Wed	18:00–20:00	P2	**2D Materials: Electronic structure, excitations, etc. – Poster (joint session O/TT)**
O 72.1–72.6	Wed	18:00–20:00	P2	**2D Materials beyond graphene: Growth, structure and substrate interaction – Poster (joint session O/TT)**
O 73.1–73.6	Wed	18:00–20:00	P2	**Graphene: Growth, structure and substrate interaction – Poster**
O 74.1–74.9	Wed	18:00–20:00	P2	**Graphene: Electronic structure, excitations, etc. – Poster (joint session O/TT)**
O 75.1–75.1	Thu	9:30–10:15	TRE/PHYS	**Topical Talk Bibes (joint session O/TT)**
O 76.1–76.7	Thu	10:30–12:15	HSZ/0201	**Electronic structure of surfaces: Spectroscopy, surface states II**
O 77.1–77.7	Thu	10:30–12:15	HSZ/0204	**Nanostructures at surfaces:1D, 2D, networks II**
O 78.1–78.6	Thu	10:30–12:15	HSZ/0401	**Vacuum Science & Technology: Theory and Applications I**
O 79.1–79.7	Thu	10:30–12:15	HSZ/0403	**Plasmonics and nanooptics: Light-matter interaction, spectroscopy III**
O 80.1–80.5	Thu	10:30–13:00	TRE/PHYS	**Gerhard Ertl Young Investigator Award Competition**
O 81.1–81.7	Thu	10:30–12:15	TRE/MATH	**Catalysis and surface reactions II**
O 82.1–82.6	Thu	10:30–12:30	WILL/A317	**Focus Session: Unoccupied States by Inverse Photoemission III**
O 83.1–83.10	Thu	15:00–17:30	HSZ/0201	**Organic molecules on inorganic substrates: electronic, optical and other properties III**

O 84.1–84.11	Thu	15:00–17:45	HSZ/0204	**2D Materials: Electronic structure, excitations, etc. III (joint session O/HL/TT)**
O 85.1–85.7	Thu	15:00–17:00	HSZ/0401	**Vacuum Science & Technology: Theory and Applications II**
O 86.1–86.10	Thu	15:00–17:45	HSZ/0403	**Surface dynamics**
O 87.1–87.9	Thu	15:00–17:15	TRE/PHYS	**Solid-liquid interfaces: Structure, spectroscopy**
O 88.1–88.11	Thu	15:00–17:45	TRE/MATH	**Catalysis and surface reactions III**
O 89.1–89.12	Thu	15:00–18:00	WILL/A317	**Spins on surfaces at the atomic scale II**
O 90	Thu	17:15–18:15	HSZ/0401	**Members' Assembly of the Vacuum Science and Technology Divison (VA)**
O 91	Thu	19:00–19:30	HSZ/AUDI	**Members' Assembly**
O 92	Thu	19:30–20:30	HSZ/AUDI	**Post-Deadline Session**
O 93.1–93.10	Fri	9:30–12:00	HSZ/0201	**Electronic structure of surfaces: Spectroscopy, surface states III**
O 94.1–94.11	Fri	9:30–12:30	HSZ/0204	**Oxides and insulators: Adsorption and reaction of small molecules**
O 95.1–95.12	Fri	9:30–12:30	HSZ/0401	**2D Materials: Stacking and heterostructures (joint session O/HL/TT)**
O 96.1–96.12	Fri	9:30–12:30	HSZ/0403	**Plasmonics and nanooptics: Fabrication, characterization and applications**
O 97.1–97.11	Fri	9:30–12:30	TRE/PHYS	**Solid-liquid interfaces: Reactions and electrochemistry III**
O 98.1–98.10	Fri	9:30–12:15	TRE/MATH	**Ultrafast electron dynamics at surface and interfaces IV**
O 99.1–99.12	Fri	9:30–12:30	WILL/A317	**Spins on surfaces at the atomic scale III**
O 100.1–100.1	Fri	13:15–14:00	TRE/PHYS	**Closing Talk Steinrück**

Members' Assembly of the Vacuum Science and Technology Divison (VA)

Thursday 17:15–18:15 HSZ/0401

Members' Assembly of the Surface Science Division

Thursday 18:00–19:00 HSZ/AUDI

Sessions

– Invited, Topical, Contributed Talks, and Posters –

O 1: Topical Talk Wulfhekel (joint session O/TT)

Time: Monday 9:30–10:15 Location: TRE/PHYS

Topical Talk O 1.1 Mon 9:30 TRE/PHYS

Vortices, inter-band coupling and inelastic QPI in two band superconductors — •Wulf Wulfhekel — Physikalisches Institut, Karlsruhe Institute of Technology

The majority of superconductors have more than one Fermi surface, on which the electrons pair below the critical temperature, yet their behavior can be well described by a single-band Bardeen-Cooper-Schrieffer theory. This is mostly due to interband scattering, especially in superconductors in the dirty limit, rigidly linking the pairing amplitude of the bands. We here lift this constrain and study the behavior of the ultra-pure two-band superconductor Pb. We show that at low temperatures, it is neither of type I nor type II and superconducting vortices of arbitrary flux quanta can be formed. We show that on the non-spherical Fermi surfaces, a modified index theory is needed for the description of in gap states in vortices. Further, the two condensates are only weakly coupled and can be individually manipulated. By studying stacking fault tetrahedra, we demonstrate local tuning of interband coupling ranging from weak to strong and the modification of the superconducting order parameters from two well separated gaps to one merged gap around defects. The experiments critically test the theory of multiband superconductors and give a route to access a wide range of predicted quantum effects in these systems. Finally, we demonstrate that quasi particle interference is also possible in the inelastic tunneling channel enabling the imaging of standing phonons with STM.

O 2: Electronic structure of surfaces: Spectroscopy, surface states I

Time: Monday 10:30–12:30 Location: HSZ/0201

O 2.1 Mon 10:30 HSZ/0201

Unveiling the spin texture of the topological surface state in Sb(111) — •Xin Liang Tan[1], Arthur Ernst[2], Anders Christian Mathisen[1], Stefanie Suzanne Brinkman[1], Fabian Göhler[1], Chul Hee Min[1], and Hendrik Bentmann[1] — [1]Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, 7491 Trondheim, Norway — [2]Institut für Theoretische Physik, Johannes Kepler Universität, A 4040 Linz, Austria

Spin-resolved momentum microscopy is a powerful tool for mapping the complete Fermi surface and spin texture of two-dimensional electronic states. Here, we present spin- and momentum-resolved Sb(111) surface state, a benchmark system exhibiting strong spin-orbit coupling and a non-trivial topology. Using a continuous-wave vacuum-ultraviolet laser ($h\nu = 6eV$) for photoexcitation, we achieve efficient k-space mapping of the in-plane spin-polarization components over the full surface Brillouin zone. We will present experimental data obtained for different light polarizations. Our results are compared to first-principles calculations.

[1] X.L. Tan et al., Ultramicroscopy 253, 113820 (2023).
[2] C. Tusche et al., Ultramicroscopy 159, 520 (2015).
[3] D. Hsieh et al., Science 323, 919-922(2009).
[4] H. Ishida. Phys., Rev. B 90, 235422 (2014).

O 2.2 Mon 10:45 HSZ/0201

Surface Electronic Structure of Magnetic Kagome Metal GdV_6Sn_6 — •Robin P. Forster[1], Honey Boban[1], Mohammed Qahosh[1], Xiao Hou[1], Yishui Zhou[2], Yixi Su[2], Gustav Bihlmayer[3], Claus M. Schneider[1], and Lukasz Plucinski[1] — [1]PGI-6 Forschungszentrum-Jülich — [2]JCNS Forschungszentrum-Jülich — [3]PGI-1 Forschungszentrum-Jülich

The magnetic Kagome metal GdV_6Sn_6 combines in a single material phenomena such as van Hove Singularities [1,2,3], local moments of the 4f electrons of Gd, and itinerant V 3d electrons [4], providing a platform to study their complex magentic and electronic interactions. We have performed termination-dependent micro-ARPES measurements of paramagnetic GdV_6Sn_6 with 20 μm real-space resolution at 20 K [5]. A series of scans over a photon energy range between 75 eV and 200 eV enabled the distinction between surface and bulk states. We have chosen $h\nu$ of 80 and 130 eV for detailed ARPES scans. In addition, XPS measurements and DFT-GGA slab calculations were performed, which can be used to investigate surface terminations. Preliminary circular-dirchroic ARPES maps exhibit multiple sign inversions that stem from a combination of initial state orbital angular momenta and photoemission final state scattering [6].

[1] PRL 127, 266401 (2021) [2] RRL 17, 2300083 (2023) [3] Sci. Adv. 8, 38 (2022) [4] JPSJ 90, 124704 (2021) [5] PRB 104, 235139 (2021) [6] arXiv:2410.19652 (2024).

Invited Talk O 2.3 Mon 11:00 HSZ/0201

Superconducting Fermi arcs. — •Andrii Kuibarov, Susmita Changdar, Oleksandr Suvorov, Luminita Harnagea, Bernd Büchner, and Sergey Borisenko — Leibnitz Institute for Solid State and Materials Research, Dresden, Germany

$PtBi_2$ is a trigonal non-centrosymmetric material that has recently drawn attention as a natural platform for topological superconductivity, without the need for engineered heterostructures. Recent STM studies have strengthened this claim by showing a superconducting gap with size up to 20 meV and critical temperature around 45 K.

Using angle-resolved photoemission spectroscopy, we demonstrate that both terminations of $PtBi_2$ expose Fermi arc surface states, which become superconducting at approximately 15 K with a gap size up to 3 meV, while the bulk of the material remains metallic, making $PtBi_2$ a surface-only superconductor. Further momentum-resolved gap measurements have shown that the superconducting gap on the Fermi arcs is anisotropic, with the superconducting node located in the center of six Fermi arcs, making it the first *i-wave (l = 6)* superconductor. This anisotropy implies the formation of Majorana surface cones and predicts robust zero-energy flat-band Majorana states at the hinges of the crystal.

O 2.4 Mon 11:30 HSZ/0201

From low- to high-energy photoelectron diffraction: Novel theoretical approaches and Kikuchi diffraction analysis — •Trung-Phuc Vo[1], Olena Tkach[2], Didier Sébilleau[3], Olena Fedchenko[2], Hans-Joachim Elmers[2], Gerd Schönhense[2], and Ján Minár[1] — [1]Univ. of West Bohemia in Pilsen, Czech Republic — [2]Univ. of Mainz, Germany — [3]Univ. of Rennes, France

Time-of-flight momentum microscopy (ToF-MM) enables simultaneous energy- and momentum-resolved mapping of the full photoelectron distribution. Its sensitivity to the strong energy dependence of Kikuchi patterns [1,2] requires advanced theoretical modeling, especially across the broad energy range accessible with modern large-k-field setups [3]. We present a fully relativistic multiple-scattering study of fine diffraction features in core-level photoemission from Ge(100) and Si(100) over kinetic energies from 106 to 4174 eV [4]. Our one-step calculations avoid cluster-size convergence issues and include inelastic scattering to describe pattern broadening. For the first time, we reproduce circular dichroism in the angular distribution of Si(100) 1s with asymmetries up to 31%, and capture both bulk- and surface-sensitive diffraction features. The simulations show good agreement with experimental data obtained using circularly polarized light, demonstrating the robustness of our approach for high-energy photoemission and PED analysis.

[1] O. Tkach et al., Ultramicroscopy 250, 113750 (2023); [2] T.-P. Vo et al., AIP Conf. Proc. 3251, 020005 (2024); [3] T.-P. Vo et al., arXiv:2504.14758 (2025); [4] T.-P. Vo et al., npj Comput. Mater. 11, 159 (2025).

O 2.5 Mon 11:45 HSZ/0201

Fermiology and spin polarization of the topological surface states in $PtBi_2$ — •Stefanie Suzanne Brinkman[1], Anders Christian Mathisen[1], Xin Liang Tan[1], Kristian Maeland[2], Øyvind Finnseth[1], Fabian Göhler[1], Chul Hee Min[1], Grisha Shipunov[3], Anna Isaeva[2], Jorge Ismael Facio[4], and Hendrik Bentmann[1] — [1]Center for Quantum Spintronics, Department of Physics, NTNU, Norway — [2]Institute for Theoretical Physics and Astrophysics, University of Würzburg, Germany — [3]Institute of Physics, University of Amsterdam, The Netherlands — [4]Instituto Balseiro, National University of Cuyo, Argentina

Weyl semimetals host topologically protected Weyl nodes in the bulk, that are connected by Fermi arcs on the surface. In $PtBi_2$, recent reports indicate superconductivity in the surface Fermi arcs at elevated temperatures [1]. In this talk, we will present results from spin- and angle-resolved VUV photoemission experiments for both inequivalent surface terminations of $PtBi_2$. Our measurements,

combined with first-principles calculations, establish vastly different low-energy dispersion relations of the Fermi arcs depending on surface termination. Furthermore, we provide evidence for spin polarization of the Fermi arcs. We will discuss the implications of our results for the emergence of unconventional superconductivity on the surface of $PtBi_2$.

[1] Andrii Kuibarov et al., Evidence of superconducting Fermi arcs. Nature **626**, 294-299 (2024)

O 2.6 Mon 12:00 HSZ/0201

Multi-technique research ecosystem structured around electronic band structure analysis — Takahiro Hashimoto[1], Andreas Janzen[2], •Hrag Karakachian[2], Eleni Anargirou[2], Timo Wätjen[1], and Martin Schmid[1] — [1]Scienta Omicron AB, Danmarksgatan 22, 75323 Uppsala, Sweden — [2]Scienta Omicron GmbH, Limburger Strasse 75, 65232 Taunusstein, Germany

The discovery and control of novel quantum materials are essential to the progress of modern technology. These materials frequently show complex behaviours that demand multiple, complementary techniques to fully understand their properties. For example, the electronic band structure, which is central to understanding emerging quantum materials, is typically investigated using angle-resolved photoemission spectroscopy (ARPES) or momentum microscopy.

Here, we describe how a surface-science research ecosystem centred on ARPES can be established by integrating state-of-the-art capabilities such as molecular beam epitaxy (MBE) for thin-film growth, X-ray photoemission spectroscopy (XPS) for chemical-state analysis, and scanning probe microscopy (SPM) for real-space imaging. Materials innovation is accelerated by combining these complementary techniques, leveraging both laboratory-based and user-facility instrumentation, and developing new tools to extend commercial systems.

We will present several research scenarios focused on electronic band-structure analysis and highlight application examples involving 2D materials and topological materials.

O 2.7 Mon 12:15 HSZ/0201

The TXPES Beamline at SESAME * A New Facility for Advanced Soft X-ray Photoelectron Spectroscopy — •ZEYNEP REYHAN OZTURK — SESAME

The Turkish X-ray Photoelectron Spectroscopy (TXPES) beamline, newly installed at the SESAME synchrotron, is dedicated to advanced soft X-ray photoelectron spectroscopy (XPS/UPS) for surface and interface analysis. Designed for high-resolution measurements across a broad photon energy range, TXPES enables detailed investigation of electronic structure, chemical composition, and oxidation states in complex materials.

The end station features interconnected UHV chambers for sample preparation, analysis, and in situ or near-ambient pressure experiments. Equipped with a hemispherical analyzer, ion gun, LEED, and LEIS, it allows comprehensive surface characterization with variable depth sensitivity.

TXPES provides a powerful platform for studying surface oxidation, adsorption, catalysis, and band alignment under controlled environments, including realistic gas conditions via its high-pressure cell. Currently in commissioning, the beamline will support diverse research on functional oxides, thin films, catalysts, and magnetic materials, highlighting the collaborative effort between Turkish institutions and SESAME toward full user operation.

O 3: Scanning probe techniques: Method development I

Time: Monday 10:30–12:15 Location: HSZ/0204

O 3.1 Mon 10:30 HSZ/0204

Single-Molecule Insights into On-Surface C-C Bond Formation: Radical Control via Sequential Dehalogenation — Qigang Zhong[1], Daniel Kohrs[2], Jannis Jung[3], Daniel Ebeling[1], Doreen Mollenhauer[3], Hermann Wegner[2], and •Andre Schirmeisen[1] — [1]Institute of Applied Physics, Justus-Liebig University Giessen, Giessen, Germany — [2]Institute of Organic Chemistry, Justus Liebig University Giessen, Giessen, Germany — [3]Institute of Physical Chemistry, Justus Liebig University Giessen, Giessen, Germany

On-surface synthesis through dehalogenative coupling provides a powerful route to construct carbon-carbon bonds with atomic precision. Using a combination of scanning tunneling microscopy (STM), atomic force microscopy (AFM), and density functional theory (DFT), we investigated the radical intermediates and coupling pathways of brominated polyaromatic precursors, specifically BBPN and BPIN, on Ag(111). Controlled thermal and tip-induced dehalogenation enabled the selective generation of phenyl and naphthyl radicals, which were subsequently characterized at the single-molecule level. Statistical analysis of tip-induced reactions reveals that cyclization leading to C-C bond formation occurs preferentially when the first dehalogenation takes place at the naphthyl group. Computational modeling demonstrates that radical alignment and flexibility govern the feasibility of C-C coupling. These findings highlight the interplay between precursor structure, radical generation sequence, and surface interactions in steering on-surface coupling chemistry.

O 3.2 Mon 10:45 HSZ/0204

Scanning probe microscopy investigation on cyclocarbons — •Jakob Eckrich[1], Lisanne Sellies[1], Marco Vitek[3], Yueze Gao[2], Fabian Paschke[1], Florian Albrecht[1], Leonard-Alexander Lieske[1], Harry L. Anderson[2], Igor Rončević[3], and Leo Gross[1] — [1]IBM Research Europe - Zurich, Rüschlikon, Switzerland — [2]Oxford University, Oxford, UK — [3]University of Manchester, Manchester, UK

I will discuss our recent investigations of cyclocarbons by means of scanning tunneling microscopy (STM) and atomic force microscopy (AFM). Cyclocarbons, molecular carbon allotropes consisting of a ring of two-fold coordinated carbon atoms, have been synthesized on surface using tip-induced chemistry [1-3], and the formation of larger cyclocarbons by dimerization of precursors was shown [3]. This talk will focus on the generation and investigation of large cyclocarbons.

[1] K. Kaiser et al., Science, 365, 1299-1301 (2019) [2] L. Sun et al., Nature, 623, 972-976 (2023) [3] F. Albrecht et al., Science, 384, 677-682 (2024)

O 3.3 Mon 11:00 HSZ/0204

Machine Learning Models Tailored for Scanning Probe Microscopy Topographic Data — •Lovis Hardeweg, Johanna Matusche, Johannes Schwenk, Christoph Sürgers, Wolfgang Wernsdorfer, and Philip Willke — Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany

Modern machine learning methods have great potential to automate processes in scanning probe microscopy (SPM). An important step for any automated operation of SPM is the accurate extraction of meaningful information, such as the position and type of adsorbates, from topographic data. Existing frameworks, that localize and identify adsorbates on the surface [1], often rely on large models developed by the traditional computer vision community. Therefore, their application to SPM topographies has certain drawbacks.

Here, we present two machine learning architectures that are adapted specifically for their application to high-resolution low-temperature SPM data. The first model predicts a semantic segmentation on samples with heterogeneous surface material, Ag(001) and MgO/Ag(001) in particular. The second model is trained to identify adatoms, molecules and possible clusters adsorbed on the surface. Both models achieve high accuracy. Additionally, due to their reduced size, they require fewer resources during training and application than models, that have not been purpose-built for their respective tasks.

[1] J. Am. Chem. Soc, 147, 39, 35232-35243 (2025)

O 3.4 Mon 11:15 HSZ/0204

Exploring Dissipation in Single-Molecule Manipulation — •Norio Okabayashi[1], Alfred J. Weymouth[2], Sophia Schweiss[2], Thomas Frederiksen[3,4], and Franz J. Giessibl[2] — [1]Kanazawa University, Ishikawa 920-1192, Japan — [2]University of Regensburg, Regensburg D-93053, Germany — [3]Donostia International Physics Center, San Sebastián 20018, Spain — [4]Basque Foundation for Science, Bilbao 48013, Spain

Single-molecule manipulation with scanning probe microscopy (SPM) offers a well-defined platform for studying nanoscale friction. While previous work has focused mainly on the forces driving molecular motion [1], the corresponding dissipation processes remain less explored. Here, we investigate a single CO molecule on Cu(110) using STM, AFM, LFM, and DFT at low temperatures. DFT identifies the preferred adsorption sites and the switching pathway (top-bridge-top), which are confirmed experimentally by IETS and by dissipation signals during AFM and LFM oscillations. In AFM [2], dissipation appears only along specific manipulation paths, whereas in LFM it also arises along trajectories associated with molecular switching. The switching rate is evaluated from STM as a function of lateral tip position, giving the manipulation probability per LFM oscillation cycle. Combining this cycle-resolved rate with the measured dissipation per cycle allows us to quantify the energy dissipated per manipulation event.

[1] M. Ternes et al., Science 319, 1066 (2008)
[2] N. Okabayashi et al., PRL 131, 148001 (2023)

O 3.5 Mon 11:30 HSZ/0204

A direct measurement of weak lateral trapping over a C_6 ring — •Alfred John Weymouth[1], Maximilian Titl[1], Shinjae Nam[1], Lukas Hörmann[2], Oliver Hofmann[3], and Franz J. Giessibl[1] — [1]University of Regensburg, Germany — [2]University of Warwick, U.K. — [3]TU Graz, Austria

Six-membered carbon rings (C_6 rings) can be found in a multitude of systems from graphite to organic molecules. Graphitic surfaces are so flat that they have been used to explore superlubricity, where one important aspect of their fric-

tional response is the trapping of a single atom in an individual C_6 ring. This trapping also plays a role in the lateral movement of adsorbates on these surfaces. However, studies investigating trapping on these surfaces often focus only on strongly-bound adsorbates. We experimentally measure the trapping of a weakly-bound single atom asperity using lateral force microscopy with a CO-tip and simulate this system with DFT-based methods. Surprisingly, we observe a uniform lateral spring constant within individual C_6 rings over heights of tens of picometers for a range of systems. To precisely determine the surface trapping, we re-evaluate the lateral spring constant of the CO at the tip apex. With this value, we determined a very weak lateral spring constant of a particle within a C_6 ring.

O 3.6 Mon 11:45 HSZ/0204

Atomic scale energy dissipation as a function of temperature measured with LFM — •Sophia Schweiss[1], Lukas Hörmann[2], Franz Giessibl[1], and Alfred Weymouth[1] — [1]University of Regensburg, Regensburg, Germany — [2]University of Vienna, Vienna, Austria

One method of studying atomically resolved surfaces and adsorbates is small amplitude FM-AFM. With this technique, the conservative (frequency shift, Δf) and non-conservative (dissipated energy, E_{diss}) components of the tip-sample interaction are measured. Lateral force microscopy (LFM) is a related technique in which the tip oscillates laterally. Tip preparation for standard FM-AFM experiments at low temperature often includes the pickup of a CO molecule at the tip apex, which results in an inert tip with enhanced imaging properties. [1] These tip preparation techniques are also available for LFM. Over individual chemical bonds, LFM yields a measurable E_{diss} signal which we interpret as the CO snapping over the bond. [2]

Here, a CO-terminated tip is used to investigate the bonds of PTCDA molecules deposited on a Cu(111) surface with LFM. E_{diss} is measured for different temperatures in the range of 5.3 K to 6.5 K. Certain bonds exhibit a distinct T-dependence, whereas others do not.

[1] Gross et al., Science, 325, 1110 (2009)
[2] Weymouth et al., Phys. Rev. Lett., 124, 196101 (2020)

O 3.7 Mon 12:00 HSZ/0204

Bond-resolved STM with density-based methods — Emiliano Ventura-Macias[1], Jose Martinez-Castro[2], Guillermo Haas[1,3], •Jara Trujillo-Mulero[1], Pablo Pou[1], Markus Ternes[2], Ruslan Temirov[2], Frank Stefan Tautz[2], and Rubén Pérez[1] — [1]Departamento de Física Teórica de la Materia Condensada and Instituto de Física de la Materia Condensada (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425, Jülich, Germany — [3]Grenoble INP-Phelma, 3 Parv. Louis Néel, 38000 Grenoble, France

Bond-resolved STM (BRSTM) combines scanning tunneling microscopy with the intramolecular resolution of CO-functionalized ncAFM. We introduce a simple, broadly applicable method for simulating BRSTM images and apply it to new measurements of PTCDA on Ag(111) acquired with unprecedented tip-sample control (~10 pm). Our approach integrates the Full-Density-Based Model (FDBM) for high-resolution AFM with Chen's derivative approximation, capturing both σ and π tunneling channels while accounting for CO-tip deflection. It accurately reproduces experimental images of PTCDA/Ag(111) and TOAT/Cu(111), including subtle distance-dependent features. We also show that substrate-induced changes in orbital occupation and CO relaxation significantly influence BRSTM contrast.

O 4: Metal & Semiconductor substrates: Adsorption and reaction of small molecules I

Time: Monday 10:30–12:15 Location: HSZ/0401

O 4.1 Mon 10:30 HSZ/0401

Increasingly incoherent: Effects of adatoms on the structure and characterisation of physisorbed aromatic molecules on Cu(111) — •Henry Thake[1], Matthew Stoodley[1,2], Mariia Radova[1], David A. Duncan[2,3], Lukas Hörmann[4], and Reinhard J. Maurer[1,4] — [1]University of Warwick, UK — [2]Diamond Light Source, UK — [3]University of Nottingham, UK — [4]University of Vienna, AT

X-ray standing wave (XSW) is a quantitative structural characterisation technique for hybrid metal-organic interfaces, providing species-dependent adsorption heights at picometer accuracy. Alongside adsorption heights, XSW measurements provide information on the coherence of the signal, directly related to the structural disorder of the overlayer. A series of recent XSW experiments on physisorbed poly-aromatic hydrocarbons (PAHs) revealed surprisingly low coherent fractions that are inconsistent with structural models produced by Density Functional Theory (DFT) calculations. In this talk, we investigate a hypothesis that this apparent increase in disorder may be related to molecular interactions with surface adatoms that are omnipresent at ambient conditions. Using a frozen transfer learned interatomic potential trained on DFT data of PAHs on Cu(111), we probe the influence of adatoms on dynamic adsorption at the interface. Spectroscopic measurements of these systems reveal perturbations in the electronic structure that are consistent with the co-adsorption of PAHs with adatoms. The inclusion of Cu adatoms to Cu(111) consistently increases the disorder for the PAHs, in line with XSW measurements.

O 4.2 Mon 10:45 HSZ/0401

Interfacial Processes in Ionic Liquid-Modified Catalysts — •Laura Ulm, Cynthia C. Fernández, Hans-Peter Steinrück, and Florian Maier — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg

Solid catalysts with ionic liquid layers (SCILL) provide a powerful route to tailor the selectivity of catalytic reactions. In this context, we study the elementary reaction steps involved in the hydrogenation of 1,3-butadiene to 1-butene, a reaction in which high selectivity is crucial for hydrocarbon processing. We recently demonstrated that ionic liquids (ILs) selectively modify the adsorption of 1,3-butadiene over 1-butene, that is, the initial step of the hydrogenation of 1,3-butadiene on Pt(111). Herein, we now address the next reaction step, namely, how ultrathin layers of the IL $[C_8C_1Im][PF_6]$ influence olefin displacement from Pt(111). Ultrathin films of IL with thicknesses < 1 nm are prepared in situ by physical vapor deposition. Using temperature-programmed X-ray photoelectron spectroscopy (TPXPS), we track structural and compositional film changes and olefin desorption with increasing temperature. We find that i) IL deposition onto a saturated 1-butene layer enhances the displacement and desorption of 1-butene by a factor of 2.8; ii) 1,3-butadiene remains unaffected by the IL; and iii) IL decomposition on Pt(111) is shifted to higher temperatures by 80 ± 10 K.

O 4.3 Mon 11:00 HSZ/0401

Investigating CO Oxidation on Rh(111)/(332) with High-Repetition-Rate Velocity Resolved Kinetics — •Johannes Diedrich, Arved Dorst, and Tim Schäfer — Georg-August-Universität Göttingen, Institut für Physikalische Chemie, Tammannstr. 6, 37077 Göttingen

Velocity resolved kinetics (VRK) allows measuring the temporal evolution of reaction products from surfaces. A recent development is high repetition rate (HRR)-VRK [1]. By using more ionization pulses per molecular beam pulse, the signal-to-noise ratio is significantly improved and data acquisition accelerated.

An ultra-high-vacuum apparatus used for conventional VRK was modified to HRR-VRK by using a 100 kHz femtosecond laser for multiphoton nonresonant ionization and a TimePix3 event camera. This setup enables measururement of the full time of flight spectrum for every laser pulse.

Preliminary results are presented for the oxidation of CO on Rh(111) and (332) facets. This system allows comparison of conventional and HRR-VRK for a previously investigated reaction [2]. Thermal and hyperthermal CO2 channels are distinguished and deviations from the single-exponential decay are discussed. In future work, the decomposition of hydrazine on Ir will be investigated to gain a deeper understanding of Ir-based monopropellant thruster catalysts.

[1] F. Nitz et al., Rev. Sci. Instrum. 96, 055106 (2025).
[2] A. C. Dorst, PhD diss. (Georg-August-University Goettingen 2025).

O 4.4 Mon 11:15 HSZ/0401

First-principles structure search study of multi-component alloys for electrocatalysis — Lei Jia, •Guo-Xu Zhang, and Zhenbo Wang — MIIT Key Laboratory of Critical Materials Technology for New Energy Conversion and Storage, School of Chemistry and Chemical Engineering, Harbin Institute of Technology, Harbin, P. R. China

Multi-component alloys (MCA) have gained increasing attention as electrocatalysts due to their tunability of catalytic properties, while vast composites and diverse active sites make them highly challenging to identify configurations of molecules on surfaces. Here, we combined first-principles calculations with an active machine learning approach, Bayesian Optimization Structure Searching (BOSS), which enables efficient and accurate identification of molecular adsorbate structures on the MCA surfaces. This strategy utilizes smart sampling of adsorption energy surface (AES), constructs a surrogate model to predict the AES landscapes, and continuously refines the models to search global and local minima of adsorption configurations. The performance of first-principles calculations with BOSS was illustrated by benchmark data against single-atom, binary and ternary alloy catalysts. The good predictive power of our method suggests an effective way towards large-scale molecular adsorption for MCA electrocatalysts.

O 4.5 Mon 11:30 HSZ/0401

Surface effects during plasma-activated nitrogen splitting for catalytic ammonia formation — •Sabine Auras and Roland Bliem — ARCNL, Amsterdam, The Netherlands

Plasma-assisted catalysis (PAC) enables the activation of stable molecules, e.g. N_2 or CO_2, by generating reactive species that interact with a catalyst, thereby lowering dissociation barriers and creating new reaction pathways. For ammonia synthesis, PAC is particularly attractive as it can operate under milder conditions than the conventional Haber-Bosch process, potentially improving efficiency while reducing energy input. However, plasma fundamentally alters the reaction environment, which limits the applicability of concepts from thermal catalysis. Therefore, in-situ studies of surface properties and adsorbate evolution are needed to understand the surface chemistry under plasma conditions.

Here, we present the first in situ XPS data of Ru and Rh surfaces during N_2 plasma exposure, as well as mixed N_2/H_2 plasmas. To correlate surface processes and plasma properties, we further characterize the plasma composition by optical emission spectroscopy and monitor gas-phase products using mass spectrometry. The results reveal distinct differences in how activated N_2 species interact with the catalytic surface. This allows us to identify surface intermediates, assess reaction kinetics, and propose a mechanism for NH_3 formation, taking into account the role of different plasma species. Our findings highlight the need for a combined approach to identify the role that plasma and catalytic surfaces play - and thus to understand the interactions driving plasma-assisted catalysis.

O 4.6 Mon 11:45 HSZ/0401

Bonding properties of a CO molecule with metallic adatoms — •Fabian Stilp, Marco Weiss, Mia Fuerst, Maximilian Krueger, Luis Vendolsky, Nicolas Wirth, Hendrik Weinert, and Franz J. Giessibl — Department of Physics, University of Regensburg, Germany

CO terminated AFM tips are often used to investigate molecules on surfaces as they are a powerful tool to make the internal structure of such molecules visible. Their chemical inertness results in high resolution of the single atoms and bonds in such molecule via Pauli repulsion. However, it was shown by Huber et al. [1] that CO terminated tips can form weak bonds to some species of adatoms on a Cu (111) sample such as Fe and Cu. In contrast, Si adatoms only interact via van der Waals attraction and Pauli repulsion.

Can one predict the strength of the bond between the CO molecule and an arbitrary atom just from its electron configuration? To set the rules for this prediction we expand our collection of AFM measurements with various atomic species.

In total the interaction between the CO molecule and the adatom shows up to five different regimes, two attractive and three repulsive. The forces are distinctly pronounced, which allows to group the atoms in four different types.

We analyze the different atomic species for their different barrier before forming the bond, directionality of the bond and electrostatic interactions.

[1] Huber et al., Science 366, 235-238 (2019).

O 4.7 Mon 12:00 HSZ/0401

Online monitoring of the oxygen adsorption on Cu(110) with PEEM and DRS — •Robert Heller, Thorsten Wagner, and Peter Zeppenfeld — Johannes Kepler University, Institute of Experimental Physics, Surface Science Division, 4040 Linz, Austria

We studied the dissociative adsorption of oxygen on the Cu(110) surface using Photoelectron Emission Microscopy (PEEM) and Differential Reflection Spectroscopy (DRS) simultaneously. Unlike many experiments carried out already in the 1970s and 1980s, our approach focusses on real-time monitoring. For oxygen exposures up to ~100L, at temperatures between 350K and 420K, the process saturates at an oxygen coverage of 0.5 with a well-ordered (2×1)O superstructure. At intermediate coverages, a regular pattern of alternating Cu and CuO stripes is formed [1].

We used a PEEM with a xenon lamp (Xe) to study changes in the electron yield (EY) during the exposure. Oxygen adsorption causes a decrease in EY and, hence, an increase in the work function. Since our DRS setup uses the same light source as the PEEM, we can synchronously record the change of the reflectance and reliably compare the two signals. Interestingly, the normalised adsorption curves are not identical, indicating that the PEEM and/or the DRS signals are not directly proportional to the oxygen coverage. This could be related to the effect of the formation of the nanostructured Cu-CuO stripe pattern upon oxygen adsorption [1].

[1] K. Kern et al., Phys. Rev. Lett. 67, 855 (1991).

O 5: Focus Session: Mineral-water interfaces I

The Focus Session discusses recent advances in the understanding of mineral-water interfaces. These interfaces are ubiquitous in nature, host of many geological and biological processes, intimately linked to the global carbon cycle, and therefore highly relevant for Earth*s climate. For example, silicate weathering removes carbon dioxide from the atmosphere on geological timescales, acting as a stabilizing feedback mechanism since weathering rates increase with temperature. In the oceans, carbonates dissolve and precipitate in response to changing atmospheric carbon dioxide concentrations, thus far mitigating part of the anthropogenic impact of CO_2 emissions. In addition, numerous industrial and technological processes involve mineral-water interfaces, including seawater desalination, scaling and incrustation prevention, as well as various biochemical applications. However, and despite their importance, many fundamental aspects of mineral-water interfaces remain poorly understood, including water binding and diffusion, structure formation, ice nucleation, growth, or desorption.

This DPG Focus Session will address these aspects at the molecular level, elucidating fundamental processes involving both single water molecules and bulk water in contact with mineral surfaces. The session brings together scientists investigating mineral-water systems under ultrahigh vacuum conditions as well as at mineral-water interfaces in bulk aqueous environments. We aim for a balanced Session with contribution from both renowned experts and young investigators active in the field.

Organized by Philipp Rahe (U Osnabrück), Angelika Kühnle (U Bielefeld), Jan Balajka (TU Vienna), Wolf Gero Schmidt (U Paderborn).

Time: Monday 10:30–12:30 Location: HSZ/0403

Invited Talk O 5.1 Mon 10:30 HSZ/0403

Can the mineral-water interface save the world? Mineral carbonation, enhanced weathering and negative emissions — •Philip Pogge von Strandmann — Johannes Gutenberg University, Mainz

The rising atmospheric CO2 concentrations are clearly having a significant impact on the climate, and will continue to do so. The currently only foreseeable method by which anthropogenic climate change will not be completely catastrophic (i.e. limited to 1.5-2°C warming), is if we implement global "negative emissions" technologies, that is the artificial removal of CO2. Two such technologies directly rely on the mineral-water interface: mineral carbonation and enhanced weathering. Both require the dissolution of silicate minerals in mildly acidic water, and the subsequent precipitation of carbonate secondary minerals, but without too much precipitation of silicate secondary minerals, which hinder the reaction. In fact, the reaction is more complex than that, because numerous reactions occur at the mineral-water interface: dissolution, sorption, exchange, co-precipitation and incorporation into interstitial sites in mineral lattices. Each of these reactions has significant consequences for the efficiency of the reaction and the CO2 drawdown. This presentation will examine these reactions, including the aspects we currently understand and can measure, and those where our knowledge and analytical abilities are still lacking.

O 5.2 Mon 11:00 HSZ/0403

Reconstruction of calcite (10.4) manifests itself in the tip-assisted diffusion of water — •Klausfering Lea, Schneider Florian, Bechstein Ralf, and Kühnle Angelika — Bielefeld University, 33615 Bielefeld, Germany

Calcite is the most common carbonate in the Earth*s crust and plays a fundamental role in environmental and industrial processes. The most stable cleavage plane of calcite is the (10.4) plane. This surface has already been extensively stud-

ied in liquid environments as well as under ultra-high vacuum (UHV) conditions. Under UHV conditions, the surface exhibits a (2 x 1) reconstruction. Due to this reconstruction, there are two energetically different adsorption sites for adsorbates, such as water. Here, we present an atomic force microscopy (AFM) study in which the diffusion of individual water molecules on the calcite (10.4) surface was investigated under UHV conditions at a temperature of 140 K. The positions of individual water molecules could be precisely determined in several consecutive atomically resolved images, allowing the diffusion of the water molecules to be observed. We found that the AFM tip has an influence on the diffusion of the water molecules, but that diffusion only occurs between one type of adsorption positions.

O 5.3 Mon 11:15 HSZ/0403

Nanoscopic insights on ice nucleation on microcline (001) — •Florian Schneider[1], Rasmus Väinö Erik Nilsson[2], Ralf Bechstein[1], Bernhard Reischl[2], Thomas Koop[1], Angelika Kühnle[1], and Tobias Dickbreder[3] — [1]Bielefeld University, Bielefeld, Germany — [2]University of Helsinki, Helsinki, Finland — [3]University of Vienna, Vienna, Austria

Heterogeneous ice nucleation plays a crucial role in various environmental and technological processes. An in-depth understanding of the nucleation at the atomic scale can greatly enhance our capability to create materials with particular ice-nucleating properties and improve our climate models. In the atmosphere, a particularly active ice nucleating particle is dust from the feldspar mineral microcline [1]. However, why microcline outperforms other mineral dust particles in its ice-nucleating ability still remains a puzzle. Here, we present atomic force microscopy images of ice crystals growing from the vapor phase on the (001) surface of microcline at low temperature. In contrast to the prevailing view of active sites such as step edges or cracks being responsible for ice nucleation, we observe ice growth at random positions on the bare terrace. For the closely related feldspar sanidine, in contrast, ice nucleation is prevalent at step edges as expected. This comparison underscores the exceptional ice nucleating ability of microcline as it demonstrates ice nucleation even in the absence of surface defects and raises important questions regarding the different ice nucleation mechanisms on these two feldspar mineral surfaces.

[1] Harrison, A. D. *et al.*, Atmos. Chem. Phys., 16, 2016.

Invited Talk O 5.4 Mon 11:30 HSZ/0403

Machine learning exploration of water binding and ice nucleation at silicate and carbon surfaces — •Mie Andersen — Department of Physics and Astronomy, Aarhus University, Denmark

Mineral-water interfaces play a central role in environments ranging from the interstellar medium to Earth's surface and subsurface. In astrochemistry, the chemical evolution of star-forming regions is controlled by gas-grain interactions on dust grains that may be partially or fully covered by water ice. A key quantity underlying these processes is the binding energy (BE) of adsorbates, which determines desorption and diffusion rates and controls chemical kinetics.

In this contribution, we explore computational strategies to quantify BE distributions at complex, partially ice-covered mineral surfaces. Using graphene and forsterite as model grain substrates, we combine atomistic simulations with machine-learning interatomic potentials to generate realistic surface structures and to efficiently sample BEs. The modelled ice structures range from amorphous structures generated by low-temperature molecular dynamics simulations to highly stable crystalline structures generated by global structure optimization. The resulting BE distributions are analyzed in terms of surface heterogeneity, ice coverage and hydrogen bonding.

While motivated by astrochemical applications, the presented methodology is broadly transferable to mineral-water interfaces under terrestrial conditions. The approach offers a general framework for linking molecular-scale interfacial structure to macroscopic transport and reaction models across disciplines.

O 5.5 Mon 12:00 HSZ/0403

Chiral water structures on dolomite(104) surfaces — •Jonas Heggemann[1], Paul Laubrock[1], Jie Huang[2], Adam S. Foster[2,3], and Philipp Rahe[1] — [1]Institute of Physics, Osnabrück University, Osnabrück, Germany — [2]Department of Applied Physics, Aalto University, Helsinki, Finland — [3]Nano Life Science Institute (WPI NanoLSI), Kanazawa University, Kanazawa, Japan

The formation mechanisms of dolomite ($CaMg(CO_3)_2$), an abundant rock-forming carbonate mineral with rhombohedral structure [1], are still poorly understood in the earth's crust [2]. The lack of replicating mineral growth under geological conditions in the laboratory is a further characteristic of the "dolomite problem" [2]. Consensus could be reached that dolomite formation only occurs in the presence of water [3] and it is further known that (104) is the most stable surface [4].

Here, we unravel a chiral character of dolomite(104) surfaces from non-contact atomic force microscopy data acquired with CO terminated tips. Backed by density functional theory and probe-particle model calculations, the presence of two surface enantiomers is identified. We further investigate water adsorption, with coverage ranging from single molecules to a full monolayer. Preferred water adsorption is found at calcium and magnesium surface sites; yet, the geometries carry a clear chiral property.

[1] L. S. Land, AAPG **24**, 1 (1982)
[2] J. A. Roberts, Nature Geoscience **17**, 716 (2024)
[3] S. E. Kaczmarek *et al.*, Sedimentology **61**, 1862 (2014)
[4] N. H. De Leeuw, Am. Mineral. **87**, 679 (2002)

O 5.6 Mon 12:15 HSZ/0403

Atomically Resolved Imaging of the Gypsum (010) surface — •David Kugler, Andrea Conti, Tun Sinner, Florian Mittendorfer, Michael Schmid, Gareth S. Parkinson, Ulrike Diebold, and Jan Balajka — Institute of Applied Physics, TU Wien, Vienna, Austria

Gypsum ($CaSO_4{\cdot}2H_2O$), the dihydrate of calcium sulfate, is the most abundant sulfate mineral in Earth's crust and it is widely used as a fertilizer and as a construction material. Its bulk crystal structure consists of alternating calcium sulfate bilayers and bilayers of crystal water. While the water in the bulk has been extensively studied, a comprehensive understanding of surface processes is still missing. Water is, however, present on all surfaces in ambient environment and influences surface chemistry. Because the adjacent layers are linked only by hydrogen bonds, gypsum cleaves readily along the (010) plane, exposing large, atomically flat terraces. In this work, noncontact atomic force microscopy (nc-AFM) with a qPlus sensor was used to resolve the atomic structure of the cleaved gypsum (010) surface and to visualize the configuration of adsorbed water. Our results indicate that one of the surface crystal water molecules rotates into a lower energy orientation, forming a hydrogen bond with the second crystal water molecule within the unit cell. Preliminary ab-initio modeling suggests that the first adsorbed water layer preserves the periodicity of the bulk structure by forming hydrogen bonds with the surface crystal water.

O 6: Organic molecules on inorganic substrates: Adsorption and growth I

Time: Monday 10:30–12:30 Location: TRE/PHYS

O 6.1 Mon 10:30 TRE/PHYS

Support-dependent reactivity of Fe-DCA 2D Metal-Organic Frameworks — •Dominik Hrůza[1], Zdeněk Jakub[1], Jakub Planer[1], Tadeáš Lesovský[2], Ayesha Jabeen[1], Pavel Procházka[1], and Jan Čechal[1,2] — [1]CEITEC - Central European Institute of Technology, Brno University of Technology, Purkyňova 123, Brno 61200, Czechia — [2]Institute of Physical Engineering, Faculty of Mechanical Engineering, Brno University of Technology, Technická 2896/2, Brno 61200, Czechia

2D Metal-Organic Frameworks (2D MOFs) are promising materials for applications in catalysis, sensing and spintronics. 2D MOFs based on 9,10-dicyanoanthracene (DCA) linker molecules are particularly intriguing due to their recently demonstrated magnetic and topological properties. Here, we study the reactivity of Fe-DCA supported on two weakly-interacting supports: graphene/Ir(111) and Au(111). Using Scanning Tunneling Microscopy (STM), X-Ray Photoemission Spectroscopy (XPS) and Low-Energy Electron Microscopy/Diffraction (LEEM/LEED), we test how the Fe-DCA reacts with carbon monoxide and molecular oxygen. When the Fe-DCA is supported on graphene, the CO adsorbs on the Fe-sites at temperatures below 200 K, while O2 exposure causes structural collapse of the 2D MOF at room temperature. In contrast, when the Fe-DCA is supported on Au(111), it appears inert to CO adsorption. Overall, our results show how the chemical reactivity of 2D MOFs depends on the supporting surface, providing critical insights for the potential integration of MOFs into functional devices.

O 6.2 Mon 10:45 TRE/PHYS

LT-STM investigation of azulene-based molecular architectures on metal surfaces — •Suchetana Sarkar[1,4], Natasha Khera[1], Kwan Ho Au-Yeung[1,5], Renxiang Liu[1,2,3], Ji Ma[1,2,3], Xinliang Feng[1,2,3], and Francesca Moresco[1] — [1]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [2]Chair of Molecular Functional Materials and Faculty of Chemistry & Food Chemistry, TU Dresden, 01062 Dresden, Germany — [3]Max Planck Institute of Microstructure Physics, Weinberg 2, Halle, Germany — [4]Present address: Department of Chemistry, Philipps-Universität Marburg, 35032 Marburg, Germany — [5]Present address: Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany

Azulene-based molecules offer a unique platform for probing on-surface self-assembly and electronic structure due to their non-benzenoid topology and intrinsic dipole. Presented here are the investigations of two related systems:

a cyclopenta[cd]azulene trimer (CPAT) and a phenyl-functionalized analogue (CPAT-Ph), using low-temperature scanning tunneling microscopy and spectroscopy. CPAT forms well-ordered homochiral domains on Au(111), whereas CPAT-Ph exhibits weak adsorption and high mobility on Au(111) and shows no ordered phases on Cu(110). Spectroscopy reveals clear electronic differences between the molecules and substrate-induced shifts for CPAT-Ph. Finally, the results of thermally induced ring-closing reactions are also shown, discussing routes toward on-surface synthesis of non-benzenoid nanographenes.

O 6.3 Mon 11:00 TRE/PHYS

Surface study of heteromolecular layers for charge injection: deprotonated carboxylic acids mixed with pentacene — •Jakub Planer[1], Veronika Stará[1], Pavel Procházka[1], and Jan Čechal[1,2] — [1]Central European Institute of Technology, Brno University of Technology, Czech Republic — [2]Institute of Physical Engineering, Brno University of Technology, Czech Republic

Heteromolecular organic films represent promising candidates for efficient charge-injection layers in organic optoelectronic devices. Using surface-science experiments together with ab-initio modeling, we investigate the structural and electronic properties of intermixed layers composed of fully deprotonated carboxylic acids and pentacene (PEN) on Ag(100) and Ag(111) substrates. Our work demonstrates that these molecules form blends capable of modulating the electrode work function by up to 0.5 eV, depending on the mixing ratio, while remaining stable during subsequent organic-semiconductor deposition. These findings underline the potential of mixed carboxylate–PEN layers as practical, robust charge-injection modifiers and show that various carboxylic acids can be effectively used in such heteromolecular interfaces [1,2].

[1] Stará, Veronika, et al. *Tunable Energy-Level Alignment in Multilayers of Carboxylic Acids on Silver.* Physical Review Applied, **18**, (2022)

[2] Krajňák, T. et al. *Robust Dipolar Layers between Organic Semiconductors and Silver for Energy-Level Alignment.* ACS Appl. Mater. Interfaces, **16**, (2024)

O 6.4 Mon 11:15 TRE/PHYS

Orientational Order of Phenyl Rotors on Triangular Platforms on Ag and Au(111) — Richard Berndt[1], Richard Berndt[2], Richard Berndt[2], Richard Berndt[3], and •Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, CAU Kiel, Germany — [2]Otto-Diels-Institut für Organische Chemie, CAU Kiel, Germany — [3]Centro de Física de Materiales, Donostia-San Sebastián, Spain

We investigated trioxatriangulenium functionalized with phenyl on Ag(111) and Au(111) using low-temperature scanning tunneling microscopy (STM). On Ag, the molecules form hexagonal arrays and the orientations of the phenyl moieties are resolved. Moreover, STM images suggest a dimerization of the molecules. Density functional theory calculations reproduce the experimental data. Van der Waals interaction is the dominant binding mechanism. The apparent dimerization results from an asymmetry of the phenyl wavefunction, which reflects intramolecular hydrogen bonding between the ligand and an oxygen atom of the triangulenium platform. Direct long-range interaction between phenyl moieties across molecules and the intramolecular H bonding are decisive for the orientations of the phenyl moieties. Similar experimental results were obtained on Au(111).

O 6.5 Mon 11:30 TRE/PHYS

Adsorption and Isomerization of Azobenzene Tetramers on Au(111) — •Natasha Khera[1], Ebru Cihan[1], Franz Plate[1], Soyoung Park[2], Ningwei Sun[2], Dmitry A. Ryndyk[1,2], Franziska Lissel[2,3], and Francesca Moresco[1] — [1]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [2]Leibniz Institute of Polymer Research Dresden, Germany — [3]Institute for Applied Polymer Physics, TU Hamburg, 21073 Hamburg, Germany

This work investigates the manipulation and voltage-induced switching of star-shaped azobenzene tetramers [1] on Au(111) using low-temperature ultra-high vacuum scanning tunneling microscopy (LT-UHV STM) to study their adsorption behavior and cis-trans isomerization. On terraces, molecules in the trans state are highly mobile and difficult to image stably, whereas voltage induced switching to the cis state makes them immobile for reliable measurement. The study also utilizes step-edge sites where trans molecules are more stable and can be addressed without prior switching. Voltage pulses with the STM tip produces reproducible switching between high-contrast and low-contrast STM signatures, consistent with the cis-trans isomerization of the azobenzene core. Electric-field-dependent measurements are also performed by retracting the STM tip and recording tip-height vs bias characteristics, providing insight into the electric-field driven response of the molecules.

[1]. M. Baroncini, et al. Nature Chemistry 7, 634-640, (2015)

O 6.6 Mon 11:45 TRE/PHYS

Steering interfacial molecular self-assembly by substrate-molecule charge transfer — •Benjamin Achatz, Matthias Zeilerbauer, Marco Thaler, and Laerte Patera — Department of Physical Chemistry, University of Innsbruck, Innsbruck, 6020, Austria

Scanning probe microscopy studies of organic molecules on metal substrates have furthered our understanding of substrate-molecule charge transfer processes [1]. On surface self-assembly of the electron acceptor C_{60} is driven by an interplay of short-range attractive Van der Waals forces and long-range repulsive electrostatic interactions [2]. Here we report the formation of an intermixed phase composed of C_{60} and Zn(II)-5,10,15,20-tetrakis(4-aminophenyl)porphyrin (Zn-TAPP) molecules on Ag(111). An approach combining scanning tunneling spectroscopy (STS) and Kelvin probe force microscopy (KPFM) was used to investigate the degree of substrate-molecule charge transfer for C_{60} in close-packed islands and a row-like intermixed structure. Analysis of our tunneling and force spectroscopy measurements revealed that mitigation of the coulomb repulsion drives the formation of the intermixed phase and promotes additional charge transfer to the C_{60} molecules. These results demonstrate that controlling long-range Coulomb interactions can steer the formation of distinct self-assembled structures on metal substrates, offering insights for the design of new charge-optimized molecular nanostructures.

[1] R. Otero et al., Surf. Sci. Rep. 72, 105 (2017).

[2] M. Švec et al., Phys. Rev. B 86, 121407 (2012).

O 6.7 Mon 12:00 TRE/PHYS

Nanostructuring of organic radicals on cobalt surfaces — •Arkaprava Das and M. Benedetta Casu — Institute of Physical and Theoretical Chemistry, University of Tübingen, Tübingen, Germany

Organic radicals are potential candidates for groundbreaking applications like energy storage, quantum computing, and spintronics. To investigate the nature of the adsorption of the radical derivative molecules on cobalt surfaces, we investigate their electronic structure and morphology. The electronic structure at the interface is investigated by using X-ray photoelectron spectroscopy (XPS), and the morphology is studied with scanning electron microscopy. The radical/Co interface interactions have resulted in different nanostructures crucial for device fabrication, whereas changes in line shape of core level spectra confer direct evidence of changed electronic properties at the interface. Considering ecological requirements, we also endeavour to minimize the materials consumption by making the Co substrate reusable, which is in line with the principles of closed-loop circular economy.

O 6.8 Mon 12:15 TRE/PHYS

Competition between dative bonds and aromatic gains — •Jonas Brandhoff[1], Richard Berger[2], Felix Otto[1], Maximilian Schaal[1], Lorenz Brill[1], Oliver T. Hofmann[2], Peter Puschnig[3], Torsten Fritz[1], and Roman Forker[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany — [2]Institute of Solid State Physics, Technical University Graz, Petersgasse 16, 8010 Graz, Austria — [3]Institute of Physics, University of Graz, Universitätsplatz 5, 8010 Graz, Austria

Upon molecular adsorption on a surface, a variety of interactions can occur. Identifying which mechanisms dominate this complex quantum-mechanical landscape is crucial for understanding molecule – surface coupling. One key factor in many π-conjugated systems is aromaticity – a fundamental concept in chemistry describing the energetic stabilization that arises from particular π-electron arrangements. To investigate how aromaticity competes with other adsorption-driven interactions, we study 5,7,12,14-pentacenetetrone (P4O) on different metal surfaces as a model system. P4O is a prototypical molecule expected to undergo aromatic stabilization upon adsorption, where charge transfer from the substrate modifies the topology of the occupied π-system and leads to a more energetically favorable configuration. Using photoemission orbital tomography measurements combined with density functional theory calculations, we show how hybridization with the surface can outweigh a potential aromatic stabilization, *not* necessarily maximizing the latter. We reveal a mechanism in which the unoccupied π-system of the molecule forms dative bonds with the substrate.

O 7: 2D Materials: Electronic structure, excitations, etc. I (joint session O/HL/TT)

Time: Monday 10:30–12:30 Location: TRE/MATH

Invited Talk O 7.1 Mon 10:30 TRE/MATH

Magnetic Order in 2D Materials Beyond Bulk Constraints — •Jeison Fischer — II. Physikalisches Institut, Universität zu Köln

Even though exfoliated microflakes remain widely used in 2D magnetism research, their bulk origin restricts access to many potentially interesting phases, an obstacle that molecular beam epitaxy (MBE) can overcome. MBE enables the controlled synthesis of single-layer materials directly related to, yet often distinct from, their bulk counterparts.

In my talk, I will present structural characterization and discuss the mechanisms behind the formation of such novel 2D materials grown via MBE on graphene. [1-2] The emerging magnetic properties of these new 2D materials will be exemplified with two cases: Cr_2S_3-2D and Fe_2S_2-2D. Cr_2S_3 forms a covalently bonded NiAs-type structure without van der Waals gaps. Using spin-polarized scanning tunneling microscopy (STM) and X-ray magnetic circular dichroism (XMCD), we show that it hosts ferromagnetic coupling within the plane with magnetic moments pointing out-of-plane, combined with A-type antiferromagnetic coupling between different Cr planes. Fe_2S_2 exhibits a unique hexagonal phase, in which Fe atoms occupy tetragonally coordinated sites. Spin-polarized STM reveals that the moments are noncollinear within the plane. We map the in-plane components of two distinct magnetic configurations and find that the moments are confined to the 2D plane, forming a Néel state and a 2Q state.

[1] Knispel et al. Small, 2025 21, 2408044.
[2] Safeer et al. Adv. Funct. Mater. 2025, 202500907.

O 7.2 Mon 11:00 TRE/MATH

Ab initio modeling of magnons and magnon-phonon coupling in 2D magnetic materials — Ali Esquembre-Kucukalic[1], Khoa Le[2], Hsiao-Yi Chen[3], Ivan Maliyov[2], Jin-Jian Zhou[4], Davide Sangalli[5], and •Alejandro Molina-Sánchez[1] — [1]ICMUV, University of Valencia, Valencia, Spain — [2]CALTECH, California, USA — [3]Tohoku University, Japan — [4]Beijing Institute of Technology, Beijing, China — [5]ISM-CNR, Roma, Italy

Understanding spin-wave excitations in two-dimensional magnetic materials is essential for advancing spintronic and quantum information technologies. Chromium trihalides and related 2D magnets provide a platform where the choice of halide influences on the magnetic behavior, yet its impact on magnon properties is not completely understood. We present first-principles calculations of magnon dispersions and wave functions in monolayer Cr trihalides using the Bethe-Salpeter equation (BSE), resolving key features such as the topological gap at the Dirac point. The BSE analysis reveals that magnons originate from electronic transitions spanning a wider energy range than excitons, offering new insight magnon character and enabling the extraction of Heisenberg exchange parameters. Building on this framework, we develop an ab initio description of mag-ph coupling by deriving BSE-based mag-ph interaction matrices and applying them to monolayer CrI3 and hydrogenated graphene. We show that mag-ph and electron-phonon couplings differ markedly, identifying specific phonon modes that dominate magnon scattering.

O 7.3 Mon 11:15 TRE/MATH

Electron-phonon interaction in transition-metal dichalcogenides — •Gerrit Johannes Mann, Thorsten Deilmann, and Michael Rohlfing — Institute of Solid State Theory, University of Münster, Germany

Electron-phonon interaction is a crucial effect in solid state physics, in particular in two-dimensional materials. We developed a generally applicable ab-initio implementation on top of density functional theory using a basis set of localized Gaussian orbitals. It combines finite differences calculations with the perturbative Allen-Heine-Cardona framework in order to calculate the temperature-dependent renormalization of the electronic bandstructure due to electron-phonon interaction. Our implementation circumvents the limiting problems of previous implementations and allows to evaluate Debye-Waller contributions beyond the rigid-ion approximation [1], which are usually neglected.

In addition to the renormalization of the electronic bands, electron-phonon interaction introduces a line broadening due to finite-lifetime effects, which have recently been incorporated into our implementation. In this presentation, we discuss our results, including those with finite-lifetime effects, for two-dimensional transition-metal dichalcogenides, where the renormalization of the electronic bandstructure due to electron-phonon interaction can be as large as several hundreds of meV.

[1] Mann et al., Phys. Rev. B **110**, 075145 (2024)

O 7.4 Mon 11:30 TRE/MATH

Surface-state engineering for nonlinear charge and spin photocurrent generation — •Javier Sivianes[1], Peio Garcia-Goiricelaya[2], Daniel Hernangómez-Pérez[3], and Julen Ibañez-Azpiroz[1,4,5] — [1]Centro de Física de Materiales (CSIC-UPV/EHU), Donostia, Spain — [2]University of the Basque Country UPV/EHU, Leioa, Spain — [3]CIC nanoGUNE BRTA, San Sebastián, Spain — [4]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — [5]Donostia International Physics Center (DIPC), Donostia, Spain

We systematically explore the generation of nonlinear charge and spin photocurrents using spin-orbit-split surface states. This mechanism enables net DC flow along the surface plane even in centrosymmetric bulk environments like the Rashba prototype Au(111), where we characterize the main quadratic contributions by combining model predictions with density functional calculations. We further identify the Tl/Si(111) surface as a prime scenario for experimental verification; with slight doping, it develops metallic surface states featuring remarkable relativistic properties deviating from the Rashba paradigm, while the bulk remains semiconducting. Its nonlinear charge photocurrent reveals a distinct angular signature and a magnitude comparable to bulk ferroelectrics, highlighting the potential of surface-state photocurrents for low-bias optoelectronic applications. Moreover, the non-trivial spin texture of its surface states enables the generation of pure out-of-plane spin-polarized currents, offering a highly versatile nonlinear spin-filtering functionality beyond the conventional spin Hall effect.

O 7.5 Mon 11:45 TRE/MATH

Influence of Vanadium Doping on WSe_2, as seen through ARPES — •Jana Kähler[1,2], Florian K. Diekmann[1,2], Matthias Kalläne[1,2,3], Tim Riedel[1,2], Adina Timm[1,2], Anja Yalim[1,2], Jens Buck[1,2], Meng-Jie Huang[2], Jules M. Knebusch[1,2], Luka Hansen[1,3], Jan Benedikt[1,3], and Kai Rossnagel[1,2,3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Spintronics offers a compelling, energy-efficient alternative to traditional electronics with potential applications in communications, sensing, and information processing. The vanadium-doped layered transition metal dichalcogenide $2H$-WSe_2 is particularly promising as a room-temperature magnetic semiconductor with gate-tunable transport properties. Here, we use a combination of 11 eV laser, 21.2 eV He-lamp, and soft X-ray synchrotron ARPES to highlight the influence of a fairly small vanadium doping on the electronic structure of WSe_2. Both the pristine and doped compounds were grown by chemical vapor transport in our own laboratory.

O 7.6 Mon 12:00 TRE/MATH

Engineering sulfur vacancy dimers in monolayer WS_2 — •Daniel Jansen[1], Guangyao Miao[1], Jan Keienburg[1], Jeison Fischer[1], Thomas Michely[1], Hannu-Pekka Komsa[2], and Wouter Jolie[1] — [1]Institute of Physics II, University of Cologne, Cologne, Germany — [2]Faculty of Information Technology and Electrical Engineering, University of Oulu, Oulu, Finland

Sulfur vacancies [1] and sulfur vacancy dimers in nearest-neighbor distance [2] in monolayer WS_2 have been experimentally proven to yield bright and stable photon emission, thus holding promises for the development of quantum technologies.

Here we investigate dimers of sulfur vacancies in different configurations in monolayer WS_2 created with the tip of a scanning tunneling microscope [3]. Scanning tunneling spectroscopy reveals strong hybridization of the sulfur vacancy electronic in-gap states, validated by density functional theory calculations. For dimers in nearest-neighbor configuration we find that inelastically tunneling electrons can induce sulfur atom migration, resulting in a rotary motion of the dimer. This motion is studied in detail by analyzing the emerging telegraph noise in the junction. Lastly, we elaborate on scenarios to make use of the dimer motion for the design of vacancy structures and lattices.

[1] Schuler et al., Sci. Adv. **6**, 38 (2020)
[2] Sun et al., Nature Commun. **15**, 9476 (2024)
[3] Jansen et al., Phys. Rev. B **109**, 195430 (2024)

O 7.7 Mon 12:15 TRE/MATH

Alkali-metal doped transition metal chlorides confined in bilayer graphene: Insights from first-principles calculations — •Munawar Ali[1], Arkady V. Krasheninnikov[2], Giovanni Cantele[1], and Mahdi Ghorbani-Asl[2] — [1]Università degli Studi di Napoli "Federico II," Dipartimento di Fisica "Ettore Pancini," Complesso di Monte S. Angelo, via Cinthia, 80126 Napoli, Italy — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany

The intercalation of atomic and molecular species into layered materials has emerged as a powerful strategy for synthesizing novel two-dimensional systems with tunable electronic, magnetic, and energy-storage properties. Encapsulating transition-metal halides into bilayer graphene has proven effective for stabilizing 2D magnetic phases that are otherwise thermodynamically unstable. Using density functional theory, we systematically investigate the intercalation of

metal chlorides (TCl_3, T = Fe, Cu, Mo, Al) doped with alkali metals (Li, Na, K, Rb, Cs) across a range of concentrations. Li- and Na-doped $FeCl_3$, $CuCl_3$, and $MoCl_3$ monolayers exhibit the highest thermodynamic stability, whereas $AlCl_3$ remains unstable even under doping. Bader charge analyses reveal substantial charge transfer from the graphene host to the intercalated layers, particularly in the case of $CuCl_3$, which also shows the strongest binding. These findings provide a theoretical framework for understanding the stability of these heterostructures and highlight alkali-metal-intercalated graphene systems as a platform for engineering tunable 2D magnetic materials.

O 8: Nanostructures at surfaces:1D, 2D, networks I

Time: Monday 10:30–12:30 Location: WILL/A317

O 8.1 Mon 10:30 WILL/A317

Quantum confinement of excited states in a two-dimension metal-organic coordinated network — •Lu Lyu[1], Martin Anstett[2], Wei Yao[3], Tobias Eul[1], Martin Aeschlimann[2], and Benjamin Stadtmüller[1] — [1]Experimentalphysik II, Institute of Physics, Augsburg University, Universitätsstraße 2, 86159 Augsburg, Germany — [2]Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau, Erwin-Schrödinger-Straße 46, 67663 Kaiserslautern, Germany — [3]Institute of Advanced Light Source Facilities, Shenzhen 518107, China

Quantum confinement effects of surface electrons in two-dimensional metal-organic coordinated networks (2D-MOCNs) provide a highly tunable platform for exploring the laws of quantum mechanics in condensed matter systems. Here, we focus on a porous network formed by coordinating pyridine-functionalized T4PT molecules with Co atoms on Au(111). One-photon photoemission (1PPE) experiments reveal a substantial energy shift of the Shockley surface state (SS) that is indicative of a hybridization with Co centers. This hybridization is responsible for a leaky channel for electrons between adjacent pores, which prevents the quantum confinement of SS electrons. In contrast, excited electrons into the unoccupied image potential states (IPS) reveal clear signatures of a substantial quantum confinement in a two-photon photoemission (2PPE) experiment. These contrasting observations of SS and IPS can be attributed to the 3D nature of the quantum well potential of the 2D-MOCNs and the distinct surface-perpendicular wave function distribution in the SS and the IPS.

O 8.2 Mon 10:45 WILL/A317

On-surface prepared 2D MOFs as models of single-atom catalysts: Fe-N_3 vs. Fe-N_4 — •Zdeněk Jakub[1], Jakub Planer[1], Dominik Hrůza[1], Ayesha Jabeen[1], Tadeáš Lesovský[1], and Jan Čechal[1,2] — [1]CEITEC, Brno University of Technology, Brno, Czechia — [2]Faculty of Mechanical Engineering, Brno University of Technology, Brno, Czechia

What defines the reactivity of the so-called single-atom catalysts? Here, we utilize 2D Metal-Organic Frameworks (MOFs) synthesized on an inert graphene support to address this fundamental question. By temperature-dependent scanning tunneling microscopy and density functional theory, we quantify the CO adsorption strengths on threefold-coordinated (Fe-N_3) and fourfold-coordinated (Fe-N_4) iron sites embedded within Fe-DCA and Fe-TCNQ 2D MOFs. A significant 0.5 eV difference in CO binding strengths is found, despite the fact that the electronic parameters like Fe oxidation state, spin configuration, occupancy of the individual d-orbitals and their positions with respect to Fermi level are almost identical prior to CO adsorption. We trace the origin of the different reactivity to the higher structural flexibility of the Fe-N_3 sites compared to Fe-N_4. These results highlight the key role of local coordination and demonstrate that reactivity cannot be reliably predicted from electronic structure parameters alone.

Invited Talk O 8.3 Mon 11:00 WILL/A317

Controlling nanostructures on surfaces via intermolecular interactions — •Yunjun Cao — Physical Chemistry I, Ruhr-Universität Bochum, D-44801 Bochum, Germany

Synthesizing sophisticated nanostructures on surfaces requires precise control over intermolecular interactions ranging from strong covalent bonds to weak van der Waals interactions. In the first part of the talk, I will present an irreversible, multi-step covalent coupling strategy for reactive molecules. By precisely controlling the reaction sequence, we synthesize highly branched nanostructures on a metal surface [1]. As a complementary approach, I will then introduce a reversible, multi-step self-assembly protocol for sterically crowded molecules, highlighting how intermolecular van der Waals interactions steer the formation of well-separated cyclic nanostructures with an unprecedented high yield [2]. Finally, I will turn to the single-molecule level and discuss how to control via van der Waals interactions the configuration of individual molecules [3] and the potential energy landscape of a dynamic chirality switch [4]. Our studies highlight how tunable intermolecular interaction strengths control the synthesis of tailored nanostructures on surfaces.

[1] Y. Cao et al., Nat. Commun. in press (2025). [2] Y. Cao et al., ACS Nano 19, 21942 (2025). [3] Y. Cao et al., Phys. Rev. B 111, 115426 (2025). [4] Y. Cao et al., Nat. Commun. 14, 4500 (2023).

O 8.4 Mon 11:30 WILL/A317

Autonomous Nanoworld: Building Nanostructure Without Human Intervention — •Bernhard Ramsauer[1], Qigang Zhong[2], Stefan Pranger[3], Bettina Könghofer[3], and Oliver T. Hofmann[1] — [1]nstitute of Solid State Physics, NAWI Graz, Graz University of Technology, Graz, 8010, Austria — [2]Institute of Functional Nano & Soft Materials, Soochow University, Suzhou, 215006, China — [3]Institute of Applied Information Processing and Communications, Graz University of Technology, Graz, 8010, Austria

In this contribution, we present atomically precise molecular nanostructures fabricated without human intervention. We demonstrate that simultaneous control of molecular position and orientation is attainable - both are prerequisites for constructing covalently bonded nanostructures in the future. We employ deep reinforcement learning agents to learn the complex tip-molecule-surface interactions by determining the optimal manipulation parameters for moving and rotating molecules. Because exhaustive sampling of all possible manipulation parameters is impossible, we generate a simulation based on selected experiments. This simulation allows us to train robust agents that even generalize to unseen adsorption conditions and arbitrary nanostructures. With this strategy, we autonomously assemble molecular building blocks into arbitrary geometries, establishing a reliable platform for automated molecular assembly.

O 8.5 Mon 11:45 WILL/A317

The Tale of a Band Melting in a Low-Dimensional Nanostructure — •Lenart Dudy[1,2], Julian Aulbach[2], Joerg Schaefer[2], Ralph Claessen[2], Victor Rogalev[2,3], and Piotr Chudzinski[4,5] — [1]Synchrotron SOLEIL, France — [2]U Würzburg, Germany — [3]Diamond Light Source, UK — [4]Queen's U Belfast, UK — [5]Polish Academy of Sciences, Poland

We explore the unusual phenomenon of "band melting" in the quasi-one-dimensional nanostructure Si(553)-Au. Using angle-resolved photoemission spectroscopy (ARPES) and scanning tunneling spectroscopy (STM), we observe a striking disappearance of a well-defined electronic band upon increasing temperature, while the atomic structure remains unchanged. Such dramatic temperature-driven changes are rare and typically associated with strongly correlated systems like Kondo or Mott phases.

Our findings point to electronic disorder and suppressed quantum coherence along one dimension. Supported by theoretical insights, we interpret this behavior within a phenomenological framework involving Luttinger-liquid physics and frustrated (pseudo-)spin interactions. This work sheds light on the interplay between dimensionality, correlations, and disorder in low-dimensional materials, opening new perspectives for understanding emergent electronic phases in nanostructures.

O 8.6 Mon 12:00 WILL/A317

Iron-porphyrin coordination network with surface-bound dysprosium adatoms: implications for long-range magnetic ordering — •Pierre Josse[1,2], Massine Kelai[1,2], Caroline Hommel[1,2], Lukas Spree[1,2], and Fabio Donati[1,3] — [1]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS), Seoul 03760, Republic of Korea — [2]Ewha Womans University, Seoul 03760, Republic of Korea — [3]Department of Physics, Ewha Womans University, Seoul 03760, Republic of Korea

Ordering spins on surfaces offers significant promise for spintronic, magnetic, magnetoelectric, and magneto-optic technologies. One effective approach is to employ spin-active centers embedded within molecular frameworks capable of self-organizing on surfaces. Porphyrins, with their exceptional chemical versatility and tunability, stand out as particularly suitable candidates for this purpose. Various strategies can be used to achieve such spin ordering, including molecular self-assembly, metal-ligand coordination, and on-surface synthesis involving the formation of C-C bonds. In this work, we present the specific strategies we use to organize spins on surfaces and examine how these methods influence long-range magnetic ordering.

O 8.7 Mon 12:15 WILL/A317

On-Surface Synthesis on Oxide — •Sonja Bohl[1], Kassandra Zoltner[1], Leonard Neuhaus[1], Stefan R. Kachel[1], Agustina Heredia[2], Cissie Slopianka[1], Sophie Schäfer[1], Lisa Arnold[1], Doris Grumelli[2], Sabine Wenzel[1], and J. Michael Gottfried[1] — [1]Fachbereich Chemie, Universität Marburg — [2]INIFTA, Universidad Nacional de La Plata

Oxide surfaces offer the advantage of weak molecule-substrate interactions, enabling a more direct and undistorted probing of the properties of adsorbed molecules compared to metal substrates. However, the reduced adsorption energies represent a central challenge for on-surface synthesis, requiring adjusted precursor strategies to prevent premature desorption from the oxide substrates. In this work, we explore approaches to enable on-surface reactions on thin-film oxides and well-defined bulk oxides. While various nano-carbon structures have previously been synthesized on metal surfaces, we investigate whether analogous processes can be realized on oxides. Furthermore, we examine how metal-organic nanostructures interact with bulk oxide surfaces and whether the substrate can induce changes in their coordination environment. Our methodology combines on-surface synthesis with scanning tunneling microscopy (STM), X-ray photoelectron spectroscopy (XPS), and temperature-programmed desorption (TPD).

O 9: Organic molecules on inorganic substrates: electronic, optical and other properties I

Time: Monday 15:00–18:00 Location: HSZ/0201

O 9.1 Mon 15:00 HSZ/0201

Adsorption-induced chirality of an otherwise highly-symmetrical molecule — •Jannis Lessmeister[1], Chetana Badala Viswanatha[1], Andreas Windischbacher[2], Christian S. Kern[2], Lu Lyu[3], Vitaliy Feyer[4], Iulia Cojocariu[4], Daniel Baranowski[4], Martin Aeschlimann[1], Peter Puschnig[2], and Benjamin Stadtmüller[3] — [1]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, 67633 Kaiserslautern, Germany — [2]Institute of Physics, University of Graz, 8010 Graz, Austria — [3]Institute of Physics, University of Augsburg, 86159 Augsburg, Germany — [4]Peter Grünberg Institute (PGI-6), Jülich Research Centre, 52428 Jülich, Germany

Chirality is a fundamental concept with far-reaching implications across chemistry, biology and materials science. In condensed matter, interest has grown around the chiral-induced spin selectivity (CISS) effect, which promises spin-dependent functionality in chiral molecules without magnetic or heavy-metal components. So far, however, the role of the interface for CISS remains unclear.

To illuminate the interactions at chiral metal-molecular interfaces, we explore how the highly-symmetrical molecule pentacene adsorbes on a naturally chiral copper surface. Employing momentum microscopy we identify changes of the emission pattern of the frontier molecular orbitals of pentacene adsorbed on chiral Cu(643) versus achiral Cu(110). In conjunction with density functional theory calculations, we can attribute these observations to a twisting of pentacene and thus to an adsorption-induced chirality of the otherwise symmetric molecule.

O 9.2 Mon 15:15 HSZ/0201

Explaining Principles of Tip-Enhanced Raman Images with Ab Initio Modeling — •Krystof Brezina[1], Yair Litman[2], and Mariana Rossi[1] — [1]Max-Planck-Institut für Struktur und Dynamik der Materie, Hamburg, Germany — [2]Max-Planck-Institut für Polymerforschung, Mainz, Germany

Tip-enhanced Raman spectroscopy (TERS) is an emerging method for imaging vibrational motion and chemically characterizing surface-bound molecular adsorbates. Existing approaches to TERS simulation often build on strong approximations, including a simplification or neglect of the underlying metallic substrate, often leading to discrepancies with experiments. In this work, we present a new, *ab initio* finite-field formulation of a TERS simulation framework [1] that can efficiently address large-scale, realistic systems under periodic boundary conditions [2]. This treatment is essential as it eliminates known artifacts in simulated TERS images stemming from substrate approximations, as shown by our benchmarks on adsorbates and surface defects, and allows for simulations directly comparable to experiments. In this direction, our simulations of Mg(II)-porphine on Ag(100) correctly explain the spatial intensity variation of experimental TERS images and provide an insight into the fundamental principles that define substrate contribution to the scattering cross section in TERS. Our infrastructure is generally applicable to any solid substrate, is computationally efficient and available within the FHI-aims electronic structure code.

[1] Litman Y. et al. *J. Phys. Chem. Lett.*, 14, 6850–6859 (2023)
[2] Brezina K., Litman Y. and Rossi M. *arXiv:2509.13075* (2025)

O 9.3 Mon 15:30 HSZ/0201

Periodic Potential Engineering of 2D Superlattices for Enhanced Photocatalysis — •Qun Yang — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle

Atomically thin semiconductors hold great promise for photocatalytic solar energy conversion, yet often face key challenges such as rapid electron-hole recombination, inappropriate band gaps, and misaligned energy levels to redox potentials. We introduce a general design strategy based on symmetry-defined periodic potentials for 2D photocatalyst engineering. These long-range modulations reshape the band structure and induce robust electron-hole separation without altering the material lattice. Applied to a monolayer InSe photocatalyst, we show that experimentally achievable moiré patterns, such as those formed with twisted hBN, enable miniband formation and tunable spatial charge separation. Moreover, the periodic potential modulates local adsorption energetics, providing a new handle to enhance catalytic activity for both photocatalytic hydrogen and oxygen evolution reactions. Our results provide a path toward the realization of high-efficiency solar-to-chemical energy conversion in a broad range of 2D materials.

O 9.4 Mon 15:45 HSZ/0201

Supramolecular organisation of thermolabile $TbPc_2$ derivatives at surfaces — •Patrick Lawes[1], Joachim Reichert[1], Anthoula C. Papageorgiou[1,3], Joe Komeda[4], Svetlana Klyatskaya[4], Andreas Walz[1,2], Annette Huettig[1,2], Hartmut Schlichting[1,2], Rochio Sánchez-de-Armas[6], Nicolas Montenegro-Pohlhammer[6,7], Carmen J. Calzado[6], Jean-Pierre Bucher[5], Johannes V. Barth[1], and Mario Ruben[4,8] — [1]TU Münich, DE — [2]pureions GmbH, Gilching, DE — [3]National and Kapodistrian University of Athens, GR — [4]Karlsruhe Insitute of Technology, DE — [5]IPCMS Université de Strasbourg FR — [6]Universidad de Sevilla, ES — [7]DIC, CIBQA, Universidad Bernardo OHiggins, CL — [8]CESQ, ISIS, Université de Strasbourg, FR

Creation and study of novel materials towards the goal of quantum information processing, involves sophisticated chemistry integrated into useful architectures. The self-organization of single-molecule magnets, is widely studied and reported. Utilizing electrospray ion beam deposition permits the study of thermolabile, functionalised bis(phthalocyaninato) terbium complexes on surfaces. This work aims to tailor the lattices of spin centres. Complex ligand tuned structures were characterised by scanning tunneling microscopy allowing for potential study into quantum criticality and quantum technologies.

O 9.5 Mon 16:00 HSZ/0201

Orbitals of Artificial Atoms in a Gapped Two-Dimensional Vacuum — Mong-Wen Gu[1,2], Aizhan Sabitova[1,2], Taner Esat[1,2], Christian Wagner[1,2], F. Stefan Tautz[1,2,3], Aleksandr Rodin[4,5], and •Ruslan Temirov[1,2,6] — [1]PGI-3, Forschungszentrum Jülich, Germany — [2]JARA, Fundamentals of Future Information Technology, Germany — [3]RWTH Aachen, Germany — [4]NUS, Singapore — [5]Yale-NUS College, Singapore — [6]University of Cologne, Germany

Artificial atoms–engineered nanostructures that confine electronic states–offer a route toward atom-by-atom design of electronic functionality. In this work, we use low-temperature STM and STS to study single-molecule vacancies in a commensurate PTCDA/Ag(111) monolayer, which act as attractive potentials for the two-dimensional interface-state electrons.

Using feature-detection STS [1,2], we directly image the vacancy-induced bound states and identify artificial analogues of *s*- and *p*-orbitals that split from the parabolic band minimum and hybridise when two vacancies are brought into proximity. Beyond these conventional orbital analogues, the periodically corrugated interface-state band hosts partial band gaps that support additional quasi-localised states with no counterparts in natural atoms. Tight-binding simulations reproduce these high-energy states and reveal their origin in the gap regions of the 2D dispersion.

[1] A. Sabitova, et. al., PRB 98, 205429 (2018), [2] J. Martinez-Castro, Commun. Mater. 3, 57 (2022)

O 9.6 Mon 16:15 HSZ/0201

Thermal and photo-induced one-dimensional switching of azobenzene derivatives on a graphite surface — •Thiruvancheril Gopakumar[1], Hariom Birla[1], Showkat H. Mir[1], Khushboo Yadav[1], Thomas Halbritter[2], Alexander Heckel[2], and Jayant K. Singh[3] — [1]Department of Chemistry, Indian Institute of Technology Kanpur, Kanpur 208016, India — [2]Institute for Organic Chemistry and Chemical Biology, Goethe-University Frankfurt, Max-von-Laue-Str. 9, 60438 Frankfurt, Germany — [3]Department of Chemical Engineering, Indian Institute of Technology Kanpur, Kanpur 208016, India

In this presentation we demonstrate an unusual one-dimensional (1D) cascade effect in the thermal- and photo-induced switching of azobenzene derivatives deposited on graphite surface. Upon thermal- and photo-induction, molecules switch between their geometric states (trans and cis) along a selected lattice within the assembly up to several hundreds of nanometres. Generally, such directionality is observed only for a length scale of few nanometres. It is revealed that the strong intermolecular interaction along one of the lattices compared to the other is at the origin of the 1D cascading effect. Harnessing cooperative switching opens possibilities for engineering the responses of molecular film

to external trigger and provides opportunities to control the directionality of switching/reactions, and novel nanostructures.

O 9.7 Mon 16:30 HSZ/0201

Accessing Energetically Restricted Optical Transitions in a Single Free-Base Porphyrin Molecule — •Eve Ammerman, Nils Krane, and Bruno Schuler — Empa - nanotech@surfaces Laboratory, 8600 Dübendorf, Switzerland

Charge transfer between a single molecule and the electrodes of an STM leads to a series of excitation and relaxation processes, including radiative relaxation from the molecule's optically active excited states. Utilizing the STM tunnel junction in electroluminescence experiments enables optical characterization on sub-molecular length-scales. However, the electroluminescence phenomenon is constrained by the alignment of ionization and optical state energies. Here, we show how positive ion resonance energy of a free-base tetrabenzoporphyrin (H2TBP) can be tuned relative to the optical emission energy through local gating by the STM tunnel junction or by work function engineering. The tuning of the energy level alignment allows us to produce optical emission from H2TBP on Ag(111), where electroluminescence is energetically restricted, or on Ag(110) where the molecule becomes bright.

O 9.8 Mon 16:45 HSZ/0201

Optical characterisation of single chlorophyll molecules at the sub-nanometre scale — Thiago G. L. Brito[1], •Daniel Arribas[1], Myriam Wadsack[1], Claudia Leticia Gómez Flores[1], Victor Feitosa[1], Klaus Kuhnke[1], Klaus Kern[1,2], Kelvin Anggara[1], and Anna Rosławska[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

As one of the main biomolecules harvesting light in photosynthetic organisms, chlorophyll plays a crucial role in biological systems, ultimately sustaining life on Earth. Therefore, the fundamental understanding of its optical properties has attracted widespread interest from the scientific community. However, traditional spectroscopic experiments, often probing complexes, only provide an averaged understanding of the rich photophysics of chlorophyll, where the effects of each possible molecular configuration and the local environment are smeared out. In this work, we address this by exploiting the sub-nm resolution of scanning tunnelling microscopy and the highly-localised plasmonic enhancement of the picocavity in the tunnelling junction. We characterise individual chlorophyll molecules, deposited by electrospray ion beam deposition on a Ag(111) surface with NaCl islands as decoupling layer. By analysing the fluorescence emission excited by the tunnelling electrons, we observe the structural dependency of the molecular opto-electronic properties. Our investigation opens new opportunities for the fundamental understanding of light-harvesting during photosynthesis with unprecedented sub-molecular resolution.

O 9.9 Mon 17:00 HSZ/0201

Polaronic transport through a molecular system with scanning probe microscopy — •Laëtitia Farinacci[1,2,3], Gaël Reecht[3], Christian Lotze[3], and Katharina Franke[3] — [1]University of Wuerzburg, Wuerzburg, Germany — [2]Carl-Zeiss-Stiftung Center for Quantum Photonics Jena-Stuttgart-Ulm, Stuttgart, Germany — [3]Freie Universitaet Berlin, Berlin, Germany

Polarons are quasi-particles in which electron excitations couple to distortions of the local ions network surrounding them. Typically, they are studied in metal oxides where they heavily influence charge transport and thereby often are key to understand and characterize the materials' properties. Here, we use scanning tunneling microscopy and atomic force microscopy to study the properties of Fe-porphine-chloride (FeP-Cl) molecules adsorbed on Pb(111). We observe distinct properties in the dI/dV signal that are indicative of polaronic transport.

More precisely, we find that the FeP molecules form islands in which Cl adatoms are trapped between the molecules. This leads to an effective gating of the molecules by local electric fields that stabilize either of two electronic configurations. Some FeP molecules display sharp peaks in their dI/dV reminiscent of vibrational modes. Importantly, the mapping of these peaks in dI/dV reveal the key role of the electric field and the necessity to account for charge transport through the island. These ingredients are the fundaments of polaron formation and will provide complementary understanding of the fundamental phenomena at the origin their formation in organic/inorganic interfaces.

O 9.10 Mon 17:15 HSZ/0201

Debromination and π-radical formation by single-electron injection on an insulator — •Ye Liu[1], Felix Giselbrecht[1], Lucía Gómez-Rodrigo[2], Manuel Vilas-Varela[2], Tzu-Chao Hung[1], Diego Peña[2], and Jascha Repp[1] — [1]University of Regensburg, Germany. — [2]Universidade de Santiago de Compostela, Spain.

The creation of π-radicals in nanostructures offers promising opportunities in spintronics and quantum technologies1,2, yet their controlled formation on an insulator remains challenging3. Here, we investigated the charge-induced reaction of 11-bromo-11H-benzo[b]fluorene on thick NaCl films (> 20 monolayers) using non-contact atomic force microscopy. The injection of only one electron from the microscope's tip induces debromination, which yield an open-shell structure and a bromide anion. In contrast, removal of an electron from the precursor results in a cation without bond cleavage. The voltage threshold for debromination depends on the molecular adsorption geometry, specifically on whether the bromine atom points upward or downward, reflecting opposite orientations of the molecular dipole moment. We present a feasible tip-induced synthesis strategy for generating a π-radical in molecule on an insulator, offering a promising route toward constructing larger open-shell nanostructure with multiple π-radicals on such surfaces.

O 9.11 Mon 17:30 HSZ/0201

Intramolecular cyclization of helicenes towards non-benzenoid nanographenes via formation of radicals — •Daniel Rothhardt[1], Ming-Lun Pan[2], Christian Wäckerlin[3,4], Hans Josef Hug[1], Yao-Ting Wu[2], Karl-Heinz Ernst[1,5,6], and Miloš Baljozović[1] — [1]Empa, Dübendorf, Switzerland — [2]National Cheng Kung University, Tainan, Taiwan — [3]PSI, Villigen PSI, Switzerland — [4]EPFL, Lausanne, Switzerland — [5]The Czech Academy of Sciences, Prague, Czech Republic — [6]University of Zurich, Zurich, Switzerland

On-surface synthesis has recently become a leading tool for controllable C-C bond formation that would otherwise hardly be accessible by conventional solution chemistry. The advancement of on-surface synthesis gave rise to a novel class of magnetic materials, namely open-shell magnetic nanographenes. The magnetism here mostly stems from the formation of unpaired electrons (radicals) due to a sublattice imbalance, topological frustration or aromatic stabilization. Such carbon-based spin systems are often considered promising candidates for spintronics applications due to their weak spin-orbit coupling and hyperfine interaction, allowing for long spin-lifetime and spin diffusion lengths. Here we demonstrate that the radical formation within the non-planar hydrocarbons such as helicenes leads to intramolecular bond formation and reorganization on Au(111) substrate resulting in non-benzenoid nanographenes. The products are identified using ToF-SIMS, STM and nc-AFM, corroborating the proposed radical-induced cyclization mechanism.

O 9.12 Mon 17:45 HSZ/0201

A Molecule with Half-Möbius Topology — Igor Roncevic[1,2], Fabian Paschke[3], Yueze Gao[2], Leonard-Alexander Lieske[3], Lene A. Gödde[2], Jascha Repp[4], Florian Albrecht[3], Harry L. Anderson[2], and •Leo Gross[3] — [1]Department of Chemistry, The University of Manchester, Oxford Road, Manchester, United Kingdom — [2]Department of Chemistry, Oxford University, Chemistry Research Laboratory, Oxford, United Kingdom — [3]IBM Research Europe - Zurich, Rüschlikon, Switzerland — [4]Institute of Experimental and Applied Physics and Halle-Berlin-Regensburg Cluster of Excellence CCE, University of Regensburg, Regensburg, Germany

Stereoisomers of $C_{13}Cl_2$ exhibiting helical orbitals around a ring of carbon atoms were synthesized by atom manipulation on bilayer NaCl on Au(111). We resolved the enantiomeric geometries of the closed-shell singlet states by atomic force microscopy and mapped their helical orbital densities by scanning tunnelling microscopy. A π-orbital basis of the helical, non-planar singlets that twists by 90° in one circulation is consistent with a half-Möbius topology. In such a topology, the π-orbital basis changes sign with respect to two circumnavigations and is periodic with respect to four circumnavigations. This is in contrast to a topologically trivial Hückel basis, which shows no twist, and a Möbius basis, which twist by 180° in one circulation. We demonstrate reversible switching of the topology, between the two singlets of oppositely threaded half-Möbius topology, and the planar, topologically trivial, triplet state.

O 10: 2D Materials beyond graphene: Growth, structure and substrate interaction (joint session O/HL/TT)

Time: Monday 15:00–17:45 Location: HSZ/0204

O 10.1 Mon 15:00 HSZ/0204

A virtual super-moiré: $MnBr_2$ on graphene on Ir(110) — Affan Safeer[1], Oktay Güleryüz[1], Nicolae Atodiresei[2], •Thomas Michely[1], and Jeison Fischer[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich, Germany

$MnBr_2$ on Gr/Ir(110) constitutes a three lattice system, giving rise to a super-moiré pattern – a moiré of moirés. The super-moiré of Gr/$MnBr_2$/Ir(110) is unique, as it involves a virtual moiré of $MnBr_2$ with the Ir(110) surface lattice

– two lattices not in contact with each other. Using a careful Fourier analysis of the bias dependence of scanning tunneling microscope topographs, scanning tunneling spectroscopy, the known properties of Gr/Ir(110), and the results of ab initio calculations, the origin of the virtual moiré is uncovered and related to the inhomogeneous binding of Gr to Ir(110). Comparative experiments with $MnBr_2$ on Gr/Ir(111) show similar growth and structure as on Gr/Ir(110), but highlight the unique properties of the $MnBr_2$/Gr/Ir(110) super-moiré.

O 10.2 Mon 15:15 HSZ/0204

Magnetism of monolayers of $FeCl_2$ and $FeBr_2$ Epitaxially Grown on Bi_2Se_3 — •Sebastien E. Hadjadj[1], Weibin Li[2], Pierluigi Gargiani[2], Cinthia Piamonteze[3], Oleksandr Stetsovych[4], Pavel Jelínek[4], Maxim Ilyn[1], and Celia Rogero[1] — [1]Materials Physics Center(MPC - CFM), Donostia, Spain — [2]ALBA Synchrotron Light Source, Barcelona, Spain — [3]Paul Scherrer Institut, Villigen, Switzerland — [4]FZU - Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic

Two-dimensional transition metal dihalides exhibit novel magnetic and electronic properties. By combining 2D magnetic semiconductors with topological insulators (TIs) novel quantum and spintronic phenomena can be investigated. Here, we report the uniform and epitaxial growth of monolayer $FeCl_2$ and $FeBr_2$ on the TI Bi_2Se_3. Structural and electronic characterization via LEED, STM, and STS measurements revealed a material-specific moiré pattern resulting from lattice mismatch, as well as a position-independent bandgap of 4 eV. Synchrotron-radiation-based XAS and XMCD measurements confirm robust ferromagnetic order down to the monolayer limit, with an intrinsic reduction of the effective spin magnetic moment by 40-50%. These magnetic vdW heterostructures provide a platform for investigating magnetic proximity effects and moiré-induced modifications of topological surface states. [1] S. E. Hadjadj et al., Chem. Mater., 35, 23, 9847*9856,(2023) [2] S. Kerschbaumer et al., Adv. Science, e08262,(2025)

O 10.3 Mon 15:30 HSZ/0204

Rise and fall of 1T-TaS_2: Epitaxial growth of monolayer TaS_2 on Au(111) — •Lars Buss[1], Cathy Sulaiman[1], Raquel Sánchez-Barquilla[1], Iulia Cojocariu[2], Marcin Szpytma[3], Tevfik Onur Menteş[2], Andrea Locatelli[2], Jens Falta[4], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Cottbus, Germany — [2]Elettra-Sincrotrone Trieste S.C.p.A, Basovizza, Trieste, Italy — [3]Faculty of Physics and Applied Computer Science, AGH University of Krakow, Poland — [4]Institute of Solid State Physics, University of Bremen, Germany

Two-dimensional TaS_2 has attracted extensive research interest due to its ability to exhibit electron correlation effects, including charge density waves (CDWs). In particular, 1T-TaS_2 is of interest as it shows a CDW at room temperature. However, when grown on metal substrates, only 2H-TaS_2 has been reported. To elucidate the reasons for the apparent lack of 1T-TaS_2 growth in the literature, we have investigated the growth of TaS_2 on Au(111) employing *in situ* low-energy electron microscopy (LEEM) and micro-diffraction (μLEED) as well as X-ray photoemission electron microscopy (XPEEM) [1]. We show that at elevated temperatures TaS_2 nucleates and grows in the metastable 1T-TaS_2 phase, which transforms into the stable 2H-TaS_2 phase via a temperature-activated process and then continues to grow at a considerably lower rate. Furthermore, we observe CDW-like ordering in 1T-TaS_2/Au(111), though it is suppressed in 2H-TaS_2/Au(111).
[1] L. Buß et al. Phys. Rev. Materials **9**, 074006 (2025).

O 10.4 Mon 15:45 HSZ/0204

Band-Like Transport and its Modulation by Nitrogen Doping in Transferable Semi-Conducting 2D-imine Covalent Organic Framework — •Vijay Bahadur Yadav, Diksha Srivastava, Satya Veer Singh, Itu Pandey, Manabendra Chandra, and Thiruvancheril G. Gopakumar — Indian Institute of Technology Kanpur

Two-dimensional (2D) imine-based covalent organic frameworks (COFs) are promising semiconductors for thin-film electronics and sensing due to their extended in-plane π-conjugation, enabling efficient charge transport. Here, we investigate two highly crystalline 2D imine COF films synthesised via quasi-equilibrium Schiff base condensation. By selecting molecular precursors, we tuned the nitrogen content, producing COFs with ten and six nitrogen atoms per unit cell (10N-COF and 6N-COF). The films are chemically stable in organic solvents and water, mechanically robust, and transferable onto various substrates, allowing fabrication over areas of tens of square centimeters. Electrical measurements using silver electrode arrays show linear current*voltage behaviour, indicating band-like transport, with consistent responses across multiple regions. The conductivity of 10N-COF is ~36 times higher than that of 6N-COF. Density functional theory calculations reveal similar band gaps but enhanced band dispersion near the Fermi level in 10N-COF, improving charge carrier mobility. Nitrogen incorporation thus effectively tunes charge transport in 2D COFs.

O 10.5 Mon 16:00 HSZ/0204

Co_2S_2: a new 2D material and its phase transitions — •Abdallah Karaka, Max Wolfertz, Affan Safeer, Guangyao Miao, Wouter Jolie, Thomas Michely, and Jeison Fischer — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Cologne, Germany

Using molecular beam epitaxy under ultra high vacuum conditions, 2D materials can be synthesized under conditions far from equilibrium for which no bulk parent compound exists.

Co_2S_2-2D is such an example. Using scanning tunneling microscopy and low energy electron diffraction we characterize this new single-layer 2D material crystallizing in the CuI structure (space group: $P\bar{3}m1$ trigonal), when grown on graphene on Ir(111) using molecular beam epitaxy. We found it can be synthesized phase pure upon low temperature growth and moderate annealing with a lattice constant of 3.66 ± 0.05 Å and a height of 6.2 Å. Beyond the single-layer limit it transforms into a new hexagonal crystal structure with a distinctly different lattice parameter of 3.52 ± 0.05 Å and a height of 11.7 Å. This transition typically occurs between 650 and 750 K, although the exact temperature depends on the annealing conditions. The phase transition is accompanied by the emergence of a 2x2 superstructure in the high temperature phase.

O 10.6 Mon 16:15 HSZ/0204

Tailored growth of 2D alloy transition metal dichalcogenides with tunable optical and electrical properties using liquid precursors — •Md Tarik Hossain[1], Axel Printschler[1], Nhat Lam Duong[1], Julian Picker[1], Rahul Sharma[1], Christof Neumann[1], Mona Sedighi[2], Johannes Biskupek[2], Muhammad Sufyan Ramzan[1], Caterina Cocchi[1], Ute Kaiser[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Jena, Germany — [2]University of Ulm, Ulm, Germany

Doping or alloying of two-dimensional (2D) transition metal dichalcogenides (TMDs) provides a promising route to tune the optical, magnetic, and electronic properties. Here, we present a liquid-precursor-based chemical vapor deposition (CVD) for the controlled growth of large-area monolayer ($V_xW_zMo_{1-x-y}$)S_2 alloys with tunable optical and electrical properties. Comprehensive characterization using atomic force microscopy, transmission electron microscopy, Raman spectroscopy, photoluminescence (PL) spectroscopy, and ab initio calculations confirms the structural and optical quality. Notably, PL shows a noticeable defect exciton peak at room temperature in the V-doped monolayer. Furthermore, by adjusting the composition, we modulate the carrier type of these monolayers from n-type to p-type or even make the monolayers metallic for high vanadium concentrations, which is deduced from electrical transport measurements and density functional theory calculations. This work demonstrates high potential of liquid-precursor CVD as a platform for the tailored growth of complex 2D TMD alloys for next-generation optoelectronic devices.

O 10.7 Mon 16:30 HSZ/0204

CVD growth and characterization of WSe_2 monolayers on Au(111) and their conversion to Janus SeWS — •Julian Picker[1], Jonas Brandhoff[2], Maximilian Schaal[2], Felix Otto[2], Christof Neumann[1], Torsten Fritz[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, Germany — [2]Institute of Solid State Physics, Friedrich Schiller University Jena, Germany

Transition metal dichalcogenides (TMDs) exhibit distinctive optical and electronic properties in the two-dimensional monolayer limit. Recently, Janus TMDs have attracted significant attention because their asymmetric chalcogen composition breaks the out-of-plane symmetry and enables properties not attainable in conventional TMDs. In this work, we initially investigate the structural and electronic characteristics of WSe_2 monolayers grown on Au(111) via ambient-pressure chemical vapor deposition (CVD). Surface-sensitive techniques - including scanning tunneling microscopy (STM), low-energy electron diffraction (LEED), X-ray photoelectron spectroscopy (XPS), and angle-resolved photoelectron spectroscopy (ARPES) - were employed to characterize the properties of these monolayers. Subsequently, the WSe_2 monolayers were transformed into Janus SeWS monolayers through selective chalcogen replacement at the WSe_2/Au interface. A comparative analysis reveals the structural and electronic differences between the two systems.

O 10.8 Mon 16:45 HSZ/0204

Controlling polymorphism in the growth of 2D manganese sulfide on graphene via substrate interaction — •Max Wolfertz, Abdallah Karaka, Nicolas Georgopoulos, Oktay Güleryüz, Affan Safeer, Thomas Michely, and Jeison Fischer — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Cologne, Germany

We investigate the epitaxial growth of single-layer manganese sulfide on graphene/Ir substrates grown via molecular beam epitaxy. Morphology, crystal structure and electronic properties are examined using scanning tunneling microscopy and - spectroscopy and low energy electron diffraction. While bulk MnS exists in the three polymorphs, α-(rock-salt structure), β-(zincblende structure), and γ-MnS (wurtzite structure), its structure in a single-layer is unknown, as fabrication using exfoliation methods cannot be applied. We find that

when grown by molecular beam epitaxy on Gr/Ir substrates manganese sulfide grows in two competing phases: manganese sulfide in trigonal CuI-structure (space group P-3m1) and MnS in thin platelets of a cubic rock-salt structure (space group Fm-3m). Their in-plane lattice parameters are 4.16 Å, and 3.63 Å respectively. We show that the substrate exerts a strong influence on the phase selected. While the growth on Gr/Ir(111) results in a large share of cubic MnS, the Gr/Ir(110) substrate favors the formation of single layer trigonal manganese sulfide. Also, the use of seeding methods for avoiding loss of Mn into the bulk Ir crystals is discussed.

O 10.9 Mon 17:00 HSZ/0204

Low Temperature MOCVD Growth of two-dimensional InSe and InSe/WS2 Heterostructures — •Robin Guenkel, Nils Langlotz, Matvei Kislitsyn, Juergen Belz, and Kerstin Volz — mar.quest|Marburg Center for Quantum Materials and Sustainable Technologies, Philipps University Marburg, Germany

Two-dimensional van der Waals heterostructures offer powerful opportunities for engineered optoelectronic functionality, particularly when type-II band alignment enables efficient charge separation and interlayer transitions. InSe and WS* are especially promising in this regard because their band structures allow for the formation of a type-II interface at the Γ point, which avoids momentum mismatch. This is an essential requirement for robust radiative processes in 2D stacks. This talk presents a low-temperature metal-organic chemical vapor deposition (MOCVD) approach for synthesizing high-quality InSe and vertically integrated InSe/WS2 heterostructures. Using DTBSe and TMIn at 350 °C, we synthesize homogeneous, single-phase InSe films on 2-inch sapphire substrates and extend the process to directly grow on monolayer WS2. Atomic force microscopy, Raman spectroscopy, and energy-dispersive X-ray spectroscopy provide insight into the morphology, crystallinity, and composition of the films, offering a detailed understanding of the growth behavior and the influence of the substrate surface chemistry.

O 10.10 Mon 17:15 HSZ/0204

Synthesis of Vertically Stacked 2D-hBN/Borophene Heterostructures on Ir(111) via Intrinsic Segregation — •Marko Kriegel, Karim Omambac, Smruti Mohanty, Birk Finke, Frank-J. Meyer zu Heringdorf, and Michael Horn-von Hoegen — University Duisburg-Essen and Center for Nanointegration Duisburg-Essen (CENIDE), Lotharstr. 1, 47057 Duisburg, Germany

Research efforts on 2D materials increasingly target complex architectures built from high-quality heterostructures. A key challenge remains the reliable and scalable in-situ fabrication of such systems. In this work, we use high-resolution spot-profile analysis LEED (SPA-LEED) and -microscopy (LEEM) to investigate a synthesis route for an hBN/borophene heterostructure on Ir(111) based on *intrinsic segregation*. At elevated temperatures, boron dissolves into the Ir subsurface region during exposure to the borazine precursor $B_3N_3H_6$ in a CVD process [1], thereby creating a boron reservoir. Increasing the precursor pressure drives the chemical balance toward formation of a complete hBN layer across the Ir surface [2]. Upon cooldown, the decreasing boron solubility induces segregation, resulting in the growth of a continuous borophene layer beneath the hBN overlayer. This one-step CVD approach establishes a promising, scalable pathway for the controlled synthesis of high-quality 2D heterostructures. [1] K. Omambac et al., ACS Nano **15** (2021) 7421 [2] K. Omambac et al., ACS Nano **17** (2023) 17946

O 10.11 Mon 17:30 HSZ/0204

MBE growth and characterization of high-quality monolayer MoS2 on stepped Au surface — •Sayan Debnath, Ram Prakash Pandeya, Konstantin Shchukin, Patrik Staudenmayer, and Alexander Grüneis — Optoelektronische Materialien Institut für Festkörperelektronik, TU Wien, 1040 Wien, Austria

In the present work, we investigate the growth of sub-monolayer MoS2 on Au(788) and Au(111), using molecular beam epitaxy. Sample growth quality is characterized using low-energy electron diffraction, X-ray photoemission spectroscopy, and scanning electron microscopy. Furthermore, a comparative study of the electronic properties was performed by studying the band structure using angle-resolved photoemission spectroscopy (ARPES), and the vibrational properties were measured by angle-resolved polarized Raman (ARPR) spectroscopy.

Our study reveals superior crystalline quality, with fewer S deficiencies, and better azimuthal order of MoS2 grown on the stepped Au(788) substrate compared to the Au(111). In the case of ARPES, we observed more resolved band dispersion on MoS2/Au (788), confirmed by probing the spin-orbit splitting at the Brillouin zone boundary (K point). On the other hand, ARPR of the first Raman mode E2g on MoS2/Au (788) deviates from the symmetry of freestanding MoS2, suggesting the effect of the stepped surface on the vibrational properties. We discuss the role of increased catalytic activity at step edges in promoting the growth of high-quality TMDCs, such as MoS2 and WS2, on stepped surfaces.

O 11: Metal & Semiconductor substrates: Adsorption and reaction of small molecules II

Time: Monday 15:00–17:00 Location: HSZ/0401

O 11.1 Mon 15:00 HSZ/0401

Ethylene on Si(001) revisited: New insights from XPS, STM, and Monte Carlo Simulations — •Jannick A. Peters, Sophie Göbel, and Michael Dürr — Institut für Angewandte Physik and Zentrum für Materialforschung, Justus-Liebig-Universität Giessen, Germany

The adsorption of ethylene - the smallest organic molecule with a C=C double bond - on Si(001) seems straightforward and is widely used as reference, e.g., for the determination of absolute surface coverage. On the other hand, there is ongoing discussion about adsorption configurations, coverage dependence, and in particular the site-selective adsorption based on strongly reduced reactivity on the partially covered surface, leading to two-step adsorption kinetics. In this study, the adsorption of ethylene on Si(001) was investigated at 300 K by means of XPS and STM with special focus on the coverage dependence, and was further modelled by means of Monte Carlo simulations. We can show that the first step of the two-step adsorption kinetics results in a saturation coverage of 0.7 ML, which is significantly higher than the commonly referenced coverage of 0.5 ML. STM measurements show that this behaviour is caused by a combination of adsorption statistics, nearest-neighbour interactions, and site-selective hindrance. Higher coverage up to 1 ML is then reached with a significantly higher dose due to the reduced reactivity of the remaining surface sites. Monte Carlo simulations taking into account a limited set of reaction channels accurately describe the complete coverage dependence as well as the local order of the adsorbates on the surface.

O 11.2 Mon 15:15 HSZ/0401

The Influence of Doping on Inelastic H Atom Scattering from Silicon — •Malte Opfermann, Kerstin Krüger, Sophia Tödter, and Oliver Bünermann — Institut für physikalische Chemie, Georg- August-Universität Göttingen, Tammannstraße 6, 37077 Göttingen

Inelastic H atom scattering experiments on the semiconducting Ge(111)c(2x8) surface have revealed a bimodal energy-loss distribution consisting of a narrow low energy-loss component and a broad high energy-loss component with an onset equal to the surface band gap. Theoretical calculations attribute the low energy-loss component to an adiabatic scattering mechanism at the adatom. The high energy-loss component is explained by a non-adiabatic scattering mechanism involving electron transfer across the surface band gap from the rest atom to the adatom.

Recently, we extended our studies to scattering experiments from the Si(100)2x1 surface. Although the experimental energy loss distributions resemble the bimodal behavior of Ge(111)c(2x8), the first component is broader, and the second exhibits a visible but less well-defined onset at the surface band gap. To gain further insight, we carried out scattering experiments from n-doped and p-doped surfaces. The first component shifts to lower energy losses for n-type doping and to higher energy losses for p-type doping, whereas the second component remains essentially unaffected. Based on the theoretical results for Ge(111)c(2x8), we propose a scattering mechanism for the Si(100)2x1 surface.

O 11.3 Mon 15:30 HSZ/0401

***Ab initio* insights into the OER activity of pristine and metal-supported Co_3O_4(111)** — •Muhammad Munawar[1,2] and Rossitza Pentcheva[1] — [1]Department of Physics and Center for Nanointegration (CENIDE), Universität Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — [2]IMPRS SusMet, Max Planck Institute for Sustainable Materials GmbH, Max Planck-Straße 1, 40237, Düsseldorf, Germany

Co_3O_4 is a promising anode material for the oxygen evolution reaction (OER), yet the role of metallic supports on its electronic properties and performance remains elusive. Here, we employ density functional theory with a Hubbard U term (DFT+U) to investigate the structural, electronic, and catalytic properties of pristine Co_3O_4(111) and Co_3O_4(111) grown on Pt(111). Using *ab-initio* thermodynamics, we determine that the Co tetrahedral termination is the most stable Co_3O_4(111) surface across a broad range of oxygen chemical potentials. Our results reveal that a built-in electric field emerges when Co_3O_4(111) is grown on a metallic substrate like Pt(111), that shifts the valence band maximum in the surface layer toward the Fermi level. Moreover, the work function increases monotonically with applied strain. Furthermore, we compare the OER activity of the pristine Co_3O_4(111) and Co_3O_4(111)/Pt(111) surface. These results provide atomic scale insight into structure-property relationships at oxide and oxide/metal interface, offering guidance for the rational design of next generation oxide-based electrocatalysts.

O 11.4 Mon 15:45 HSZ/0401

Through Stronger Hinderance to Higher Reactivity: Influence of the Alkyl Chains on the Activation Energy of Ether Cleavage on Silicon — Timo Glaser[1], Gustav F. Nolte[1], Tamam Bohamud[1], Philip Keller[1], Mathieu G. Silly[2], Hendrik Weiske[3], Ralf Tonner-Zech[3], and •Michael Dürr[1] — [1]Institut für Angewandte Physik und Zentrum für Materialforschung, Justus-Liebig-Universität Giessen, Germany — [2]Synchrotron SOLEIL, Gif sur Yvette, France — [3]Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Germany

Reactivity in surface chemistry is often discussed in terms of the interaction between surface states and the functional groups of the reacting molecule. Herein we demonstrate that for finite submonolayer coverage, i.e., surface coverage at which the molecular adsorbates cannot be treated as isolated molecules anymore, the seemingly innocent side chains of the adsorbate can also play a decisive role. For the example of ether cleavage on Si(001), which represents the surface analogue of an S_N2-type reaction, we show both experimentally by means of real-time XPS as well as based on ab-initio calculations that steric hindrance by the side chains determines the activation energy for C-O dissociation into the final state. In contrast to a simple expectation, the *stronger* steric hindrance of the butyl group in butyl methyl ether leads to a *lower* activation energy for ether cleavage on Si(001) when compared to diethyl ether. This effect was traced back to different degrees of destabilization of the precursor and the transition state [1].

[1] T. Glaser, et al., Angew. Chem. Int. Ed. e19990 (2025).

O 11.5 Mon 16:00 HSZ/0401

Frontier Orbitals Control Adsorbate Bonding to Stepped Transition Metal Surfaces — •Florian Nitz[1], Stefan Hörandl[1], Dmitriy Borodin[2], and Alec Wodtke[1] — [1]Institute for Physical Chemistry, Georg-August University of Goettingen, Tammannstraße 6, 37077 Goettingen, Germany — [2]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS), Seoul 03760, South Korea

Developing intuitive models of bonding and reactivity lies at the heart of physical chemistry. While such models have been developed for atoms and molecules, we still lack concepts to explain bonding and reactivity in the solid state, including surface chemistry and catalysis. Here, we address this gap and present a model of covalent bonding between molecular orbitals of an adsorbate and symmetry-specific bands on a metal surface atom, analogous to frontier orbital theory in molecular chemistry. We apply the model to the adsorption of three molecules–CO, NO, and NH_3–on stepped platinum surfaces of varying step density and compare its predictions to experimental adsorption energies. The experiment reveals that the adsorption energies vary systematically with step density, an unexpected phenomenon that can only be explained by the frontier orbital model. Correlations of the adsorbate bond strength with the mean energy of the metal d-electrons or with surface strain fail to describe the experimental observations. This highlights frontier orbitals as a powerful concept to rationalize bonding and reactivity in condensed-phase systems.

O 11.6 Mon 16:15 HSZ/0401

Memory friction and zero-point motion in hydrogen surface diffusion — •George Trenins and Mariana Rossi — MPI for the Structure and Dynamics of Matter, Hamburg, Germany

By virtue of their small mass, hydrogen atoms readily manifest quantum dynamical effects under typical experimental conditions. In particular, hydrogen diffusion on metal surfaces is strongly influenced by nonadiabatic interactions with the conduction electrons. Such "electronic friction" is incorporated into numerical simulations via the generalized Langevin equation (GLE). Additionally, hydrogen possesses substantial zero-point energy and can undergo quantum tunnelling. This is accurately described by "ring-polymer molecular dynamics" (RPMD), an atomistic simulation approach rooted in the path-integral formulation of quantum mechanics. Using a rigorous combination of the GLE and RPMD frameworks, we show that a combination of zero-point motion and non-Markovian (memory) friction are key to the temperature dependence of H-atom diffusion on copper surfaces [1]. In a limited temperature range, the two effects happen to mask each other almost perfectly, creating the appearance of classical, memoryless dynamics. Outside this range, the experiment displays non-Arrhenius behaviour that is not captured by classical dynamics but is readily explained when quantum effects are taken into account. [1] G. Trenins, M. Rossi, Phys. Rev. Lett. **134**, 226201 (2025).

O 11.7 Mon 16:30 HSZ/0401

When plasma meets surfaces - Nitrogen plasma-induced surface transformations on copper — •Ester Perez Penco and Roland Bliem — ARCNL, Amsterdam , The Netherlands

Inside EUVL setups, materials are exposed to challenging conditions, most importantly a plasma generated by the interaction of EUV radiation with the main background gas, hydrogen, and trace elements such as nitrogen. The reactive nature of plasma environments causes even trace gases to significantly influence material properties and affect the condition of surfaces. Copper is widely used in semiconductor technology, including applications as functional parts of the latest generation of chip manufacturing tools using extreme ultraviolet lithography (EUVL), therefore, it is relevant to study its behaviour in such reactive environment.

In this surface science study, we investigate the interaction of plasma-activated nitrogen with Cu(111) surfaces using in situ X-ray photoelectron spectroscopy (XPS) and low-energy electron diffraction (LEED). By systematically comparing the effects of molecular nitrogen, neutral atoms, ions, and nitrogen plasma, we provide detailed insights into how individual plasma species modify the copper surface. Our findings reveal that while radicals modify the very surface layer, higher energy species are required to induce structural disorder and incorporate into deeper layers. The results presented in this study aid in the prediction of plasma-induced changes and the role of trace elements in the EUVL environment.

O 11.8 Mon 16:45 HSZ/0401

From Gold to Copper: N-heterocyclic Carbene Self-Assembly for Area-Selective Deposition — •Franz Thiemann[1], Patrick Melix[1], Emmett Desroche[2], Francesco Tumino[2], Cathleen Crudden[2], and Ralf Tonner-Zech[1] — [1]Wilhelm-Ostwald Institute, Universität Leipzig, Germany — [2]Carbon to Metal Coating Institute, Queen's University, Kingston, Canada

N-heterocyclic carbenes (NHCs) are promising small-molecule inhibitors for area-selective atomic layer deposition (ASD) due to their strong, selective binding to metal surfaces. Using density functional theory with PBE-D4 functionals and periodic surface slabs, this study investigates NHC adsorption on a Cu(111) surface and compares it with previously studied Au(111) systems. In both cases, experimentally observed overlayer formation could be reproduced by DFT calculations and verified using STM images, revealing a distinctive dimer pattern in which NHCs bind to extracted copper adatoms at high density (1.8 NHC/nm^2) with a tilted molecular orientation. Energy decomposition analysis for extended systems revealed the origin of the stable overlayer: strong σ-donation to the surface and π-backdonation, combined with dispersion interactions between the NHC backbones, result in a highly stable blocking layer. [1] Furlan et al. Chem. Mater., 5753, 37 (2025). [2] DesRoche et al., in Preparation. [3] Raupach et al. J. Chem. Phys., 194105, 142 (2015).

O 12: Scanning probe microscopy: light matter interaction at atomic scales

Time: Monday 15:00–17:45 Location: HSZ/0403

O 12.1 Mon 15:00 HSZ/0403

Upconversion electroluminescence in VOPc via adsorption-induced interaction of unpaired spin — •Lukas Gerhard[1], Vibhuti Rai[1], Christof Holzer[1], Carsten Rockstuhl[2], and Wulf Wulfhekel[1] — [1]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology (KIT), D-76344 Eggenstein-Leopoldshafen, Germany — [2]Institute of Theoretical Solid State Physics, Karlsruhe Institute of Technology (KIT), D-76131 Karlsruhe, Germany

Molecules with unpaired spins (radicals) promise favourable spin statistics in their electroluminescence. Here, we combine scanning tunneling microscopy induced luminescence and density functional theory to study single vanadyl phthalocyanine molecules, which are stable neutral radicals. Two distinct adsorption geometries of the molecule on NaCl/Au(111) lead to a difference in the interaction of the unpaired electron with the substrate, which in turn allows us to investigate its effects on the light emission process [1]. Remarkably, we observe that up-conversion electroluminescence is gated by the adsorption geometry of the molecule, an effect we attribute to a reordering of excited states and enhanced excited state transition probabilities. The profound influence of the unpaired electron via state reordering opens new possibilities for tuning not only molecular electroluminescence but also many other spin dependent phenomena.

[1] V. N. Rai, C. Holzer, C. Rockstuhl, W. Wulfhekel, and L. Gerhard, arXiv:2508.11501.

O 12.2 Mon 15:15 HSZ/0403

Machine Learning for Atomic-Scale Molecular Discovery from Tip-Enhanced Raman Spectroscopy — Harshit Sethi[1], Markus Juntilla[1], •Orlando J Silveira[1], and Adam S Foster[1,2] — [1]Aalto University, Espoo, Finland — [2]Kanazawa University, Kanazawa, Japan

Tip-enhanced Raman spectroscopy (TERS) combines the nanoscale spatial resolution of scanning probe microscopy with the chemical specificity of Raman spectroscopy, offering a powerful tool for resolving both molecular structure and composition. However, extracting precise atomic-scale information from com-

plex TERS hyperspectral data remains a significant challenge. In this work, we address this gap by developing an automated machine learning framework to decode simulated TERS images for molecular structure discovery. Our approach uses convolutional neural networks (CNNs) to analyze hyperspectral datasets generated by modeling the plasmonic enhancement at a probe tip and the vibrational properties of planar molecules via density functional theory. To handle varying numbers of vibrational modes, we introduce a spectral binning procedure that standardizes the input for network training. This model provides a foundational proof of concept for the autonomous identification of molecular structures from TERS data, advancing the development of automated platforms for atomic-scale materials characterization and discovery.

O 12.3 Mon 15:30 HSZ/0403

THz-induced bilayer stacking dynamics in 1T-TaS_2 — Shaoxiang Sheng[1,2], Yang Yang[3], Mohamad Abdo[1], Li Chen[4], Peize Lin[5], •Kurt Lichtenberg[1], Xinguo Ren[3,5], Sheng Meng[3,5], Susanne Baumann[1], and Sebastian Loth[1,6] — [1]University of Stuttgart, Inst. for Functional Matter and Quantum Technologies — [2]Tsientang Inst. for Advanced Study — [3]IOP, Chinese Academy of Sciences — [4]Songshan Lake Materials Laboratory — [5]Inst. of Light Resources and Environmental Science, Henan Academy of Sciences — [6]Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart

The electronic properties of layered materials change dramatically with variations in the interlayer coupling and the stacking order [1]. We employ terahertz pump-probe spectroscopy in conjunction with scanning tunneling microscopy (STM) to investigate the role of stacking order dynamics and of domain structures in layered 1T-TaS2 at the atomic scale. TaS2 exhibits diverse charge-density wave (CDW) phases and an insulating ground state at low temperatures [2]. We show that terahertz pulses can induce insulator-to-metal transitions (IMTs) and reveal hidden electronic phases in 1T-TaS2 by manipulating the bilayer stacking at femtosecond time and atomic length scales. This tunability promises unprecedented ultrafast control over the electronic phases also in other layered materials, suggesting applications in reconfigurable quantum devices and neuromorphic computing.

[1]: S.-H. Lee, PRL 122, 106404 (2019) [2]: V Petkov, J. Phys.: Cond. Matt. 34 345401 (2022)

O 12.4 Mon 15:45 HSZ/0403

Coherent coupling between molecular dipoles probed with STML — •Quentin Stein[1], Jakob Kuhlke[3], Song Jiang[1], Tomas Neuman[2], Michelangelo Romeo[1], Fabrice Scheurer[1], Katharina Kaiser[3], and Guillaume Schull[1] — [1]Université de Strasbourg, CNRS, IPCMS, UMR7504, F-67000 Strasbourg, France — [2]Institute of Physics, Czech Academy of Sciences Cukrovarnick'a 10, Prague, 16200, Czech Republic — [3]Georg-August-Universität Göttingen, Physikalishes Institut, 37077 Göttingen, Germany

The clustering of chromophores allows their excited states to hybridize, enabling the formation of coherently coupled dipoles spanning multiple molecules. This is of key importance for optical processes occurring in both artificial and natural molecular assemblies.

Probing these coherently coupled dipoles with atomic-scale precision cannot be achieved through conventional optical techniques because of the diffraction limit set by Abbe's law. This difficulty has recently been overcome by scanning tunneling microscopy induced luminescence (STML), which relies on the extreme confinement of the electromagnetic field in the plasmonic picocavity formed at the apex of a metallic STM-tip. The radiative decay rate of a molecular exciton placed in such a cavity is greatly increased, allowing for the detection of states that are typically optically dark. It also provides nanometer-resolved maps of molecular transition dipole moments, revealing the spatial character of the excitonic states with atomic precision. In this work, we used this approach to investigate the fluorescence of coherently coupled dipoles within simple molecular assemblies.

O 12.5 Mon 16:00 HSZ/0403

Continuous-wave all-optical microscopy at the atomic scale — •Valentin Bergbauer[1], Felix Schiegl[1], Svenja Nerreter[1], Valentin Giessibl[1], Fabian Sandner[1], Franz J. Giessibl[1], Yaroslav A. Gerasimenko[1], Tom Siday[2], Markus A. Huber[1], and Rupert Huber[1] — [1]Department of Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, 93040 Regensburg, Germany — [2]School of Physics and Astronomy, University of Birmingham, Birmingham B15 2TT, U.K.

Exploring matter at the most fundamental level demands optical microscopy with ever-improving spatial resolution. By confining light to the apex of a sharp metallic tip, scanning near-field optical microscopy (SNOM) circumvents the diffraction limit, though its spatial resolution is still limited by the mesoscopic tip shape, inhibiting atomic resolution. Here, we observe atomically confined optical signals with Ångström-scale lateral modulations using continuous-wave mid-infrared radiation. These signals, characterized by a picometric vertical decay and a distinct optical phase shift, are consistent with emission from lightwave-driven tunnelling currents, a mechanism recently discovered using intense THz pulses. Observing near-field optical tunnelling emission (NOTE) under continuous-wave illumination is surprising, as strong-field effects such as coherent electron driving typically require ultrafast or free-electron lasers. Demonstrating the accessibility of this tunneling-mediated contrast mechanism with standard optical setups paves the way towards routine optical imaging with atomic-scale resolution.

O 12.6 Mon 16:15 HSZ/0403

Tuning Molecular Light Emission Through Atomic-scale Control of the Local Environment — •Thiago G. L. Brito[1], Daniel Arribas[1], Sofia Canola[2], Klaus Kuhnke[1], Tomáš Neuman[2], and Anna Rosławska[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569 Stuttgart, Germany — [2]Institute of Physics, Czech Academy of Sciences, 16200 Prague, Czech Republic

Intermolecular distances, adsorption sites, and configurations define a molecule's local environment, but their combined effect on single-molecule emission across different excitation pathways remains unclear. In this study, we measure the singlet emission of zinc phthalocyanine (ZnPc) on NaCl/Ag(111) and introduce platinum phthalocyanine (PtPc) as both a controlled perturbation of the local environment and a probe of ZnPc emission via resonant energy transfer (RET). All measurements were performed using scanning tunneling microscopy induced luminescence (STML) and tip-enhanced photoluminescence (TEPL). By systematically tuning intermolecular distances, restricting molecular rotational motion, and comparing direct electrical excitation with RET-driven and photon excitations, we reveal previously inaccessible regimes of ZnPc singlet emission, including neutral exciton-libron coupling. We further disentangle the environmental factors that influence emission spectra, demonstrating how the local environment actively shapes the optical response of single molecules.

O 12.7 Mon 16:30 HSZ/0403

Dipole-dipole coupling in assembled ZnPc-molecule clusters — •Jakob Kuhlke[1], Quentin Stein[2], Song Jiang[2], Georg Traeger[1], Fabrice Scheurer[2], Tomáš Neuman[3], Katharina Kaiser[1], and Guillaume Schull[2] — [1]Georg-August University Göttingen, IV. Physical Institute, Göttingen — [2]CNRS, Institut de Physique et Chimie des Matériaux de Strasbourg, Département Surfaces et Interfaces, Strasbourg — [3]Institute of Physics, Czech Academy of Sciences Cukrovarnická 10, Prague, 16200, Czech Republic

Dipole-coupled molecules provide a promising platform to build functional structures with tailored optical properties. We use ZnPc molecules as building blocks to investigate the coupling of molecular dipoles in different molecular assemblies.

In contrast to ZnPc monomers, dimers and chains of ZnPc molecules exhibit sharper and red-shifted emission peaks, a phenomenon known as superradiance [1], [2], [3]. Here, we extend this approach to more arbitrary clusters. We use scanning tunneling microscopy-induced luminescence (STML) to study the optical properties of several cluster configurations on the nanometer scale.

[1] L. Yang, et al. Physical Review Letters 122.23 (2019)
[2] Z. Yang, et al. Nature 531.7596 : 623-627 (2016).
[3] J. Dolezal, et al. ACS nano 16.1 : 1082-1088 (2021).

O 12.8 Mon 16:45 HSZ/0403

Selectivity in tautomerization reaction pathways triggered in single molecules on ultrashort time scales — •Niklas Friedrich, Carmen Roelcke, Tzu-Chao Hung, Yaroslav Gerasimenko, Rupert Huber, and Jascha Repp — Institute of Experimental and Applied Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg, and Halle-Berlin-Regensburg Cluster of Excellence CCE, Germany

Lightwave-driven scanning tunnelling microscopy (LW-STM) is a powerful technique allowing to unravel dynamics of quantum systems on their intrinsic energy, spatial and temporal scales [1,2]. In LW-STM, the electric-field transient of ultrashort laser pulses focused into the junction of a tunnelling microscope acts as a bias-voltage transient and thereby controls tunnelling on ultrashort timescales.

Here, we explore a chemical reaction triggered on ultrashort timescales. We study free-base naphthalocyanine molecules (H2Nc) on 2ML NaCl on Cu(100). In DC-biased experiments, this system switches between different tautomers upon injection of high-energy tunnelling electrons [3]. We find that the same reaction is facilitated by ultrashort voltage transients in LW-STM for transients far exceeding the voltage of the lowest unoccupied molecular orbital. Furthermore, we observe different selectivities in the tautomerization reaction depending on the energy of the tunnelling electron that we tentatively assign to the orbital structure of H2Nc.

[1] Nat. Photon. 18, 595-602 (2024) [2] arXiv:2507.10206 (2025) [3] Science 317, 1203-1206 (2007)

O 12.9 Mon 17:00 HSZ/0403

Atomic-scale excitonic luminescence nanoscopy of moiré superlattices in van der Waals heterostructures — •Manas Pratim Biswas[1], Fábio J. R. Costa[1], Elise Jouaiti[1], Arnaud Gloppe[1], Katharina Kaiser[1,2], Fabrice Scheurer[1], Stéphane Berciaud[1], and Guillaume Schull[1] — [1]Institut de Physique et de Chimie des Matériaux de Strasbourg (IPCMS), Université de

Strasbourg (CNRS, UMR 7504), Strasbourg, France — [2]4th Physical Institute-Solids and Nanostructures, Georg-August-Universität Göttingen, Göttingen, Germany

Atomically thin two-dimensional materials are susceptible to their environment, and stacking them into van der Waals heterostructures allows precise control of their electronic and optical properties. In semiconducting transition metal dichalogenides, excitons dominate the optical response whose properties can be tuned through interfacial interactions. Twisted and/or lattice-mismatched bilayers form a moiré superlattice that periodically modulates the electronic landscape. However, diffraction-limited optical methods average over micrometer scales, concealing these nanoscale effects. To overcome this, we employ cryogenic scanning tunneling microscope-induced luminescence[1] (STML, <7K, ultra-high vacuum) to probe exciton-moiré interplay in near-aligned WSe_2/WS_2 heterobilayers[2,3]. STML enables simultaneous atomic-scale imaging and local optical readout, with the ultimate aim of demonstrating nano-optical probing of moiré-modulated systems. References: 1. Nat. Mat. 22, 482 (2023) 2. Nat. Phys. 19, 1286 (2023) 3. Nat. Mat. 20, 945 (2021)

O 12.10 Mon 17:15 HSZ/0403

Tracing vibrational anharmonicity at the submolecular level with tip-enhanced Raman spectroscopy — •Youngwook Park[1], Ikutaro Hamada[2], Martin Wolf[1], and Akitoshi Shiotari[1] — [1]Fritz-Haber Institute of the Max-Planck Society, Berlin, Germany — [2]The University of Osaka, Suita, Japan

Tip-enhanced Raman spectroscopy (TERS) can achieve atomic-scale vibrational imaging, yet overtones and combination bands remain difficult to access due to weak transition strengths. We show that point-contact TERS enables submolecular-resolution detection of intense overtones and combination bands from a single asymmetric perylene derivative on silicon. A 10-times signal increase upon tip–molecule contact allows us to resolve both mechanical and electrical anharmonicities with Å-level spatial contrast. The mapped mechanical anharmonicity reveals a site-specific vibrational energy exchange pathway, demonstrating TERS as a powerful tool for real-space tracking of intramolecular vibrational energy redistribution.

O 12.11 Mon 17:30 HSZ/0403

Orbital-resolved imaging of coherent femtosecond exciton dynamics in single molecules — •Caiyun Chen — Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart

Understanding and controlling excitonic wavepackets is fundamental to uncovering mechanisms underlying energy conversion dynamics in organic molecular systems. We present orbital-resolved imaging of coherent exciton dynamics in single metal-centered naphthalocyanine (MNc) molecules*CoNc, CuNc, and ZnNc*adsorbed on NaCl/Ag(111). Using femtosecond scanning tunneling microscopy, we directly observe time-resolved photocurrent signals and spectroscopic signatures of coherent excitons, enabling selective excitation and control of excitons in isolated and coupled molecules. In single CuNc molecules, we measure a decoherence time (~70 fs), which decreases in dimers due to intermolecular interactions. Time-resolved measurements and photocurrent imaging reveal how central metal atoms in different naphthalocyanine molecules influence decoherence dynamics of the excited electronic state. Notably, a ZnNc molecule has longer decoherence time (~ 300 fs) compared to the CuNc and CoNc (~ 30 fs). Unpaired electrons on Co in CoNc molecule leads to distinct photocurrent imaging contrasts with the closed shell ZnNc and CuNc molecules. The origin of faster decoherence times of the excited states in CoNc and CuNc molecules is linked to conical intersections. These findings underscore the applications of ultrafast STM to probe quantum coherence and energy transfer dynamics at the single-molecule level with atomic-scale spatial resolution.

O 13: Solid-liquid interfaces: Reactions and electrochemistry I

Time: Monday 15:00–18:00 Location: TRE/PHYS

O 13.1 Mon 15:00 TRE/PHYS

The Weak Spots of IrO_2: Sampling Defect Landscapes at Operation Conditions — •Jimiben V. Patel, Nikhil Bapat, Karsten Reuter, and Hendrik H. Heenen — Fritz-Haber-Institut der MPG, Berlin

Under the harsh oxidative potentials required for the oxygen evolution reaction, rutile IrO_2 surfaces undergo restructuring that leads to Ir dissolution and undermines catalyst durability, eventually impacting device performance. To mitigate the catalyst degradation via robust design principles, a fundamental atomistic understanding of how surface reconstructions initiate and propagate dissolution is urgently needed. Since high-resolution *operando* characterization remains challenging, atomistic simulations are essential for uncovering the underlying microscopic mechanisms. However, achieving realistic insight requires approaches that go well beyond conventional, idealized modeling frameworks. In this work, we employ machine-learned interatomic potentials trained on density-functional theory to systematically sample vacancy formation across a wide range of electrochemical environments. This allows us to resolve how surface defects nucleate, interact, and evolve under relevant oxidizing conditions. We find that vacancy formation becomes increasingly favorable at higher potentials, with isolated defects stabilizing and subsequently coalescing into larger surface pits – structures that likely act as precursors for accelerated dissolution. These findings provide a first link between applied potential and defect thermodynamics, offering predictive insight into potential-dependent degradation pathways of IrO_2.

O 13.2 Mon 15:15 TRE/PHYS

Electrochemical Free Energy Barriers at Constant Potential — •Elias Diesen, Karsten Reuter, and Vanessa J. Bukas — Fritz-Haber-Institut der MPG, Berlin

Simulating barriers for electrocatalytic reactions is methodologically very challenging due to the intricate dynamics at the electrified solid/liquid interface. In addition, standard atomistic simulations based on periodic density-functional theory (DFT) keep the charge of the simulation cell constant instead of allowing it to fluctuate during the reaction in order to maintain a (fixed) electrode potential. Here, we introduce a method to compute electrochemical free energy barriers under well-defined potential conditions. Our approach relies on umbrella sampling on top of DFT-based molecular dynamics to access the free energy of activation, including both enthalpic and entropic contributions [1]. By carefully sampling the work function along the reaction coordinate, a Legendre transformation of the resulting canonical (constant-charge) energetics is then used to obtain grand canonical (constant-potential) results [2]. The method is demonstrated for proton deposition over Au(111). We extract potential-dependent barriers and examine kinetic scaling relations as well as use our results to benchmark common approximations in the recent literature. This work paves the way for systematic studies under realistic electrochemical conditions at e.g. varying temperatures or considering different proton-donating species.

[1] E. Diesen *et al.*, ACS Catal. **15**, 5403 (2025).
[2] S.D. Beinlich *et al.*, J. Chem. Theory Comput. **19**, 8323 (2023).

O 13.3 Mon 15:30 TRE/PHYS

Customizable Electrostatic Potentials in DFT Supercell Calculations: Implementation and Application to Electrified Interfaces — •Samuel Mattoso[1], Jing Yang[1], Florian Florian Deissenbeck[1], Ahmed Abdelkawy[1], Christoph Freysoldt[1], Stefan Wippermann[1,2], Mira Todorova[1], and Jörg Neugebauer Jörg Neugebauer[1] — [1]Max Planck Institute for Sustainable Materials, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [2]Philipps-Universität Marburg, Renthof 5, 35032 Marburg, Germany

Electric fields drive reactions, reshape surfaces, guide protein folding and dictate selectivity in chemistry and materials science. While Density Functional Theory (DFT) is a standard tool for modelling such phenomena, introducing user-defined customizable electrostatic potentials usually requires invasive code modifications and deep coding expertise. We will present a lightweight, Python-based implementation that allows adding external electric fields to supercell DFT calculations via a new VASP-Python interface. We outline the necessary energy- and force-corrections, describe the computational setup, and provide a streamlined workflow that works entirely within VASP without altering the source code. The method's versatility is demonstrated on several case studies: molecular adsorption on charged surfaces, field-ion microscopy, electrochemical solid-water interfaces, and implicit solvent models. This approach offers a simple, flexible route for researchers to incorporate external fields into DFT simulations, enabling exploration of field-dependent phenomena across chemistry and materials science.

O 13.4 Mon 15:45 TRE/PHYS

Ion-specific charge transfer and capacitance in the compact double layer of solvated cations at metal electrodes — •Fabiola Dominguez Flores, Axel Gross, and Wolfgang Schmickler — Institute of Theoretical Chemistry, Ulm University, 89081 Ulm, Germany

A molecular-scale understanding of the compact double layer is essential for fundamental electrochemistry. Using density-functional theory with a hybrid implicit-explicit solvation model, we investigate the adsorption of solvated cations (K^+, Na^+, Ca^{2+}, Mg^{2+}) on metal electrodes. This approach captures the local hydration structure while modeling a dilute electrolyte where no diffuse layer forms. Our results reveal two distinct physical regimes: alkali ions retain their unit charge, while divalent ions exhibit substantial partial charge transfer, directly quantified by Bader analysis. This charge transfer governs the interfacial capacitance, which we calculate to be 10-20 $\mu F\,cm^{-2}$, in excellent agreement with

experiment. We demonstrate that the electrosorption valency equals the negative of this partial charge. Interpreting these results with a parallel-plate model yields an effective dielectric constant dictated by the polarizabilities of the metal and the water layer. This work provides fundamental microscopic insight into how ion-specific electronic interactions control the properties of the electrochemical double layer.

O 13.5 Mon 16:00 TRE/PHYS

Electrokinetic spectroscopy of ion dynamics near charged surfaces using modulated surface acoustic waves — •Ofer Manor, Li Yifan, and Sudeepthi Aremanda — Technion, Haifa, Israel

We use MHz-level frequency-modulated surface acoustic waves (SAWs) to study the dynamics of ions in the electrical double layer (EDL) to appear near the charged glass/electrolyte interface. The SAW travels in the solid; the EDL exists in the electrolyte; both phenomena are entangled through a field effect, a mechanical evanescent wave, which is invoked in the electrolyte by the SAW and vibrates ions in the EDL to result in the leakage of an electrical field off the glass/electrolyte interface. We show measured spectra of electrolyte comprising different types and concentrations of salts and salt mixtures. This is a spectroscopy of ion dynamics in isolated and unique EDLs.

EDLs are nanometer-thick clouds of ions that appear at the charged interface between a substrate and an electrolyte solution and determines its electrical properties. Ions migrate through the EDL within micro- to nano-seconds: These are the EDL relaxation-times for charging and discharging, which are a product of the EDL structure and ion species therein.

Ion relaxation-times similar to the SAW periodic time result in an ion electromechanical synchronization, which maximizes ion vibration and the leakage of electrical fields off the EDL. The leakage identifies ion relaxation-time spectra for different electrolytes and the presence of ions and the intrinsic rate by which they charge and discharge EDLs.

O 13.6 Mon 16:15 TRE/PHYS

Impact of the Negative Dielectric Responses on Solvation and Adsorption at Electrified Interfaces — •Zhenyu Wang[1], Mira Todorova[1], Christoph Freysoldt[1], Stefan Wippermann[2], and Jörg Neugebauer[1] — [1]Department of Computational Materials Design, Max Planck Institute for Sustainable Materials, Düsseldorf, Germany — [2]Department of Physics, Philipps-Universität Marburg, Marburg, Germany

Understanding processes at electrified solid-liquid interfaces is central to electrocatalysis, corrosion, and water-splitting, yet the dielectric response of interfacial water remains poorly understood. Using a capacitor geometry in which water is confined between oppositely charged electrodes, we perform several hundred nanoseconds-long molecular dynamics simulations to probe both the dielectric behaviour of neat water and the solvation of ions under bias. The simulations reveal pronounced oscillations in the screening of interfacial water, giving rise to regions in which the local dielectric constant becomes negative. This dielectric response gives rise to weakly bound adsorption states. By correlating the computed potential profiles with the evolution of Na^+ and Cl^- solvation shells, we demonstrate that the rate-limiting step is not related to the charge transfer barrier but originates from the reorganization of the ion solvation shell when transferring through the negative-dielectric regions. This insight bridges atomistic dielectric anomalies with macroscopic electrochemical behaviour and provides a quantitative basis to describe ion migration in the vicinity of the electrified interface.

O 13.7 Mon 16:30 TRE/PHYS

Selectivity in Electrochemical Oxidation Reactions: Challenges in Ethylene Epoxidation — •Pauline Schütt and Alexander Bagger — Department of Physics, Technical University of Denmark

Electrochemical technologies play a central role in the sustainable production of fuels and chemicals, but their applications remain limited due to significant overpotentials and challenges in controlling selectivity. Alternative oxidation reactions could potentially generate value-added products on the anode side of electrochemical cells, but typically suffer from competition with the oxygen evolution reaction (OER).[1] Density functional theory (DFT) predictions and concepts from computational catalysis provide useful tools to systematically analyze selectivity and establish trends across different catalyst and reaction systems.[2] We here discuss key challenges restricting such alternative oxidation reactions and their competition with the OER, with a focus on ethylene epoxidation.

[1] L. F. T. Novaes *et al.* Chemical Society Reviews **50**(14), 7941-8002 (2021).
[2] P. Schütt, L. Karlsson and A. Bagger, in preparation, (2026).

O 13.8 Mon 16:45 TRE/PHYS

Bias, Barriers, and Beyond: Perturbative Insights into Electrochemical Reactivity — •Nicolas G. Hörmann and Karsten Reuter — Fritz-Haber-Institut der MPG

Electrochemical processes at solid-liquid interfaces are strongly shaped by the applied potential, yet capturing these effects efficiently remains a central challenge for atomistic modelling. In this talk, I will provide an overview of recent advances made in our group, focusing on perturbative and response-based approaches for electrochemical energetics and kinetics. Building on a rigorous connection between the constant-charge and constant-potential ensembles, we establish general connections between computational formalisms and clarify how potential-dependent properties emerge.

These insights enable efficient Taylor-expanded descriptions of energetics that avoid explicit simulations at different applied biases and allow analytical assessments of non-Nernstian shifts in hydrogen underpotential deposition, potential-dependent symmetry factors and potentiostat-free barrier calculations. Implementing them into bias-aware ML potentials opens the door to long-timescale molecular dynamics and accelerated exploration of electrochemical reaction pathways.

O 13.9 Mon 17:00 TRE/PHYS

Electro-osmotic Flow in Nano-capillaries via Optical Imaging and I/V Measurements: Influence of different salts and concentrations — •Aleksei Overchenko[1], Simon Brauburger[2], Frank Cichos[1], and Ulrich Keyser[2] — [1]Leipzig University, Peter Debye Institute for Soft Matter Physics, Linnéstr. 5, 04103 Leipzig — [2]University of Cambridge, Cavendish Laboratory, JJ Thomson Ave

Electro-osmotic flow (EOF) is of great interest in solid-state nanopores (SSNPs) due to its ability to pump, mix, and separate fluids in micro- and nanofluidic devices without mechanical components. However, EOF remains insufficiently explored at the nanoscale. Although KCl, NaCl, and LiCl are the most commonly used salts for driving matter through nanopores, no systematic qualitative or quantitative study has yet evaluated how different ions and concentrations affect EOF magnitude in nanopores.

We investigated the influence of various salts and their concentrations (10 mM to 1 M) on EOF behavior in 100 nm SiO2 glass capillaries. Flow visualization was performed using dark-field optical microscopy with simultaneous I/V measurements via a custom-designed flow cell. Tracer particles included 250 nm polystyrene and AuNPs.

This study provides higher spatial resolution and more detailed characterization of EOF than previously reported, offering new insights into nanoscale behavior. Understanding EOF under different ionic conditions is essential for future applications, including controlled manipulation of single DNA molecules and proteins.

O 13.10 Mon 17:15 TRE/PHYS

Facet-dependent restructuring and catalytic activity of Cu single crystals during CO electro-oxidation — Matthias Leitner, Francesc Valls Mascaro, •Andrea Auer, and Julia Kunze-Liebhäuser — Institute of Physical Chemistry, University of Innsbruck, Austria

Understanding how surface structure relates to catalytic activity is essential for designing efficient electrocatalysts. Copper (Cu) is known to restructure under reaction conditions, yet the precise impact of this dynamic behavior on activity remains largely unclear. Here, we combine electrochemistry with in situ electrochemical scanning tunneling microscopy (EC-STM) to investigate CO electro-oxidation on Cu(111) and Cu(100) single crystals and correlate activity with facet-specific structural changes. Both surfaces undergo nanometer-scale restructuring, forming undercoordinated Cu adatoms that act as active sites. Their evolution, however, differs significantly: Cu(111) shows dynamic, reversible restructuring that maintains a high density of adatom nanoclusters, whereas Cu(100) forms clusters that evolve less reversibly, with a gradual reduction in density. Interestingly, the evolution of clusters and their density does not directly correlate with the observed catalytic activity for either facet. Instead, we propose that the differences in activity stem primarily from variations in the effective density of the catalytically active Cu adatoms and their distinct interaction with reactants, rather than from different structural motifs. These results underscore the crucial role of dynamic restructuring in guiding the design of Cu-based electrocatalysts.

O 13.11 Mon 17:30 TRE/PHYS

In-situ magneto-optical tracking of redox reactions in NiFe electrocatalysts — •Sandhya Chandola[1,2], Karuppasamy Dharmaraj[2], Jörg Rappich[2], and Norbert Esser[1] — [1]Institut für Festkörperphysik,TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Schwarzschildstr. 8, 12489 Berlin, Germany

Nickel/Iron (NiFe)-based electrocatalysts are known to be efficient catalysts for the oxygen evolution reaction (OER), involved in water splitting. By using a polarization sensitive optical spectroscopy technique, Reflection Anisotropy Spectroscopy (RAS), at near normal incidence, we show how the polarization state of the reflected light can be directly correlated with the oxidation state changes of NiFe catalysts via two entangled magnetic effects, which are the magneto-optical Kerr effect (MOKE) at the surface of the NiFe layer and Faraday rotation within the layer. The polarization state can be used to monitor phase transitions which are not observed in unpolarized absorption spectra.

Increasing amounts of Fe in the NiFe films correspond to greater changes in the RAS/MOKE intensities, up to the solubility limit of ~ 25% Fe, after which the spectra do not show any more changes. RAS/MOKE is shown to be a valuable spectroscopic technique which can probe changes in the redox states for differ-

ent NiFe ratios, due to the indirect influence of magneto-optical effects with the implied role of ferromagnetic ordering in enhancing catalytic activity.

O 13.12 Mon 17:45 TRE/PHYS

Size Dependent Stability of Pt-supported Ceria Nanoparticles in Alkaline Electrolyte — Lukáš Fusek[1], Pankaj Kumar Samal[1], Jiří Kerestеš[1], Ivan Khalakhan[1], Viktor Johánek[1], Yaroslava Lykhach[2], Jörg Libuda[2], Olaf Brummel[2], and •Josef Myslivečeк[1] — [1]Charles University, Faculty of Mathematics and Physics, V Holešovičkách 2, 180 00 Praha 8, Czech Republic — [2]Interface Research and Catalysis, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany

Ceria nanoparticles find applications in electrocatalysis as co-catalysts for alcohol and CO oxidation, and for fuel cell and water electrolysis reactions. Synergistic effects of ceria are expected to critically depend on the cerium phases established under electrochemical conditions.

We perform a combined surface science and electrochemical study of CeO2(111) nanoparticles on Pt(111). Under electrochemical operation conditions, large ceria nanoparticles exhibit a stable redox behavior, while nanoparticles smaller than 5 nm destabilize and convert to a fully hydrated phase. Both types of nanoparticles block OH adsorption and H evolution on Pt(111), but do not block H adsorption, indicating H intercalation.

Our results reveal the nature of the electrocatalytically active cerium phases [10.1039/d3cp03831a] and underline the relevance of combined surface science and electrochemical experiments [10.1021/acs.jpclett.5c01465] for obtaining in-operando information on model electrocatalyst systems.

O 14: Ultrafast electron dynamics at surface and interfaces I

Time: Monday 15:00–18:00 Location: TRE/MATH

Invited Talk O 14.1 Mon 15:00 TRE/MATH

Spin and time-resolved ARPES and the orbital angular momentum of light — Pierre Nonnon[1,2], Romain Géneaux[1], Karol Hricovini[1,2], Christine Richter[1,2], David Bresteau[1], and •Mauro Fanciulli[1,2] — [1]Cergy Paris University, France — [2]LIDYL CEA Saclay, France

I will present the recently developed Panoramix beamline at Attolab, open to users, which allows for spin, time and angle-resolved photoemission spectroscopy (STARPES) experiments. The combination of a high harmonic generation (HHG) setup with tunable repetition rate and pulse duration, and a hemispherical analyzer with a 3D spin detector, permits to study charge and spin ultrafast dynamics in material surfaces. As an example, I will compare the observation of chiroptical resonant control of spin polarized excitons in bulk 2H-WSe2, to how the spin polarization changes for electrons pumped beyond bandgap resonance in the unoccupied conduction band. In the search of ever-increasing multidimensional spectroscopic techniques, I will conclude on the possibility to further include exotic light pulses with azimuthally varying phase or polarization, and how they might affect the photoemission process.

O 14.2 Mon 15:30 TRE/MATH

Disentangling exciton resonances in 2D materials by time-resolved XUV-ARPES — •Gregor Zinke[1,2], Antonius Naujok[1], Franz Spartz[1], Sebastian Hedwig[1], Tobias Eul[2], Martin Aeschlimann[1], and Benjamin Stadtmüller[2] — [1]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern - Landau, 67663 Kaiserslautern, Germany — [2]Experimental Physics II, Institute for Physics, University of Augsburg, 86159 Augsburg

Ultrafast and coherent electron dynamics in 2D materials and their heterostructures are governed by the complex energy landscape of various excitons. These quasi-particles are often separated only by tens of meV, making them difficult to distinguish in conventional time-resolved experiments due to the spectral linewidth of ultrashort pulses. Although interferometric photoemission experiments have shown potential in resolving (coherent) excitation pathways and absorption resonances, they depend mostly on optical pulses, limiting the observable momentum space, leaving high-symmetry points of 2D materials inaccessible. To address these limitations, we present a modified version of interferometric trARPES that employs two active, phase-stabilized IR pump pulses and a fs-XUV probe pulse for photoionization. We demonstrate the capability of our approach by examining the well-known A-exciton transition energies in WSe_2 at different frequencies of our pump spectrum, showing how temporal Fourier analysis of the entire ARPES spectrum allows linking distinct transition energies to congruent excitation paths within the WSe_2 electronic band structure.

O 14.3 Mon 15:45 TRE/MATH

Multi-mode momentum microscopy for studying light-induced metastable states — •Junde Liu[1], Bent van Wingerden[1], Hashima Marukara[1], Paul Werner[1], Daniel Steil[1], G. S. Matthijs Jansen[1], Wiebke Bennecke[1], Jan Philipp Bange[1], Olena Tkach[2], Gerd Schönhense[2], and Stefan Mathias[1] — [1]Georg-August-Universität Göttingen, Germany — [2]Johannes Gutenberg-Universität Mainz, Germany

Light-induced ultrafast phase transitions characterized by domain competition involving interlayer ordering, chirality, and topological defects are attracting growing interest [1]. This calls for time-resolved momentum microscopy, which offers simultaneous spatiotemporal resolution and direct access to band structures [2]. However, conventional high-field setups near the sample are prone to field-emission and space-charge effects, particularly in the case of cleaved crystal surfaces.

Here, using cleaved bulk TaS_2 as an exemplary system, we employ a momentum microscope with a newly designed lens system [3] that minimizes the electric field at the sample in the gap-lens mode to suppress field emission, or applies a retarding field in the repeller mode to remove slow electrons and thereby mitigates space-charge effects. This development paves the way to study cleaved crystals and enables dark-field imaging capabilities of domain-resolved electronic structure, nonequilibrium pathways, and the microscopic mechanisms of light-driven phase transitions. [1] Liu et al., *arxiv:2405.02831* (2024); [2] Reutzel, Jansen, Mathias, *Adv. in Phys. X* 9, 2378722 (2024); [3] Tkach & Schönhense, *Ultramicroscopy* 276, 114167 (2025).

O 14.4 Mon 16:00 TRE/MATH

Tracking ultrafast exciton-polariton propagation and coherent energy exchange in thin WSe_2 films — •Tobias Eul[1,2], Kai Rossnagel[2,3,4], and Michael Bauer[2,3] — [1]Institute of Physics, University of Augsburg — [2]Kiel Nano, Surface and Interface Science KiNSIS, Kiel University — [3]Institute of Experimental and Applied Physics, Kiel University — [4]Deutsches Elektronen-Synchrotron DESY, Hamburg

Efficient charge transfer of electrons and holes after photogeneration is fundamental for light-induced energy conversion. The propagation of bound electron-hole pairs, i.e., excitons, can enhance this efficiency by reducing non-radiative losses before charge separation and extraction. A promising approach to improve exciton propagation is via exciton-polaritons, quasiparticles formed by the strong coupling of excitons and photons. In these hybrid states, the excitation coherently oscillates between exciton and photon character, enabling the photonic component to transport energy over extended distances. Using photoemission electron microscopy, we visualize the propagation of exciton-polaritons in a thin WSe2 film by observing the ultrafast energy exchange between excitons and photons.

O 14.5 Mon 16:15 TRE/MATH

Probing On-Chip THz Generation by Momentum Streaking in Photoelectron Emission Microscopy — •David Huber, Wolfgang Hoppe, Georg Woltersdorf, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg

THz electromagnetic radiation provides ultrafast electric fields on the femtosecond timescale. Using THz radiation as a pump in time-resolved photoemission experiments enables sub-cycle probing of induced dynamics e.g. charge and spin currents. The momentum and energy streaking of electrons in vacuum – i.e., their acceleration due to the Coulomb force – has long been shown to reliably probe electric fields and THz radiation.

In a spintronic THz emitter, we generate a spin current through the ultrafast demagnetization of a 3 nm ferromagnetic thin film, which results in a surface charge current in an adjacent 3 nm platinum film due to the inverse spin Hall effect. Similar to dipole radiation, the charge current emits THz radiation into the vacuum. By time-resolved in-plane momentum streaking of photoemitted electrons, we probe the single-cycle THz electric field in front of the surface and deduce the electric surface current. We verify our findings using simulated THz radiation and streaking.

O 14.6 Mon 16:30 TRE/MATH

Interplay between intraband acceleration and interband excitation in Bi_2Te_3 by subcycle time-resolved THz-ARPES — •Tim Bergmeier[1,2], Suguru Ito[1], Jens Güdde[1], and Ulrich Höfer[2] — [1]Fachbereich Physik, Philipps-Universität Marburg, Germany — [2]Fachbereich Physik, Universität Regensburg, Germany

Angle-resolved photoemission spectroscopy (ARPES) using THz driving fields with subcycle temporal resolution offers unique capabilities to investigate the dynamics of lateral Dirac currents in the surface state of topological insulators. Whereas low THz-frequencies result in pure intraband accelerations within the surface state [1], additional interband excitations become possible at higher frequencies [2,3].

Here, we present subcycle-resolved THz-ARPES measurements with 2D momentum imaging resolving the full Dirac cone of Bi_2Te_3. For this purpose, we

generate frequency-tunable two-cycle MIR pulses (20-40 THz) with electric field strengths up to MV/cm at the sample surface, combined with an ultrashort 400 nm two-photon probe (<15 fs), at a repetition rate of 200 kHz. For a frequency of 25 THz, we show that the momentum distribution of the field-driven intraband acceleration is strongly influenced by the Dirac cones hexagonal warping, while being superimposed with resonant interband excitations that are only possible in the materials $\overline{\Gamma M}$ direction.

[1] J. Reimann et al., Nature 562, 396 (2018).
[2] S. Ito et al., Nature 616, 696 (2023).
[3] C.P. Schmid et al., Nature 593, 385 (2021).

O 14.7 Mon 16:45 TRE/MATH

Realistic nuclear ensembles for electronic excitation dynamics — •Hannah Bertschi, George Trenins, and Mariana Rossi — MPI for the Structure and Dynamics of Matter, Hamburg, Germany

Understanding how large-amplitude anharmonic nuclear motion influences electronic excitations is essential for explaining related phenomena in weakly-bound systems. To model charge transfer and vibronic spectra, we employ real-time time-dependent density functional theory coupled to multitrajectory Ehrenfest dynamics. In this approach, nuclear anharmonicity is incorporated through the sampling of initial conditions. In contrast to more conventional methods, we generate nuclear configurations and momenta using quantum thermostat molecular dynamics [1]. The resulting distributions of nuclear positions and momenta agree well with exact quantum references obtained from path-integral molecular dynamics, even for systems with large-amplitude motion such as the water dimer. However, the quantum thermostat does not perfectly capture the anharmonic zero-point energy of every degree of freedom, which can be mitigated by carefully choosing the parametrization of the thermostat. We show that the initial nuclear conditions of a water dimer on phenanthrene have a strong impact on both the direction and magnitude of charge transfer. Moreover, the nonadiabatic dynamics can even reverse the direction of the transfer.

[1] M. Ceriotti et al., Phys. Rev. Lett. 103, 030603 (2009).

O 14.8 Mon 17:00 TRE/MATH

Laser-induced anisotropic electronic response and inverse Faraday effect in hexagonal boron nitride from real-time time-dependent density functional theory — •Cheng Wang, Markus E. Gruner, and Rossitza Pentcheva — Department of Physics, University of Duisburg-Essen

The ultrafast electronic response of hexagonal boron nitride (h-BN) is investigated using real-time time-dependent density functional theory (RT-TDDFT) within an all-electron LAPW framework of the Elk code. We vary the light polarization (in-plane vs out-of-plane), dimensionality (monolayer, bilayer, bulk) and photon energy, and resolve the time-dependent projected density of states into orbital channels and identify the microscopic pathways of carrier injection. For out-of-plane linearly polarized light, the charge transfer is suppressed in the monolayer, weak in the bilayer, and strong in the bulk. Under in-plane polarization and a photon energy slightly above the DFT band gap, we identify a direct interband excitation pathway from the N p_z to B p_z orbitals. At higher photon energy, the bulk response is dominated by a local charge redistribution within N p_x-orbitals. Circularly polarized light induces a notable orbital angular momentum, while spin contributions remain negligible.

Funding by DFG within CRC1242 (project C02) and computational time on the MagnitUDE and AmplitUDE supercomputers at the University of Duisburg-Essen are gratefully acknowledged.

O 14.9 Mon 17:15 TRE/MATH

Theory of resonantly enhanced light-induced superconducting pairing in K_3C_{60} — •Juan I. Aranzadi[1], Joseph Tindall[2], Paul Fadler[1], and Michael A. Sentef[1,3] — [1]Institute for Theoretical Physics, University of Bremen/ BCCMS — [2]Center for Computational Quantum Physics, Flatiron Institute, New York, New York 10010, USA — [3]MPSD, CFEL, Hamburg

K_3C_{60} exhibits unconventional s-wave superconductivity with a critical temperature of approximately 20K, where the superconducting state emerges from a balance between strong electronic correlations and Jahn-Teller phonon-mediated pairing [1].

Recent pump-probe measurements have shown that optical excitation induces optical signatures reminiscent of the equilibrium superconducting state at temperatures higher than Tc [2, 3]. Notably, a 10 THz resonance was observed to trigger metastable superconducting-like properties that persist for temperatures up to 300 K [4].

The mechanism underlying this non-equilibrium superconducting state remains poorly understood. To address this question, we investigate a driven three-orbital Hubbard-Kanamori model which serves as a minimal model for equilibrium superconductivity in K_3C_{60} using numerical techniques including exact diagonalization and tensor networks.

[1] Nomura, Y., et al. (2015). *Science Advances*, **1**
[2] Mitrano, M. et al. (2016). *Nature*, **530**, 461–464.
[3] Budden, M. et al. (2021). *Nature Physics*, **17**, 611–618.
[4] Rowe, E. et al. (2023). *Nature Physics*, **19**, 1821–1826.

O 14.10 Mon 17:30 TRE/MATH

Ultrafast table-top three-dimensional photoemission orbital tomography — •G. S. Matthijs Jansen[1], Wiebke Bennecke[1], Thi Lan Dinh[2], Jan Philipp Bange[1], David Schmitt[1], Marco Merboldt[1], Lennart Weinhagen[1], Bent van Wingerden[1], Fabio Frassetto[3], Luca Poletto[3], Marcel Reutzel[1], Daniel Steil[1], D. Russell Luke[2], and Stefan Mathias[1] — [1]University of Göttingen, I. Physikalisches Institut, Göttingen, Germany — [2]University of Göttingen, Institute of Numerical and Applied Mathematics, Göttingen, Germany — [3]Institute for Photonics and Nanotechnologies CNR-IFN, 35131 Padova, Italy

In photoemission orbital tomography (POT), molecular orbitals can be imaged with femtosecond resolution. Also, when combined with photon-energy-dependent measurements, POT is, so far, the only method that can probe the orbitals of adsorbed molecules in 3D. However, the study of, e.g., hybridization in organic/inorganic heterostructures [Bennecke *et al.*, arXiv:2411.14993 (2024)] by 3D-POT is extremely challenging due to the demanding nature of the experiment. Here, we present a table-top approach for 3D POT: By combining a photoelectron momentum microscope with a pulse-preserving monochromator for laser-generated extreme ultraviolet light, we speed up data acquisition. Moreover, we developed a new reconstruction algorithm that reduces the sampling requirements by about an order of magnitude [Dinh *et al.*, New J. Phys. 26 043024 (2024)]. Our first results achieved on PTCDA/Ag(110) highlight the potential for ultrafast femtosecond time-resolved 3D-POT.

O 14.11 Mon 17:45 TRE/MATH

Temporal Advancement of Photoelectrons emitted via Evanescent Waves — •Luis Maschmann, Andreas Gebauer, Tillmann Schabbehard, and Walter Pfeiffer — Bielefeld University, Universitätsstr. 25, 33615 Bielefeld

Photoelectron emission dynamics in solids is governed both by propagating and evanescent wave components. Here we employ a one-dimensional Kronig-Penney model to investigate the role of evanescent waves on the photoelectron wave packet dynamics based on time-reversed LEED states within one-step theory and time-dependent Schrödinger equation simulations. Using a Kronig-Penney potential with a large bandgap, we can clearly distinguish the dynamics for evanescent and propagating photoelectron emission channels. For emission via evanescent states, i.e., within the final state bandgap, the photoelectron appears temporally advanced and seemingly originates from the bulk-vacuum interface, although the emitter well is located well below the interface. Our results establish a direct analogy to the temporal evolution of a wave packet undergoing quantum mechanical tunneling through a potential barrier and significantly influence the interpretation of attosecond time-resolved photoemission delays.

O 15: Spins on surfaces at the atomic scale I

Time: Monday 15:00–18:00 Location: WILL/A317

Invited Talk O 15.1 Mon 15:00 WILL/A317

Tuning Spin-1/2 Interactions in Graphene: From Long-Range Coupling to Altermagnetic Order — •Beatriz Viña-Bausá[1], Manuel A. García-Blázquez[1], Antonio T. Costa[2], Joao C. G. Henriques[2], Roberto Carrasco[1], Eva Cortés-del Río[1], Diego Expósito[1], Pierre Mallet[3], Jean-Yves Veuillen[3], Joaquín Fernandez-Rossier[2], Juan J. Palacios[1], and Iván Brihuega[1] — [1]Dept. Física de la Materia Condensada, Universidad Autónoma de Madrid, Spain — [2]International Iberian Nanotechnology Laboratory, Portugal — [3]Université Grenoble Alpes, France

Here, we demonstrate that graphene, functionalized with H atoms, serves as a versatile platform for engineering and investigating long-range magnetic interactions. Through scanning tunneling microscopy, we manipulate spin-1/2 moments induced by single H atoms on graphene and quantify their coupling via spin excitations using inelastic electron tunneling spectroscopy[1]. Our measurements reveal robust ferromagnetic and antiferromagnetic exchange interactions in H pairs, extending over nanometer-scale distances. Additionally, guided by symmetry selection, we realize unconventional magnetic phases in our system, namely altermagnets and Lieb ferrimagnets[2]. Our results, supported by mean-field Hubbard and density functional theory calculations put forward hydrogenated graphene as a promising material for simulating exotic spin systems.

[1] B. Viña-Bausá, et al., arXiv:2511.06887 (2025)
[2] B. Viña-Bausá, et al., Nano Letters 25,11554-11561 (2025)

O 15.2 Mon 15:30 WILL/A317

versatile building blocks for molecular qubits on surfaces — •Saba Taherpour[1,2], Corina Urdaniz[1,3], Jisoo Yu[1,3], Jose Reina-Galvez[1,3,4], Kevin Lizárraga[1,3], and Christoph Wolf[1,3] — [1]Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul 03760, Korea — [2]Department of Physics, Ewha Womans University, Seoul 03760, Korea — [3]Ewha Womans University, Seoul 03760, Korea — [4]University of Konstanz, 78457 Konstanz, Germany

Electron spins are natural quantum objects. Molecules that host an electron spin S=1/2 can therefore be considered qubit candidates provided they have reasonable coherence times. In this work, I will show based on first-principles calculations how the charge transfer across an Ag/MgO interface can be utilized to change the charge and spin state of 3d transition-metal phthalocyanine molecules. Iron(II) phthalocyanine (FePc) emerges as a promising qubit candidate. We present density functional theory calculations and nonequilibrium quantum transport simulations based on recent developments of all electrical electron spin resonance in atomic scale magnetic transport junctions. Our results indicate that FePc on the Ag/MgO substrate can be used as molecular building block of on-surface qubit architectures.

O 15.3 Mon 15:45 WILL/A317

Creating multi-well energy landscapes from coupled orbital memory states — •Kira Junghans, Niek M. M. Aarts, Hermann Osterhage, Julián D. Rojas-Castillo, and Alexander A. Khajetoorians — Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

The interaction between atomic spins on surfaces is usually dictated by the exchange interaction. Its short-range nature strongly favors spin orientations that are either ferro- or antiferromagnetic. Recently, it was shown that memory can be created from an atomic spin using its valency [1]. Unlike the exchange interaction, it was shown that the interactions between orbital memory elements are long-range. This can lead to complex stochastic dynamics often needed in computational schemes based on theoretical neuroscience [2]. Exploiting this new functionality requires a deeper understanding of the nature of the interaction as well as the uniqueness of this material system.

Here, we study the stochastic dynamics of Co and Fe atoms on black phosphorus with scanning tunneling microscopy and spectroscopy. We quantify how the state favorability and lifetimes are influenced in dimers at different distances and by the neighboring atoms' state. We find that heterogenous dimers can also lead to complex stochastic noise, analogous to multi-well behavior. Furthermore, we investigate the dynamics of multiple coupled atoms and show that the state favorabilities can be tuned by the states of all surrounding atoms.

[1] B. Kiraly et al., Nat. Comm. 9, 3904 (2018).
[2] B. Kiraly et al., Nat. Nanotechn. 16, 414 (2021).

O 15.4 Mon 16:00 WILL/A317

Single spin control of atomic defects in monolayer MoS_2 — •Kwan Ho Au-Yeung[1,3], Wantong Huang[1,3], Johanna Matusche[1,3], Paul Greule[1,3], Jonas Arnold[1,3], Lovis Hardeweg[1,3], Máté Stark[1,3], Luise Renz[1,3], Affan Safeer[2], Daniel Jansen[2], Jeison Fischer[2], Thomas Michely[2], Wolfgang Wernsdorfer[1,3], Christoph Sürgers[1,3], Johannes Schwenk[1,3], Wouter Jolie[2], and Philip Willke[1,3] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe — [2]II. Physikalisches Institut, Universität zu Köln, Köln — [3]Center for Integrated Quantum Science and Technology, Karlsruhe Institute of Technology, Karlsruhe

Point defects in two-dimensional (2D) semiconductors host localized quantum states that can function as sensors, single-photon emitters, and qubits, but their controlled realization and individual addressability in atomically thin hosts remain challenging. Here we combine scanning tunneling microscopy with electron spin resonance (ESR-STM) to achieve single-spin control of atomic defect in a monolayer transition-metal dichalcogenide. Using STM manipulation, we create individual point defects, including sulfur vacancies and substitutional impurities in monolayer MoS_2 on graphene/Ir(111). Scanning tunneling spectroscopy and ESR measurements reveal their electronic structures and magnetic properties respectively, while pulsed ESR schemes enable quantum control of their spin states at the atomic scale. Our results demonstrate that monolayer MoS_2 provides a solid-state quantum platform that directly links 2D materials engineering with atomic-scale spin initialization, control, and readout.

O 15.5 Mon 16:15 WILL/A317

Imaging 2D ferromagnetic order with a single nickelocene molecule — •Leonard Edens[1], Trisha Sai[1], Divya Jyoti[1], Stefano Trivini[1], Fabian Schulz[1], and Nacho Pascual[1,2] — [1]CIC nanoGUNE BRTA, 20018 Donostia - San Sebastián, Spain — [2]Ikerbasque, Basque Foundation for Science, 48013 Bilbao, Spain

Lanthanide intermetallic compounds formed on coinage metal (111) surfaces exhibit ferromagnetic ground states with moments robustly aligned towards a polarization axis, even in the single monolayer limit. Characteristic of these 2D magnetic systems is the intricate dependence of the easy axis on 4f occupancy, and the formation of a moiré-induced superstructure with the support, which causes an inhomogeneous local magnetization [1]. Here, we study two representative alloys of this family of materials, $GdAu_2$ and $TbAu_2$, which respectively magnetize in- and out-of-plane. To sense their magnetic state, we employ a single nickelocene molecule adsorbed on the tip of a scanning tunnelling microscope. By quantifying the directional exchange field atom-by-atom, we characterize incommensurate order and local perturbations to the moiré-congruent magnetic texture. Further insight into the nature of the exchange field is gained by studying its dependence on vertical separation and externally applied magnetic fields.

[1] Edens et al. Advanced Materials (2025).
https://doi.org/10.1002/adma.202510753

O 15.6 Mon 16:30 WILL/A317

Two-photon transition in an Er-Ti atomic spin pair — •Dasom Choi[1,2], Yaowu Liu[1,2], Stefano Reale[2,3], Jeongmin Oh[1,2], Lei Fang[1,2], We-hyo Seo[1,2], Andreas Heinrich[1,2], Fabio Donati[1,2], and Soo-hyon Phark[1,2] — [1]Department of Physics, Ewha Womans University, Seoul, Republic of Korea — [2]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS), Seoul, Republic of Korea — [3]QuTech and Kavli Institute of Nanoscience, Delft University of Technology, Delft, The Netherlands

Multi-photon process becomes a key ingredient in quantum information science, offering a promising route to nonlinear quantum transitions and entanglement generation. Extending this to atomic spin qubits on surfaces is of great interest, yet has not been demonstrated. In this work, we investigate a spin-pair of Er and Ti atoms adsorbed on a MgO/Ag(100) surface using a scanning tunneling microscope (STM). By applying pulsed electron spin resonance in the STM, we realize two-photon resonant transitions corresponding to an angular momentum change of $\Delta m = \pm 2$ of the spin-pair, a phenomenon beyond the conventional single-photon processes as shown at the single atom level. Our work demonstrates the ability to coherently control higher-order quantum transitions at the single spin level, which provides a novel pathway towards implementing multi-quantum gate operations in atomic spin qubits, highlighting the potential of single atomic lanthanides on a surface for quantum information processing.

O 15.7 Mon 16:45 WILL/A317

Landau-Zener transitions of multilevel atomic spins — •Lukas Veldman[1,2], Henrik Lichtl[1,2], Nicolaj Betz[1,2], Johannes Schust[1], Laëtitia Farinacci[1,3], Fernando Delgado[4], Susanne Baumann[1,2], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies — [2]Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart — [3]Carl Zeiss Stiftung Center for Quantum Photonics — [4]Instituto de Estudios Avanzados IUDEA, Departamento de Física, Universidad de La Laguna, Tenerife, Spain

The ability to perform Landau-Zener (LZ) transitions is a powerful and relatively unexplored tool to study and control spins on the nanoscale. LZ transitions provide spectroscopic information about energy level crossings, state populations and can even be used as a driving mechanism for coherent control over quantum spin states. In an idealized picture of a two level system (TLS), these qualities can be relatively easily understood via the LZ model. Here, we show LZ transitions on antiferromagnetic Fe chains on Cu2N/Cu(100) induced by ramping the magnetic field emanating from the tip of a scanning tunneling microscope (STM). Using real time measurement of the spin state we distinguish between classical and quantum tunneling transition processes. We find that avoided level crossings in higher excited states play a significant role in the dynamics between the ground states, showcasing the necessity to go beyond the TLS approximation used in the standard LZ model.

O 15.8 Mon 17:00 WILL/A317

Robustness of zero-energy edge states to disorder in bottom-up designed Fe chains on a superconducting Rashba alloy — •Harim Jang[1], Daniel Crawford[2], Jens Wiebe[1], Stephan Rachel[3], and Roland Wiesendanger[1] — [1]Department of Physics, University of Hamburg, Hamburg, Germany — [2]Department of Physics and Nanoscience Center, University of Jyväskylä, Finland — [3]School of Physics, University of Melbourne, Parkville, Australia

In this talk, we report on the role of disorder for the observation of Majorana zero modes (MMs) and a topological gap in a tailored 1D magnet-superconductor hybrid (MSH) system, showing the robustness of MMs to disorder, even in cases for which the topological gap is fully suppressed. We constructed 1D spin chains from Fe atoms on the Rashba surface alloy BiAg2/Ag(111) with proximity-induced superconductivity from a Nb(110) substrate. While the Fe chains have perfect crystalline order by design, the BiAg2/Ag(111) film exhibits nano-scale potential disorder, observed by scanning tunneling microscopy. However, this doesn't prevent the emergence of zero-energy states at the Fe chain's ends, in agreement with tight-binding calculations which show that they only appear in the topologically non-trivial regime [1]. This may not only explain earlier observations of MMs in disordered MSH systems, but also provides novel perspectives for the realization of robust Majorana qubits. [1] H. Jang et al., arXiv:2506.17414 (2025)

O 15.9 Mon 17:15 WILL/A317

Coherent control of a single 4f electron spin — •Yaowu Liu[1,2], Dasom Choi[1,2,3], Stefano Reale[1,2], Jeongmin Oh[1,2,3], Lei Fang[1,2], We-hyon Soe[1,2], Andreas Heinrich[1,2,3], Soo-hyon Phark[1,2], and Fabio Donati[1,2,3] — [1]IBS Center for Quantum Nanoscience (QNS) — [2]Ewha Womans University, Seoul 03760, Korea — [3]Department of Physics, Ewha Womans University, Seoul 03760, Republic of Korea

Electron spins on surface provide an atomic scale qubit platform for quantum information science using scanning tunneling microscopy (STM). Lanthanide atoms, with their strongly localized 4f electrons, can be potential candidates for single atom qubits with a long quantum coherence. However, STM tunneling current can strongly reduce the coherence time of surface atoms if they are probed directly. To circumvent this issue, it is possible to use an alternative scheme where a Ti (S = 1/2) atom located in a position within a 1 nm distance from a single Er atom on MgO surface can sense the quantum spin states of its 4f electron shells. In this work, we performed pulsed electron spin resonance (ESR) on the Er atom and demonstrated coherent control of 4f-electron spin of a single Er atom. Moreover, we observed a tenfold enhancement of Rabi rate compared to the direct drive of Ti atom from the tip, which is ascribed to the anisotropy of exchange interaction between the two spins.

O 15.10 Mon 17:30 WILL/A317

Kondo physics of composite molecular spins made from coupled nanographenes — •David Jacob — Department of Physics, University of Alicante, Spain

Open-shell nanographenes can now be fabricated by on-surface synthesis (OSS) and stabilized on metallic substrates, enabling access to their intrinsic (multi)radical character. Scanning-tunneling spectroscopy (STS) reveals clear Kondo signatures, demonstrating that these nanographenes host quantum spins whose magnitude reflects their degree of radicality [1]. By covalently linking such magnetic nanographenes, coupled spin systems can be engineered in controlled geometries–including dimers [2], hexagons [3], chains [4], and other topologies–allowing quantum magnetism to be probed at the atomic scale. Here we investigate coupled nanographenes whose constituent units have different spin magnitudes. We show that the composite nature of the resulting effective molecular spin leads to a rich spectrum of spin excitations and to unconventional Kondo behavior.

[1] *JACS Au* **3**, 1358 (2023); *Phys. Rev. Res.* **6**, L022061 (2024).
[2] *Phys. Rev. B* **106**, 205405 (2022); *Nano Lett.* **23**, 9353 (2023).
[3] *Angew. Chem. Int. Ed.* **60**, 25224 (2021).
[4] *Nature* 588, **287** (2022).

O 15.11 Mon 17:45 WILL/A317

Site-Specific magnetism of Ho atoms on MgO — •Andrés Pinar Solé[1,2], Merve Ercelik[1,2], Jungseok Chae[1,2], Fabio Donati[3], Dmitriy Borodin[1,2], and Andreas Heinrich[3] — [1]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS) — [2]Ewha Womans University — [3]Department of Physics, Ewha Womans University

Holmium (Ho) atoms on ultrathin MgO films are model systems for single-atom magnetism, where spin stability and relaxation strongly depend on the local crystal field and adsorption site. Isolated Ho atoms on oxygen sites of Ag(100)/MgO exhibit magnetic bistability but lack clear inelastic spin-excitation features; nevertheless, their magnetic states can be switched and read electrically through spin-polarized tunneling.

By extending to Ho dimers, additional spin-flip excitations become accessible, providing deeper insight into the electronic and magnetic states of Ho on MgO. The magnetic behavior of Ho dimers reflects the intra-atomic exchange coupling between the highly localized 4f moment and the outer valence-shell spins. Certain Ho dimers exhibit pronounced inelastic conductance steps, revealing strong magnetic interactions both between the atoms and with the surrounding MgO crystal field. Using STM-based atom manipulation, we precisely assemble Ho dimers on bridge and oxygen sites and probe their magnetic and electronic properties via Kelvin probe force microscopy (KPFM) and inelastic electron tunneling spectroscopy (IETS) in a combined STM/AFM UHV setup.

O 16: Focus Session: Structure and Dynamics of Solvent at Electrochemical Interfaces – Poster

Understanding how solvent molecules organize and move at electrochemical interfaces is central to catalysis, energy conversion, and electrochemical materials science. This Focus Session will bring together experimental and theoretical leaders using complementary surface specific spectroscopies as vibrational sum frequency generation, advanced X ray/electron techniques, and multiscale simulations to reveal intermolecular structure, hydrogen bond networks, ion-solvent coupling, and field driven dynamics from single crystal electrodes to complex battery interfaces. By highlighting recent breakthroughs in time-resolved measurements and operando platforms, the session aims to connect fundamental interfacial physics with macroscopic performance in electrocatalysis, corrosion, and electrochemical energy storage.

Organized by Yujin Tong (U Duisburg-Essen) and Angelika Kühnle (U Bielefeld).

Time: Monday 18:00–20:00 Location: P2

O 16.1 Mon 18:00 P2

Ab initio study of water clusters and thin film adsorption on Bi(111) surfaces — •Yingjie Xie, Adriana Bocchini, Uwe Gerstmann, and Wolf Gero Schmidt — Universität Paderborn, Paderborn, Deutschland

Bismuth, as a semimetal with strong spin-orbit coupling, plays an important role in many electrochemical applications, including electrocatalysis, electrode materials, and seawater desalination [1]. In these environments, interaction between Bi surfaces and water is unavoidable. The Bi(111) surface is both the natural cleavage plane of bulk Bi and the preferred growth surface in epitaxial processes, and is therefore suitable for studying water adsorption. While the atomic and electronic structures of Bi(111) surfaces have been well characterized, understanding of the water-Bi interface remains incomplete, and existing theoretical studies report partially conflicting results [2,3].

In this work, we employ density functional theory (DFT) to systematically investigate the adsorption behavior of isolated water molecules, molecular clusters, and thin water films on Bi(111). We examine the interplay between water-water and water-metal interactions and determine energetically favorable adsorption sites and configurations for water clusters and ultrathin films.

[1] V. Jovanovski, *et al.*, Curr. Opin. Electrochem. **3**, 114-122 (2017).
[2] V. Ivanistsev, *et al.*, E. Lust, Surf. Sci. **609**, 91 (2013).
[3] W. Oh *et al.*, J. Phys. Chem. C, **122**, 23084 (2018).

O 16.2 Mon 18:00 P2

Structure and Dynamics of Na^+ and Cs^+ adsorbed on Cu(111) and solvated by D_2O molecules — Florian Denizer[1], Jayita Patwari[1,2], John Thomas[1], Inga Langguth[2], Karina Morgenstern[2], and •Uwe Bovensiepen[1] — [1]Fakultät für Physik, Univ. Duisburg-Essen — [2]Phys. Chemie I, Ruhr-Univ. Bochum

Alkali cations in liquid water represent widely studied model systems of solvation science in which the water-water interaction competes with the local water-cation coupling. On electrode surfaces additional interactions become relevant. In our investigation using time-resolved two-photon photoemission and low-temperature scanning tunneling microscopy we compare Na^+ and Cs^+ on Cu(111) coadsorbed with individual D_2O molecules. $D_2O/Na^+/Cu(111)$ forms 10 nm wide, flat-lying aggregates. We observe a linear increase of the electronic lifetime of the 3*s* electron transfer resonance at the Cu(111)-Na^+ interface as a function of the number n of adsorbed D_2O molecules per ion combined with a maximal energy transfer to solvent modes ΔE of 0.6 eV at $n = 6-7$ [1]. On $D_2O/Cs^+/Cu(111)$ we find exclusively one or three D_2O attached to Cs^+. This leads to a stepwise increase in the corresponding 6*s* electron lifetime with n. ΔE is half that of $Na^+/Cu(111)$ which we associate with difference in ion core diameter and modified interactions with Cu(111) [2]. Comparing both systems we identify pronounced differences rooted in the microscopic connection between structure and dynamics.

[1] Kühne et al., JPC C **129**, 2054 (2025). [2] Thomas et al., JPC C **127**, 23467 (2023).

O 17: Spins on surfaces at the atomic scale – Poster

Time: Monday 18:00–20:00 Location: P2

O 17.1 Mon 18:00 P2

Conformational Control of Spin Lifetimes of a Single Molecule Magnet on a Metal Surface — •Sufyan Shehada[1], Corina Urdaniz[2], Manuel dos Santos Dias[3], Christoph Wolf[2], Dmitriy Borodin[2], Andreas Heinrich[2], Ruslan Temirov[1], Jeongmin Oh[1], Yujeong Bae[2], F. Stefan Tautz[1], Taner Esat[1], and Samir Lounis[4] — [1]Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich, Germany — [2]IBS Center for Quantum Nanoscience (QNS), South Korea — [3]Scientific Computing Department, STFC Daresbury Laboratory, United Kingdom — [4]Institute of Physics, Martin-Luther-University Halle-Wittenberg, Germany

We present a first-principles study of a spin-engineered molecular nanostructure: a PTCDA molecule coordinated to two Fe atoms on an Ag(111) surface. This work complements recent STM-based quantum sensing experiments, where upright molecules were assembled on metallic pedestals to enable precise spin manipulation and nanoscale magnetic field detection using electron spin resonance [1-3]. Using density functional theory (DFT), we investigate how adsorption geometry influences exchange interactions and magnetic anisotropy energy in both standing and lying conformations. Incorporating DFT-derived parameters and experimental input, we developed a spin model to simulate spin relaxation dynamics [4-6]. This reveals how conformational control can regulate spin lifetimes at the single-molecule level.

[1] Esat et al., Nature '18. [2] Esat et al., PRR '23.[3] Esat et al., Nat. Nanotechnol. '24. [4] Khajetoorians et al., Science '13.[5] Delgado et al., Surf. Sci. '14.[6] Hermenau et al., Nat. Commun. '17.

O 17.2 Mon 18:00 P2

Towards faster dynamics of magnons in atomic spin chains — Christina Mier[1], Alexandra Meerovici Goryn[1], •Michael Schelchshorn[1], Lukas Veldman[2], and Sander Otte[1] — [1]Delft University of Technology, Delft, The Netherlands. — [2]University of Stuttgart, Stuttgart, Germany.

The coherent free evolution of coupled atomic spins [1] as well as electron and nuclear spins within a single atom [2] has previously been demonstrated using ESR-STM. Extending this approach to atomically assembled spin chains, provides a tunable platform for investigating magnon transport and interactions; by exploiting the spectral resolution of ESR-STM, we achieve controlled excitation and tuning of coherent spin-wave modes while pump-probe techniques allow us to directly map their dynamics on a nanosecond time scale. In particular, by engineering stronger exchange coupling both within the chain itself and to the readout atom, we observe many more oscillations within the coherence times, demonstrating dynamical timescales significantly faster than those reported by Veldman et al. [1]. This work addresses the coherent magnon dynamics within precisely engineered atomic spin chains and paves the way for probing more complex collective excitations in larger spin systems.

[1] Veldman, L.M., et al., Science, 2021. 372(6545): p. 964-968.
[2] Veldman, L.M., et al., Nature Communications, 2024. 15(1): p. 7951.

O 17.3 Mon 18:00 P2

Development of Time-Resolved Pump-probe SP-STS for Ultrafast Spin Dynamics in SAM — •Yannick Noettger[1] and Artem Odobesko[2] — [1]Wuerzburg University — [2]Wuerzburg University

Achieving coherent control of Single Atom Magnets (SAMs) is necessary for their use in quantum technologies and requires fundamental understanding of their spin dynamics on the atomic scale. Scanning tunneling microscopy (STM) provides a unique platform for probing and manipulating SAMs with atomic precision. One major challenge is minimizing coupling of the SAM to the surrounding as substrate-mediated relaxation strongly limits coherence and lifetime. Usually this is done by placing the SAM on a thin insulating layer on a metal substrate. We used an extended approach by combining the decoupling layer with a superconducting substrate, potentially enabling enhanced lifetimes due to the gap in the SC density of states. We investigate NaCl/Cu(111)/NbOx heterostructures grown by e-beam evaporation, which exhibit substrate induced superconductivity within the Cu(111)-layer up to a film thickness of 3ML. NaCl deposition on Cu(111)/NbOx was achieved, however showing very different growth characteristics than on bare Cu(111). Furthermore we implemented an all-electrical pump-probe spectroscopy scheme into our existing STM setup demonstrating functionalization and precise synchronization with the Lock-In Amplifier, although pump-probe measurements on single Fe atoms on Cu2N/Cu(001) did not yield any measurable lifetimes, highlighting limitations of our current STM setup.

O 17.4 Mon 18:00 P2

Structural characterization of $Sc_3N@C_{80}$ on Ag(111) with scanning probe microscopy — •Caroline Hommel[1,2], Seong-Hyun Hong[1,4], Andrés Pinar Solé[1,2], Merve Ercelik[1,3], Robert Ranecki[1,2], Shinjae Nam[1,2], Dmitriy Borodin[1,2], Andreas Heinrich[1,3], and Lukas Spree[1,2] — [1]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS), Seoul 03760, Republic of Korea — [2]Ewha Womans University, Seoul 03760, Republic of Korea — [3]Department of Physics, Ewha Womans University, Seoul 03760, Republic of Korea — [4]Department of Physics, Korea University, Seoul 03760, Republic of Korea

Endohedral fullerenes are a fascinating class of compounds, that consist of a number of atoms trapped inside a fullerene cage structure. Among them, the Nitride Cluster Fullerenes (NCF) stand out for their stability and relatively high production yield. $Sc_3N@I_h$-C_{80} is the most abundant species in this class. Its electronic structure and the relatively free rotation of the internal cluster make it a promising candidate for molecular electronics.

In the presented work, we use STM and AFM with a CO functionalized tip to characterize individual $Sc_3N@I_h$-C_{80} molecules on Ag(111). This allows us to resolve their adsorption configuration and study the interaction of cage, cluster, and substrate in highest detail.

Studying $Sc_3N@I_h$-C_{80} at the single molecule level provides direct access to its geometric and electronic characteristics, which are often hidden in bulk measurements.

O 17.5 Mon 18:00 P2

Study of correlated spin interactions in bottom-up assembled molecular structures — •Lars Pütz[1,2,3], Daria Sostina[1,2,3], Stefan Tautz[1,3,4], and Markus Ternes[1,2,3] — [1]Peter Grünberg Institut (PGI-3); Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Experimentalphysik II B, RWTH Aachen University, 52072 Aachen, Germany — [3]Jülich Aachen Research Alliance (JARA), Fundamenatls of Future Information Technology, 52425 Jülich Germany — [4]Experimentalphysik IV A, RWTH Aachen University, 52072 Aachen, Germany

Correlated physics hosts phenomena such as unconventional superconductivity and exotic magnetic phases, yet their theoretical description is often challenging. To provide a starting point, we investigate finite correlated systems. We study NTCDA molecules deposited on an Ag(111) surface using a low-temperature scanning tunneling microscope. These molecules can receive an additional electron from the surface, which turns each of them into a spin-1/2 system. Normally, this spin is screened by the substrate through the Kondo effect. By using molecular manipulation techniques, we built small molecular structures in which the spin-exchange interaction between two neighboring molecular spins overcomes the screening from the surface. In these structures, we observe singlet-triplet excitations. Moreover, these excitations exhibit a spatially varying bias asymmetry in scanning tunneling spectroscopy, reflecting the phase pattern of the triplet wave function and thus providing experimental access to it.

O 17.6 Mon 18:00 P2

Spectra and competing correlations in coupled magnetic impurities on superconducting substrates — •Carlos Quesada Pérez and David Jacob — Departamento de Física, Universidad de Alicante, Spain

The study of magnetic impurities in superconductors is a fundamental challenge in condensed matter physics, crucial for understanding phenomena like in-gap states such as Yu-Shiba-Rusinov (YSR) states. Systems with multiple impurities can potentially host exotic ground states relevant for topological quantum applications. Accurate numerical methods like the numerical renormalization group are computationally too demanding for solving more than two impurity levels. Recently, an efficient impurity solver was proposed, based on the exact diagonalization of a single impurity connected to discretized superconducting reservoirs [1]. In this work, we extend this model to the case of two magnetic impurities coupled to BCS superconductors. By exact diagonalization of the resulting tight-binding Hamiltonian, we study the competition between the impurity-superconductor coupling and the impurity-impurity exchange to form a singlet with the bath or a singlet between the impurities themselves. The results reveal the evolution of YSR states and spin correlations, showing transitions between distinct quantum phases driven by this competition.

[1] Phys. Rev. B **108**, L220506 (2023)

O 17.7 Mon 18:00 P2

Atomic-Scale Engineering of Spin Defects in Monolayer MoS_2 — •Johannes Schwenk[1], Wantong Huang[1], Kwan Ho Au-Yeung[1], Johanna Matusche[1], Paul Greule[1], Jonas Arnold[1], Lovis Hardeweg[1], Máté Stark[1], Luise Renz[1], Affan Safeer[2], Daniel Jansen[2], Jeison Fischer[2], Thomas Michely[2], Wolfgang Wernsdorfer[1], Christoph Sürgers[1], Wouter Jolie[2], and Philip Willke[1] — [1]Physikalisches Institut (PHI), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]II. Physikalisches Institut, Universität zu Köln, Köln, Germany

Solid-state spin defects have become a promising platform for quantum technologies, including quantum sensing, communication, and computing. However, reliably creating and addressing such defects individually remains a major challenge. Here, we create distinct defect types in monolayer MoS_2 using the tip

of a scanning tunnelling microscope, i.e. sulphur vacancies and substitutional impurities. Moreover, we characterize their spin properties using electron spin resonance scanning tunnelling microscopy (ESR-STM) and demonstrate coherent control of the spin defects. By constructing dimers of defects, we show that their spins can be coupled via magnetic exchange, which provides a path to realize larger spin structures. These results open a new avenue to design and engineer quantum states at the atomic scale for applications in quantum sensing and simulations [Nat. Nanotech.19,1782-1788 (2024)].

O 17.8 Mon 18:00 P2

Switching properties of a spin-crossover complex on Cu(111) analyzed from time traces of the tunneling current — •Katharina Biel[1], Jasmeen Jasmeen[1], Sujoy Karan[1], Karl Ridier[2], Gael Reecht[1], and Manuel Gruber[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany — [2]LCC, CNRS and Université de Toulouse, France

Spin-crossover molecules can be switched between two states associated with different spin, a low spin (LS) and a high spin (HS) state. The switching between these two states can be induced by tunneling electrons, among other triggers, which offer the possibility to use a scanning tunneling microscope (STM) to investigate the switching dynamics at the single molecular level.

Here we investigate the spin-crossover molecule $[Fe(HB(1,2,4\text{-trazolyl})_3)_2]$, which forms self-assembled islands on Cu(111) and exhibits efficient switching under electron injection. The switching is monitored via time traces of the tunneling current, exhibiting two levels corresponding to the different spin states. Statistical analysis of these traces provides a detailed view on the switching properties. In particular we studied the influence of the applied voltage and the tunneling current on the switching rate. The influence of the applied voltage and the tunneling current on the switching yield is studied in details.

O 17.9 Mon 18:00 P2

Spin-Electric Control of Individual Spins on Surfaces — Paul Greule[1], Wantong Huang[1], Máté Stark[1], Kwan Ho Au-Yeung[1], Johannes Schwenk[1], Jose Reina-Gálvez[2], Christoph Sürgers[1], Wolfgang Wernsdorfer[1], Christoph Wolf[3], and •Philip Willke[1] — [1]Physikalisches Institut (PHI), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]Department of Physics, University of Konstanz, Konstanz, Germany — [3]Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul, Republic of Korea.

Individual magnetic molecules are promising building blocks for quantum technologies because of their chemical tunability, nanoscale dimensions, and ability to self-assemble into ordered arrays. In this work, we present spin-electric coupling (SEC) for two molecular spin systems, iron phthalocyanine (FePc) and Fe-FePc complexes, adsorbed on a surface. We use electron spin resonance combined with scanning tunnelling microscopy (ESR-STM) to locally address them with the STM tip and electrically tune them using the applied bias voltage. These measurements reveal a pronounced nonlinear voltage dependence of the resonance frequency, linked to the energic onset of other molecular orbitals. We attribute this effect to a transportmediated exchange field from the magnetic tip, providing a large, highly localized, and broadly applicable SEC mechanism. Finally, we demonstrate that the SEC enables all-electrical coherent spin control: In Rabi oscillation measurements of both single and coupled Fe-FePc complexes we show that the spin dynamics can be tuned.

O 17.10 Mon 18:00 P2

Defluorination of F_{16}Cu-Phthalocyanine on Superconducting Pb(100) — •Julian Skolaut, Biswajit Pabi, Alexander Weismann, and Richard Berndt — Institute for Experimental and Applied Physics, CAU Kiel, Germany

F_{16}Cu-phthalocyanine was investigated on a superconducting Pb(100) surface using low-temperature scanning tunneling microscopy. We achieved controllable defluorination of selected lobes. A single defluorinated lobe serves as a pivot point for rotation toward eight different azimuthal orientations. Defluorination of more than one lobe eliminates the ability to rotate. The energy of the lowest unoccupied molecular orbital depends on the degree of defluorination and is lowest when two lobes have been defluorinated. We also observed Yu-Shiba-Rusinov states, which exhibit shifts depending on the adsorption configuration and azimuthal orientation.

O 17.11 Mon 18:00 P2

Investigations of FePc molecular spins on a superconducting substrate — •Luise Renz[1], Máté Stark[1], Jonas Arnold[1], Johannes Schwenk[1], Christoph Sürgers[1], Wolfgang Wernsdorfer[1], and Philip Willke[1,2] — [1]Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Center for Integrated Quantum Science and Technology (IQST), Karlsruhe Institute of Technology, Karlsruhe, Germany

Electron spin resonance (ESR) measurements performed with a scanning tunneling microscope (STM) has emerged as an excellent technique to probe quantum spin systems at the nanoscale. However, the spin lifetimes of surface spins are limited by scattering with substrate electrons[1]. This can be prevented by employing thin insulating layers[1]. Alternatively, superconducting substrates can be used for decoupling[2].

Here, we present results on FePc molecules on a superconducting substrate. First, we characterize the FePc molecules on the new substrate by investigating the Zeeman splitting and the molecular orbitals. Our findings show that FePc resembles a spin-1/2 system, and that the molecular orbitals exhibit a similar pattern as was previously reported on MgO/Ag(001)[3]. Additionally, we perform all electric pump-probe measurements on single FePc molecules. By adjusting the external magnetic field, we can switch between the normal conducting and superconducting state and investigate the influence of the superconductor on the T_1 time of the FePc molecules. [1] Nat. Phys. 13, 403 (2017) [2] Nat. Phys. 9, 765 (2013) [3] Nat Commun 16, 5208 (2025)

O 17.12 Mon 18:00 P2

Spin Screening in MoS_2 Mirror Twin Boundaries on Graphene/Ir(110) — •Kuber Vyas, Tfyeche Tounsi, Jeison Fischer, Affan Safeer, Thomas Michely, and Wouter Jolie — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

Mirror twin boundaries (MTBs) are line defects that host confined states in the bandgap of monolayer MoS_2(1). The confined states closest to the Fermi energy splits into a singly and a doubly occupied level separated by the Coulomb repulsion U, forming a spin-1/2 system. The spin of the singly occupied state is then screened by the electron bath present in the substrate below, giving rise to a Kondo resonance pinned to the Fermi energy.

In this work, we investigate spin screening in MoS_2 MTBs grown on graphene/Ir(110) using low-temperature scanning tunnelling microscopy and spectroscopy. STS spectra recorded along the boundaries show two pronounced impurity peaks separated by the Coulomb energy U, together with a zero-bias feature which can be attributed to the Kondo resonance. MTBs on Gr/Ir(110) exhibit significantly broadened impurity-level widths, indicating strong hybridization γ with the electron bath provided by the graphene/Ir(110) substrate. This enhanced hybridization results in a Kondo temperature T_K comparable to the measurement temperature (7 K), enabling us to study the phase transition between the Kondo singlet phase below and the magnetic phase above the Kondo temperature. [1] C. van Efferen et al, Nat. Phys. 20, 82-87 (2024)

O 18: New methods: Theory – Poster

Time: Monday 18:00–20:00 Location: P2

O 18.1 Mon 18:00 P2

Cost-Efficient Approach for Training MACE Potentials — •Antonia Gerstenberg[1,2], Thomas Bligaard[2], and Andreas Lynge Vishart[2] — [1]currently: Fritz-Haber-Institut der MPG, Berlin, Germany — [2]DTU, Department of Energy Conversion and Storage, Denmark

Machine learning interatomic potentials (MLIPs) such as MACE offer near DFT accuracy at a fraction of the computational cost. However, a limiting factor is the cost of generating high-quality training data. This project investigates the development of a systematic and cost-efficient approach to training robust MACE models. It is therefore explored to what extent models trained on the cheapest available structures (e.g., dimers and trimers) can extrapolate to larger structures such as nanoparticles and vice versa.

To test this, an active learning workflow was implemented, iteratively adding structures with increasing numbers of atoms. The results show that widely used training strategies, including standard active learning workflows, fail to reliably extrapolate to out-of-distribution structures. The results highlight the importance of structural diversity and weight restriction from the outset.

O 18.2 Mon 18:00 P2

The application of classical DFT for describing small molecules diffusion in porous materials. — •Mikhail Suetin and Michael te Vrugt — Institute of Physics, Johannes Gutenberg Universität-Mainz, Staudingerweg 9, 55128, Mainz, Germany.

Metal-Organic Frameworks (MOFs) are relatively new, but promising materials potentially suitable for separation of hydrocarbon molecules for chemical industry aiming reaching the Net-Zero targets. Thousands of MOFs have been obtained experimentally, and about a million computationally. In this study, we conducted computational screening of the CoRE MOF database. Classical molecular dynamics simulations are employed for considering separation via diffusion. More importantly, classical density functional theory (cDFT) approach was employed to dramatically accelerate calculations of diffusion coefficients.

O 18.3 Mon 18:00 P2

Increasing the Transferability of Machine Learning Potentials by Learning Atomic Properties — •Johann Richard Springborn[1,2], Gunnar Schmitz[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

Machine Learning Potentials (MLPs) have become an established tool for describing potential energy surfaces of complex systems. While they significantly speed up the evaluation of the energy and forces in comparison to ab-initio methods, they require high-quality reference data for training. Depending on the systems to be studied, generating this training data can become the computational bottleneck. Therefore it is of high interest to reduce the number and complexity of structures to be computed. We propose to achieve this goal by training MLPs on atomic properties instead of global quantities such as the system's total energy. This approach aims to increase the transferability of the resulting MLPs to more complicated systems while still utilizing easily accessible reference data.

O 18.4 Mon 18:00 P2

Radial Dirac-Fock solver using integral equation method — •Ernests Lazdans, Janis Užulis, and Andris Gulans — University of Latvia, Riga, Latvia

We present a relativistic generalized Kohn-Sham solver for spherically symmetric atoms. It follows the approach introduced in a multi-wavelet code [1] where the Dirac equation is represented in the integral form. The solver supports local and hybrid exchange-correlation functionals and various nuclear distributions (point-like, Gaussian, and spherical). In validation test, we find that it yields Hartree-Fock energies in full agreement for all ten digits given by Visscher *et al.* [2]. However, our numerical tests show that numerical errors in our obtained atomic energies are below 10 nHa, *i.e.*, our solver's precision exceeds that of previously published data. We use the solver for testing performance of multiple exchange-correlation functionals for predicting electron removal energies from core and valence shells in noble gas atoms. The future applications of this tool include integrating it into a linearised augmented plane wave code.

[1] Anderson J. *et al.*, J. Chem. Phys. **151**, 234112 (2019)

[2] L. Visscher *et al.*, Atomic Data and Nuclear Data Tables **67**, 207-224 (1997)

O 18.5 Mon 18:00 P2

Towards Efficient Time-Dependent Density-Functional Theory through Hubbard On- and Inter-Site Corrections — •Lydia Fichte, Karsten Reuter, and Matthias Kick — Fritz-Haber-Institut der MPG, Berlin

Density-functional theory (DFT) with a Hubbard correction (DFT+U) can mitigate self-interaction errors in a manner similar to hybrid func- tionals, but at significantly lower computational cost. This makes extending DFT+U to the time-dependent regime particularly attractive, as it allows for accurate simulations of electron dynamics at reduced computational expense. However, the on-site subspace defined by DFT+U can be too rigid to describe phenomena involving strong orbital hybridization or charge transfer between sites, necessitating a more flexible definition of the correlated subspace. To address this, we are incorporating inter-site interactions through the +V correction to enable a more complete and adaptable description. We implement this as an efficient real-time time-dependent DFT+U+V framework in the all-electron electronic-structure code FHI-aims, enabling accurate and scalable simulations of correlated electron dynamics. We discuss the current status of the implementation and highlight the pitfalls and intricacies encountered when working with a numeric atom-centered orbital basis, both in the ground state and in time-dependent simulations.

O 18.6 Mon 18:00 P2

Calculating surface energy using machine learning interatomic potentials — •Friedrich Neumann[1], Tom Barnowsky[2,3], Rico Friedrich[2,3], and Jens Kortus[1] — [1]TU Bergakademie Freiberg - Institut für Theoretische Physik, Leipziger Str. 23, 09599 Freiberg — [2]Technische Universität Dresden - Theoretische Chemie, 01062 Dresden — [3]Helmholtz-Zentrum Dresden-Rossendorf e.V., Bautzner Landstraße 400, 01328 Dresden

The surface energy of a material is a fundamental property that governs the behaviour of solid interfaces in a wide range of phenomena. While density functional theory (DFT) provides highly accurate values, its computational scaling limits its applicability for large systems and systematic surface-energy screening. In this work, a workflow was developed to estimate surface energies using machine-learning interatomic potentials (ML-IAPs). Atomic Cluster Expansion (ACE) models were fitted to DFT-based molecular-dynamics data for Al, Pt, and Au, and effective two-body contributions were extracted from the resulting potentials. These were combined with a bond-counting approach to compute surface energies and Wulff constructions. Although in our present ACE model the absolute magnitudes of the pair interactions are influenced by many-body interaction, preventing quantitative reproduction of surface energies, the approach still captures general trends and identifies the dominant facets in the Wulff constructions. In this specific formulation, the results illustrate how many-body interaction can affect the apparent pair contribution.

O 19: Vacuum Science & Technology: Theory and Applications – Poster

Time: Monday 18:00–20:00 Location: P2

O 19.1 Mon 18:00 P2

Contact-Separation phenomenon at the Silica-Gold interface: AFM and ToF-SIMS insights — •Nisha Ranjan, Tolga Acartürk, Kathrin Küster, and Ulrich Starke — Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

Contact-Separation (CS) electrification at solid interfaces constitutes a fundamental phenomenon. However, it often exhibits uncertainties and irreproducibility [1,2]. The silica-gold contact pair is a model example of a dielectric-metal system with a similar elastic modulus that shows a significant variation in charging properties such as polarity reversal among CS surfaces [3]. We aim to understand the phenomenon with interfacial interactions and chemical composition using direct microscale measurements under ultra-high vacuum conditions at the silica-gold interface. We use Atomic Force Microscope/Force Spectroscopy (AFM/FS) to quantify interfacial interactions, such as electrostatic force, van der Waals interaction, contact area, contact pressure, and deformation. Repeated approach-retraction cycles enabled the correlation of mechanical response with charge accumulation and compositional change. We use Time-of-Flight Secondary Ion Mass Spectroscopy (ToF-SIMS) for surface composition mapping to assess mechanochemistry. Our finding demonstrates that the magnitude of the force is significantly influenced by the charge accumulation. Concurrently, a change in surface composition was also observed. [1] I. Jimidar and J. Méndez Harper, Physics Today 78(8), 54 (2025). [2] D.J. Lacks, Angew. Chem. Int. Ed. 51, 6822 (2012). [3] G. Fatti et al., PRL 131, 166201 (2023).

O 19.2 Mon 18:00 P2

Simulation-Guided GIXPS: Planning faster (HA)XPS measurements while enabling depth-sensitivity — •David Capalbo[1], Oliver Rehm[1], Endrit Kusari[1], Andrei Gloskovskii[2], Christoph Schlueter[2], Lutz Baumgarten[3], and Martina Müller[1] — [1]Fachbereich Physik, Universität Konstanz, Konstanz, Germany — [2]DESY, Hamburg, Germany — [3]FZ Jülich GmbH, PGI-6, Jülich, Germany

(Hard) X-Ray Photoelectron Spectroscopy ((HA)XPS) is an established method for characterizing surfaces, interfaces, and the bulk material properties of thin films, multilayers, and devices. Such measurements, when performed at a synchrotron-based setup, can produce faster and better resolved data compared to a laboratory setup, but beamtime is limited and highly competed for. We present a simulation-based approach that enables faster and more efficient measurements by exploiting grazing-incidence (GI) angle geometries (0.3°-2°). At these GI angles, tunable depth-selective photoelectron emission becomes possible while increasing the signal by up to two orders of magnitude at characteristic angles. In our approach, an additional damping term is added to an already existing simulation model, which enables the user to simulate an accurate GI(HA)XPS response before the beamtime. This enables them to identify and prioritise configurations of interest, reduce the required aquisition time, all while keeping the expected advantages of standard (HA)XPS measurements. O.Rehm *et al.*

O 19.3 Mon 18:00 P2

Electrospray Ion Beam Deposition for Atomic Resolution Native Protein Structure Investigation at Surfaces — •Stephan Rauschenbach — University of Oxford, Kavli Institute for Nanoscience Discovery, Department of Chemistry, Sherringdon Road, Oxford

Electrospray ion beam deposition (ESIBD) enables controlled deposition of intact biomolecules from solution onto surfaces under ultrahigh vacuum conditions. We present ESIBD as a sample preparation method for cryo-EM, scanning probe, and holography applications, bridging native electrospray ionisation mass spectrometry with surface-based structural characterisation techniques.

The method combines mass-selective soft landing with controlled ice growth embedding protocols. Proteins maintain their native conformations during the gentle electrospray process and deposition. For cryoEM Ice matrix formation occurs post-deposition minimising mechanical stress and denaturation.

Here we discuss the state of the art implementation of this method on commercial and self-built platforms and demonstrate atomic resolution imaging of soluble and membrane proteins deposited on surfaces in vacuum.

O 19.4 Mon 18:00 P2

Analysis of the charge distribution of an insulating sphere in contact electrification processes — •Andre Mölleken, Hermann Nienhaus, and Rolf Möller — Experimental Physics, University of Duisburg-Essen and Center for Nanointegration Duisburg-Essen (CENIDE)

While the mechanisms of contact electrification between metals are well established, non-conductive materials present a more complex scenario due to the emergence of nonuniform surface charge distributions. This study investigates how such charge inhomogeneities on an insulating sphere like Al2O3 or quartz influence the subsequent charge transfer during contact with a planar metal or insulator electrode. We employ a redesigned experimental setup based on an established parallel-plate capacitor concept [1], enabling high-temporal-resolution measurements of induced and transferred charges as the sphere bounces on the lower electrode. By decomposing the measured signal into monopole and dipole components, we extract the net charge, quantify the dipole moment of the surface charge distribution, and determine the rotational frequency of the bouncing sphere. This approach reveals how initial charge patterns evolve dynamically and modulate the efficiency and direction of charge transfer upon impact. The new setup allows controlled manipulation of the sphere's initial surface charge distribution prior to each experiment. The results offer a novel way to study how the charge distribution on the surface influences the contact electrification process. [1] M. Kaponig, A. Mölleken, H. Nienhaus, R. Möller, Dynamics of contact electrification, Sci. Adv. 2021, 7 (22), eabg7595.

O 19.5 Mon 18:00 P2

Contact electrification between Au and hydrogen-passivated Si(111) surfaces — •Christian Gruber, Andre Mölleken, Tobias Prost, Hermann Nienhaus, and Rolf Möller — Experimental Physics, University of Duisburg-Essen and Center for Nanointegration Duisburg-Essen (CENIDE)

The charge of 1mm Au spheres bouncing on a hydrogen-passivated Si(111) surface under vacuum conditions is measured in a parallel-plate capacitor setup with fC charge sensitivity and microsecond time resolution [1]. The transferred charge between metal and semiconductor is determined as a function of impact velocity ranging from 1 to 0 m/s, of doping and of surface condition after preparation. Light exposure to the semiconductor surfaces during experiments shows no significant influence on the results. On p-doped samples the Au spheres collect a charge of typical a few 100fC with each contact. The dependence on the preparation is not as clear as on n-doped samples, on which the quality of the surface preparation clearly causes a polarity change. On n-doped samples the Au spheres collect a typical charge of a few 100 fC to over 1000 fC. However, in the limit of zero impact velocity the variations between the different samples become negligible and Au is found to be charged negative. The results are compared with predicted charge transfer between Au and Si in static Schottky diode models.

[1] M. Kaponig, A. Mölleken, H. Nienhaus, R. Möller, Dynamics of contact electrification, Sci. Adv. 2021, 7 (22), eabg7595.

O 19.6 Mon 18:00 P2

Towards nanoscale EUV spectroscopy of 2D heterostructures using interferometric coherent diffractive imaging — •Hannah Strauch, Jan Mädrich, Daniel Steil, Stefan Mathias, and G. S. Matthijs Jansen — University of Göttingen, 1st Institute of Physics, Göttingen, Germany

Time-resolved spectroscopy in the extreme ultraviolet (EUV) energy range provides element-specific insight into electronic and structural dynamics. Particularly, EUV spectroscopy of nanoscale 2D material heterostructures enables to identify the individual layer contributions due to its element-specificity. For such systems, however, a spatially resolved probe is essential: 2D material heterostructures are both intrinsically micro-scale and highly susceptible to spatial inhomogeneities. The comprehensive understanding of ultrafast dynamics in those systems therefore requires simultaneous spatial, spectral, and temporal resolution, which is a combination that remains experimentally demanding even with state-of-the-art techniques.

We will present our progress towards such a comprehensive measurement approach with our table-top EUV interferometry-based setup, which enables time-resolved spectroscopy with spatial resolution through the combination of Fourier transform holography (FTH) with interferometric Fourier transform spectroscopy (FTS). The surface sensitivity required for few-layer systems is provided through measurements in reflection geometry.

O 19.7 Mon 18:00 P2

Development of a Low Temperature Two-Level System Microscope for Superconducting Quantum Circuits — •David Mazibrada[1], Johannes Schwenk[1], Jürgen Liesenfeld[1], Hannes Rotzinger[1,2], Philip Willke[1], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut (PHI) — [2]Institut for Quantum Materials and Technologies (IQMT), Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany

Superconducting quantum circuits are among the most advanced platforms for solid-state qubits. Their performance is perturbed, however, by parasitic two-level systems (TLS). The electric fields of the qubit interact with the electrical dipole moment of the TLS, leading to an exchange of photons between the two quantum systems. TLS are mostly of an unknown nature and position, and identifying them locally would help to improve future qubits. Since TLS couple not only to the qubit's microwave field but also to externally applied electric fields, this interaction enables us to probe and localize individual TLS.

We present a microscope combining a cryogenic atomic force microscope (AFM) and a superconducting quantum circuit. By applying a local electric field with the AFM tip and performing microwave spectroscopy, we aim to identify, characterize, and map the position of individual TLS on superconducting quantum circuits.

O 19.8 Mon 18:00 P2

Prospects of ARPES measurements in an external static magnetic field — Dmitry Usanov and •Daniil Yevtushynsky — Laboratory for Quantum Magnetism, EPFL, 1015 Lausanne, Switzeralnd

Angle-resolved photoemission spectroscopy (ARPES) has traditionally been performed in magnetically shielded environments, as external magnetic fields distort electron trajectories and worsen the momentum resolution. This limitation has prevented direct observation of many field-dependent electronic phenomena. Recent studies, however, have demonstrated that applying a strongly localized static magnetic field enables ARPES measurements under external field conditions. We propose to test a newly developed compact magnetic circuit, integrated into a standard flag-type sample holder, capable of generating a high magnetic flux density at the sample position while minimizing its effect on photoelectron trajectories. In the presentation we will discuss the optical action of the designed magnetic field and subsequent aberration corrections for different types of samples. In addition, we will provide estimations of the maximum magnetic field for ARPES in the soft X-ray and VUV ranges. At the end, we will propose different test systems, where moderate magnetic fields can tune the spin order and induce pronounced modifications of the band structure near the Fermi level. Successful implementation will establish a new experimental capability - ARPES in controlled static magnetic fields - opening pathways to study field-dependent band topology and spin-charge coupling across a broad class of quantum materials and heterostructures.

O 19.9 Mon 18:00 P2

New Electrospray Ion Beam Deposition source for wellcontrolled STM sample preparation — •Niclas Przibylla[1], Markus Etzkorn[1], Stephan Rauschenbach[2], and Uta Schlickum[1] — [1]Institute of Applied Physics, TU Braunschweig, Braunschweig — [2]Kavli Institute for Nanoscience Discovery, University of Oxford, United Kingdom

High resolution imaging of complex biomolecules such as peptides, glycans, and photosynthesis building blocks are crucial for advancing their fundamental functionalities and exploring them for quantum technologies, Scanning probe microscopy techniques together with mass-selected electrospray ion beam deposition enable atomic-level structural characterization of these molecules. This project deploys a novel electrospray ion beam deposition (ESIBD) system with Python-based programmable control for depositing non-volatile molecules onto clean surfaces under ultra-high vacuum conditions. The process involves electrospray ionization, mass-to-charge filtering via quadrupole ion guides, and electrostatic focusing onto nitrogen-cooled samples. Key innovations include a modular chamber architecture allowing future expansion, alongside RF-operation using rectangular voltage waves for enhanced mass filtering precision. Frequency-asymmetric and amplitude-asymmetric waveforms will enable systematic investigation of ion stability diagram effects, advancing deposition control capabilities.

O 19.10 Mon 18:00 P2

Electronoptical Concept of ARPES and RIXS Combined in a Novel Photoelectron Microscope — O. Tkach[1], Y. Lytvynenko[1], C. Fawaz[2], T. Lacmann[3], S. Chernov[4], O. Fedchenko[1,5], H. Agarwal[1], M. Hoesch[4], J. K. Dey[4], J. Dilling[4,6], L. Bruckmeier[4,6], M. Scholz[4], J. Schunck[4,7], S. Roth[2], K. Rossnagel[4,6], M. Beye[8], M. Le Tacon[2], •G. Schönhense[1], and H.-J. Elmers[1] — [1]Univ., Mainz — [2]IQMT, KIT — [3]EPFL, Switzerland — [4]DESY, Hamburg — [5]Goethe Univ. Frankfurt — [6]CAU Kiel — [7]Univ. Hamburg — [8]AlbaNova, Sweden

The instrumentation required for ARPES and Resonant Inelastic X-ray Spectroscopy (RIXS) is usually completely different. ARPES uses electron spectrometers, primarily hemispherical ones, whereas RIXS requires high-resolution X-ray spectrometers with long optical paths to achieve the desired resolution. In a special time-of-flight photoelectron microscope, we combined photoelectron momentum microscopy (MM) - imaging of the backfocal plane of the objective lens, a powerful ARPES approach - with the concept of PAXRIXS [1]. Here, the RIXS photons are converted into photoelectrons using an ultrathin foil. The position at which a RIXS photon hit the converter is a measure for the momentum transfer. For RIXS, the converter foil is moved between the sample and the extractor with fields-of-view of >4 mm. This is facilitated by a novel type of front lens which enables various operating modes. Ultrathin Au, Ag, and Pt converter foils provide energy resolutions between 20 meV and 400 meV.

[1] Dakovski et al., J. Synchrotron Radiat. 24 (2017) 1180.

O 20: Electronic structure theory – Poster

Time: Monday 18:00–20:00 Location: P2

O 20.1 Mon 18:00 P2

From Wannier Functions to Optimal Local Orbitals: A Systematic Approach for Accurate Wavefunction Representation — •Ann Chantal Goutier and Michael Schüler — Laboratory for Materials Simulations, Paul Scherrer Institut, Villigen PSI 5232, Switzerland

Electronic structure calculations in solids are commonly carried out using DFT algorithms with large initial basis sets. These basis sets are compressed into smaller basis sets localised around atoms to calculate quantities of interest. It is desireable to be able to do this conversion with only minimal loss of accuracy. The most common algorithm for this is Wannierisation, a unitary transformation of the Hamiltonian into a space of maximally localised wave functions. Wannierisation preserves the Hamiltonian exactly, but Wannier wave functions cannot be used to construct eigenstates explicitly.

We propose new methods to create Local Orbitals directly, building on the idea of Smart Local Orbitals (Gandus, 2020). Our methods maximise the projectability of the Local Orbital basis set onto electronic eigenstates. This can be done either by blockdiagonalisation of a projectability operator, or by singular value decomposition of the overlap. It is advantageous as less information about the system is required and the Local Orbital set can be systematically improved by adjusting projectibility cut-offs. We also showcase the impact of variationally optimising the Local Orbital basis with respect to different parameters to further improve the representation of Kohn Sham states within a minimal basis.

O 21: Surface magnetism – Poster

Time: Monday 18:00–20:00 Location: P2

O 21.1 Mon 18:00 P2

Quantum confinement of spinarons in quantum corrals. — •Raffaele Aliberti[1], Juba Bouaziz[2], Ilias Klepetsans[2], and Samir Luonis[1] — [1]Institute of Physics, Martin-Luther- University Halle-Wittenberg, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, Germany

For more than two decades, cobalt atoms on noble-metal (111) sur-faces have served as a paradigm for the Kondo effect in scanning tun-nelling spectroscopy (STS) experiments. However, our recent first-principles predictions, supported by high-magnetic-field STS mea-surements, challenge this established view. We showed that the observed transport anomalies originate instead from spin excitations of Co atoms forming a distinct many-body state, the spinaron, which is a polaronic quasiparticle arising from the interaction between an excited magnetic moment and a trapped surface electron. Here, using time-dependent DFT combined with many-body perturbation theory, we investigate quantum-confinement engineering in circular and elliptical quantum corrals hosting a single Co adatom, revisiting the celebrated experiments traditionally interpreted through the lens of the Kondo effect. We demonstrate that confined electronic states significantly modify the underlying electron*boson interactions, thereby altering the amplitude and characteristics of the spinaronic states

O 21.2 Mon 18:00 P2

Spin-polarized LEED and reflectivity in altermagnetic materials — •Sourour Ayari, Aki Pulkkinen, and Jan Minar — New Technologies Research Center, University of West Bohemia in Pilsen, Plzen Czech Republic

Altermagnetic materials exhibit a characteristic non-relativistic spin splitting arising from their unconventional spin-symmetry properties [1-3], which leads to alternating spin textures in momentum space even in the absence of a net magnetization. To probe how these textures manifest at the surface, we use theoretical calculations based on the relativistic Korringa-Kohn-Rostoker multiple scattering method [4-5] to study the spin-polarized low-energy electron diffraction and angle- and spin-resolved reflectivity of electrons. These observables are sensitive to spin-dependent scattering processes and therefore provide a direct window into the surface projections of the altermagnetic spin structure. This approach enables a detailed understanding of the spin-dependent reflectivity in altermagnets and offers deeper insight into their surface electronic and magnetic properties.

References: [1] N. Dale et al., arXiv:2402.13094 (2024). [2] L. Šmejkal et al., Nat. Phys. 18, 404-408 (2022) [3]O Fedchenko, J Minár, A Akashdeep, SW D'Souza- Science advances, 2024 [4]J Krempaský, L Šmejkal, SW D'souza, M Hajlaoui- Nature, (2024) [5] J. Minár & H. Ebert, J. Electron Spectrosc. Relat. Phenom. 190, 159-170 (2013).

O 22: Surface dynamics – Poster

Time: Monday 18:00–20:00 Location: P2

O 22.1 Mon 18:00 P2

Tracing light-induced dynamics of correlated charge order at the atomic scale — •Luis Enrique Parra Lopez[1], Alkisti Vaitsi[1], Vivien Sleziona[1], Fabian Schulz[2], Martin Wolf[1], and Melanie Müller[1] — [1]Fritz Haber Institute, Berlin, Germany — [2]CIC nanoGUNE, Donostia-San Sebastian, Spain

Terahertz-driven scanning tunneling microscopy (THz-STM) is a versatile technique that enables the study of ultrafast dynamics in quantum materials with simultaneous nanometer spatial and femtosecond temporal resolution. Here, we use THz-STM to investigate the local ultrafast response of the charge density wave (CDW) phase in 1T-TaS2. Optical-pump THz-probe measurements reveal coherent oscillations of the THz-driven tunneling current at 2.5 THz, consistent with the amplitude mode of the CDW. In addition, we observe a previously unreported 1.3 THz mode in the vicinity of a structural defect, consistent with predictions for interlayer phonons. Beyond these ultrafast collective dynamics, our measurements uncover an additional slower effect: THz-induced long-lived changes of the local density of states (LDOS). These metastable modifications appear as LDOS peak shifts indicative of local stacking changes. They do not arise from the coherent CDW response, but from a local THz-induced perturbation of the CDW lattice. We demonstrate that these changes appear predominantly near lattice inhomogeneities and are consistent with local misalignments of the stacking configuration. Together these findings highlight THz-STM as a platform for imaging and controlling nonequilibrium quantum phases at their intrinsic spatial and temporal scales.

O 22.2 Mon 18:00 P2

Photonic Structures for Purcell-Enhanced Driving of a Structural Phase Transition — •Nandana Veena Uday[1], Florian Spickmann[1,2], Sebastian Zafra Koch[1,2], Felix Kurtz[1], Claus Ropers[1,2], and Hannes Böckmann[1] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]University of Göttingen, 4th Physical Institute, Göttingen, Germany

Direct integration of silicon photonics with low-dimensional materials connects tailored light-matter interaction with surface-sensitive probing. Here, we explore the remote optical driving of a prototypical Peierls insulator, adsorbed on the surface of a silicon photonic waveguide. Optical gratings couple infrared light to guided modes of a silicon slab, while ultrafast low-energy electron diffraction probes the waveguide-mediated optical quench of the periodic lattice distortion in adsorbed atomic indium chains. These experiments constitute first steps towards engineering photonic environments for surface phase control using tailored lithographic fabrication techniques. Potential avenues range from Purcell-enhanced photoinduced phase transitions to driven states of matter obtained by interfacing surface structures with integrated micro-resonator cavities. [1] Böckmann, Hannes, et al. Structural Dynamics 9.4 (2022)

O 22.3 Mon 18:00 P2

Non-equilibrium phonon dynamics of the kagome metal CsV_3Sb_5 — •Felix Kurtz[1,2], Lukas Jehn[1,2], Alp Akbiyik[1,2], Matthieu Le Tacon[3], Amir-Abbas Haghighirad[3], and Claus Ropers[1,2] — [1]Department of Ultrafast Dynamics, Max Planck Institute for Multidisciplinary Sciences, D-37077 Göttingen — [2]4th Physical Institute, University of Göttingen, D-37077 Göttingen — [3]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, D-76021 Karlsruhe

Tracking the equilibration processes that follow photoexcitation in materials can reveal couplings between and among electrons and lattice degrees of free-

dom. Thus, a variety of femtosecond electron or X-ray diffraction techniques are used to follow non-equilibrium structural dynamics. Recently, we have introduced ultrafast low-energy electron diffuse scattering (ULEEDS), a surface-sensitive method capable of tracing momentum-dependent phonon populations with out-of-plane polarization [1]. Here, we employ ULEEDS to a second material, the kagome metal CsV_3Sb_5, and reveal non-thermal phonon occupations whose subsequent equilibration is driven by phonon-phonon scattering. Comparing these results to our previous study of $TiSe_2$, we find that while a rapid buildup near the Brillouin-zone boundary still precedes a slower emergence of zone-center acoustic modes, the relaxation times in CsV_3Sb_5 are confined to a much narrower distribution.

[1] F. Kurtz *et al.*, Nat. Mater. **23**, 890-897 (2024)

O 22.4 Mon 18:00 P2

Extending Surface Phase Diagrams to Non-Equilibrium Plasmas — •Maximilian Wünschek, Alper T. Celebi, and Markus Valtiner — Institute of Applied Physics, Vienna University of Technology, Wiedner Hauptstrasse 8-10/E134, Vienna 1040, Austria

Surface phase diagrams are widely used to visualize the stability of surface reconstructions under equilibrium gas conditions. However, many growth and treatment processes use plasmas that operate far from equilibrium, where activated and ionized species are present in substantial concentrations. Examples such as ZnO have shown that unique reconstructions can be found outside the stability range defined by conventional chemical potential axes, highlighting the need to extend surface phase diagrams to non-equilibrium regimes.

Using GaN as a model system, we compile a large dataset of reconstructions for polar GaN surfaces under hydrogen, nitrogen, and oxygen environments. Building on these results, we introduce a framework for applying surface phase diagrams to plasma conditions by incorporating non-thermal species into the chemical potential landscape. A minimal kinetic model estimates plasma composition, and thermochemical properties of the constituent species are combined into an effective plasma chemical potential.

The resulting extended diagrams show how radicals and ions shift phase boundaries and stabilize surface structures inaccessible under equilibrium. This approach provides a basis for understanding and predicting surface configurations formed during plasma-assisted processing.

O 22.5 Mon 18:00 P2

Atomic vibrations in the icosahedral quasicrystal AlPdMn studied with femtosecond electron diffraction — •Moritz Schlechtriem[1,2], Victoria C. A. Taylor[2], Hyein Jung[1,2], Ralph Ernstorfer[1,2], and Yoav William Windsor[1,2] — [1]Technische Universität Berlin — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Quasicrystals (QCs) are materials in which the atomic arrangement lacks periodicity but exhibits perfect spatial order. QCs therefore produce sharp diffraction patterns with unconventional features such as 5-fold rotational symmetry. Due to the aperiodic nature of QCs, phonons are insufficient to fully describe atomic vibrations. Phasons are quasiparticles related to atomic motion in the presence of aperiodicity, and their group velocity can exceed the speed of sound. The resulting enhanced thermal conductivity gives rise to potential applications of QCs, e.g. in nanoelectronics.

Here we use pump-probe femtosecond electron diffraction (FED) to study ultrafast atomic vibrations in QCs. This enables us to study the femtosecond evolution of photoinduced atomic motion, shedding light on the coupling mechanisms between electrons, phonons and phasons.

In this presentation we focus on the icosahedral QC alloy AlPdMn. FED results, in which different high-symmetry directions (e.g. the 5-fold rotation axis) are probed, will be presented.

O 22.6 Mon 18:00 P2

Thermo-osmotic flows at the Chemically Patterned Surfaces — •Neerdhi Goswami and Frank Cichos — Universität Leipzig Linnestr. 5 04103 Leipzig Germany

The boundary flows at a solid-liquid interface are governed by the interaction of the solid and liquid, specifically by the excess enthalpy of these interactions. Consequently, chemical modification of surfaces alters boundary flow fields. By generating spatially dependent patterns of solid-liquid interactions, we can not only shape various flow fields but also directly compare excess interaction enthalpies between modified and unmodified regions.

This study analyzes opto-thermo-osmotic flow fields at a thiol-patterned gold-water interface to provide a quantitative microscopic picture of dynamic interfacial interactions through comparative analysis. Thiol stripes were generated through micro-contact printing, creating alternating patterns of modified and unmodified gold regions. Surface plasmon resonance (SPR) imaging confirmed thiol addition by detecting the characteristic frequency shift upon adsorption.

This quantitative characterization of interfacial interactions provides fundamental insights into how surface chemistry modulates boundary flows, with implications for designing responsive microfluidic systems and optimizing interfacial processes in precision separation and manipulation applications.

O 23: Catalysis and surface reactions – Poster

Time: Monday 18:00–20:00 Location: P2

O 23.1 Mon 18:00 P2

Investigating Single Atomic Catalytic Sites within Metal- Coordinated Supramolecular Networks via Submolecular Imaging in correlation with Electrochemical Analysis — •Duong Tran[1], Philipp Wiesener[1], Ying Pan[2], Nieves López- Salas[2], and Harry Mönig[1] — [1]Physikalisches Institut, Universität Münster, Germany — [2]Department of Chemistry, Sustainable Materials Chemistry, Universität Paderborn, Germany

Metal-organic layers serve as an excellent platform for creating single-atom catalysts (SACs). This study focuses on a heat-induced deprotonation reaction of a melem precursor and the formation of a heptazine-based metal-organic network on an Au(111) substrate. To overcome thermal desorption challenges hindering chemisorption, we developed a vacuum reactor chamber with a high-flux evaporator for precursor deposition. The resultant heptazine-based Au-nitride network aligns with previous results on Cu(111) using the same precursors. In particular, the interaction of Au(111) atoms with dehydrogenated nitrogens results in a gold atom flexibly suspended between two nitrogen atoms, indicating promising active sites for oxygen reduction reaction (ORR). Scanning tunneling microscopy (STM), noncontact atomic force microscopy (nc-AFM) with an oxygen-terminated copper tip, and X-ray photoelectron spectroscopy (XPS) confirm the strong chemisorption and stability of the network. A comparison of the catalytic performance of heptazine-based metal-nitride networks on Au(111) and on Cu(111) under ambient conditions enhances the understanding of the ORR electrochemical applications.

O 23.2 Mon 18:00 P2

Support-Dependent Thermal Activation of Pt17 Clusters on HOPG and CeO2: For-mation of Active CO Oxidation Catalysts — Papri Chakraborty[1,2,3], •Johannes Seibel[2], Nicola Da Roit[4], Artur Böttcher[2], Ajai Raj Lakshmi Nilayam[1], Christian Kübel[1], Silke Behrens[4], and Manfred Kappes[1,2,3] — [1]Institute of Nanotechnology, KIT, 76344 Eggenstein-Leopoldshafen, Germany — [2]Institute of Physical Chemistry, KIT, 76131 Karlsruhe, Germany — [3]Institute of Quantum Materials and Technologies, KIT, 76344 Eggenstein-Leopoldshafen, Germany — [4]Institute of Catalysis Research and Technology, KIT, 76344 Eggenstein-Leopoldshafen, Germany

Atomically precise ligand-protected metal clusters are attractive precursors for heterogeneous catalysts, potentially allowing for the precise control of the initial active site composition. However, the transformation from the protected cluster to the active catalyst, specifically the removal of the ligand shell, remains a poorly understood process that depends heavily on the support material. Here, we present a comparative study of the thermal activation of $Pt_{17}(CO)_{12}(PPh_3)_8(NO_3)_2$ on inert graphite, on reactive ceria CeO2 surfaces and in gas phase. For this we combined thermal desorption spectroscopy with high-resolution mass and ion mobility spectrometry to map the decomposition pathway of the cluster. Additionally we probed clusters supported on CeO2 before and after CO oxidation catalysis with transmission electron microscopy. This revealed dissociation of clusters and dispersion of the Pt atoms on the oxide support under certain reaction conditions.

O 23.3 Mon 18:00 P2

From model to powder systems: Sm-doped ceria for CO_2 conversion. — •Raquel Sánchez-Barquilla[1], Sichen Liu[1], Alexander Contreras-Payares[2], Pablo G. Lustemberg[2], Dominic Guttmann[1], Carlos Morales[1], Fabian Rachow[1], Verónica Ganduglia-Pirovano[2], and Jan Ingo Flege[1] — [1]Brandenburg University of Technology, Cottbus-Senftenberg, Germany — [2]Instituto de Catálisis y Petroleoquímica, Madrid, Spain

Reducible oxides are crucial in many heterogeneously catalyzed redox reactions because they can store and release oxygen during the catalytic cycle. Among these, cerium oxide (CeO_2) stands out due to its facile transition between the Ce^{4+} and Ce^{3+} oxidation states. Furthermore, the Ce^{3+} cations have been suggested to provide the active sites for CO_2 activation. Consequently, the catalytic performance of ceria-based catalysts may be significantly enhanced by promoting and stabilizing these sites, e. g., by alloying with trivalent rare-earth (RE) metals that also form cubic sesquioxides (RE_2O_3), such as samarium.

Here, we present a model system composed of (111)-oriented Sm-doped ceria nanoislands studied using X-ray photoelectron spectroscopy under near-ambient pressure. We show that Sm is crucial for CO_2 activation. This activation is accompanied by a charge-transfer process that modifies the measured Ce^{3+}/Ce^{4+} ratio, as explained by density functional theory calculations. Once the reaction mechanism was established, we performed *operando* absorption spectroscopy on powder catalysts with different Sm/Ce ratios to examine the effect of Sm doping under more realistic conditions.

O 23.4 Mon 18:00 P2

Digital Catalysis: Accelerated Discovery Through Human in the Loop — •Charles Pare[1], Aybike Terzi[2], Christian Kunkel[1], Frederik Rüther[2], Frederic Felsen[1], Robert Baumgarten[2], Esteban Gioria[2], Raoul Naumann d'Alnoncourt[2], Christoph Scheurer[1], Frank Rosowski[2,3], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]BasCat - UniCat BASF JointLab, Berlin — [3]BASF SE, Catalysis Research, Ludwigshafen

Catalyst promoters are often key components of stable and efficient industrial heterogeneous catalysts, yet most commercial systems rely mostly on one or two promoters and predominantly leverage their isolated rather than their synergistic effects. This limitation frequently results from the laborious empirical research needed to identify formulations with jointly acting components that enhance performance. To address this challenge, we implement an accelerated catalyst discovery approach that adaptively explores a large catalyst design space using only a limited number of experiments. Its foundation lies in an efficient Design-of-Experiment (DoE), parallelized testing, and iterative integration of experimental feedback. New and competitive promoter chemistries for the non-oxidative propane dehydrogenation to propylene over supported Pt are discovered within a constrained experimental campaign. The results demonstrate the potential of adaptive DoE strategies for directed, data-efficient knowledge generation and optimization in complex catalytic systems of both academic and industrial relevance.

O 23.5 Mon 18:00 P2

Automatic Kinetic Equation Discovery from Experimental Data — •Maryke Kouyate, Gianmarco Ducci, Karsten Reuter, and Christoph Scheurer — Fritz-Haber-Institut der MPG, Berlin

Optimizing and controlling industrial catalytic processes requires effective kinetic models that are both robust and interpretable, capable of predicting how key operating variables affect reactor behavior. We introduce a model-based, adaptive design-of-experiments (DoE) framework that efficiently learns parsimonious, mechanistically meaningful rate expressions from data. At each step, it selects feed conditions to maximize expected information gain.[1,2] Profile reactors further boost per-run information by providing spatio-temporally resolved composition profiles along the reactor axis. Applied to CO oxidation on Pt, the framework automatically constructs a robust, chemically interpretable kinetic model that reproduces the characteristic mid-reactor transition in concentration profiles and reveals the need for a nonlinear term to capture the observed shift from CO poisoning to a non-poisoned regime.

[1] G. Ducci *et al.*, J. Chem. Phys. **162**, 114118 (2025).
[2] M. Kouyate *et al.*, J. Chem. Phys. (in press), DOI: 10.1063/5.0289751

O 23.6 Mon 18:00 P2

Structural development of new defective titanium carbon phosphorus hybrid composites by soft x-ray spectroscopy — •Hesham Hamad — City of Scientific Research and Technological Applications, Alexandria, Egypt — Elettra Sincrotrone Trieste, Trieste, Italy

The discovery of "black" TiO2 nanoparticles with enhanced solar absorption in the visible and near-infrared regions has sparked growing interest in solar energy applications. However, their properties remain incompletely understood. In this work, we explore a sustainable defective titanium*carbon*phosphorous (TCPH) hybrid nanocomposite for photocatalytic applications. TCPH was synthesized and applied in the degradation of methyl orange (MO) dye, a model organic pollutant. Characterization revealed the presence of Ti3+ species, oxygen vacancies, and a core-shell structure, along with a significant increase in surface area. These features enhance charge transport and separation, leading to excellent photocatalytic activity. X-ray photoelectron spectroscopy (XPS) confirmed the Ti3+ modifications in TCPH. To further probe its properties, synchrotron-based X-ray absorption fine structure (XAFS) spectroscopy was employed. This advanced technique provides insights into unoccupied and occupied states, particularly the O 2p and Ti 3d hybrid orbitals, revealing the electronic and crystalline structures of anatase, rutile, Ti metal, and TCPH. The combination of XAFS with complementary methods, including XRD, XPS, and HRTEM, enables a comprehensive understanding of TCPH's morphology, crystallinity, and local electronic structure.

O 23.7 Mon 18:00 P2

Cooperative Co-Fe Effect on the OER Activity of $CoFe_2O_4$ (100), (001) and (111) surfaces — Shohreh Rafiezadeh, •Aparna Chaitram, and Rossitza Pentcheva — Department of Physics, University of Duisburg-Essen, Duisburg

Water splitting, a key method for green hydrogen production, is limited by the sluggish anodic half process - the oxygen evolution reaction (OER) [1]. This necessitates finding efficient and affordable electrocatalysts which can reduce the overpotential. Using density functional theory calculations with an on-site Hubbard U term, we study the OER activity of the $CoFe_2O_4$ (001), (100), and (111) surfaces, exploring a wide range of potential active sites and the effect of solvation. The lowest overpotential of 0.20 V is found for an octahedral Co at the A-layer termination of the (100) surface, which contains both Fe and Co. This is attributed to the synergistic stabilization of the *OOH intermediate by binding to a neighbouring Fe site[2]. Remarkably, sites with higher catalytic activity are found to retain bulk like oxidation states. Our results show that such bonding configurations that break the OER scaling relationships reveal new routes to designing catalysts for water splitting.

We acknowledge funding by DFG within CRC TRR 247.

[1] J. Rossmeisl, Z. W. Qu, H. Zhu, G. J. Kroes, and J. K. Nørskov, *J. Electroanal. Chem.* 607, 83 (2007).
[2] S. Rafiezadeh, A. Chaitram, R. Pentcheva, *ChemCatChem* (2025), DOI: 10.1002/cctc.202501290.

O 23.8 Mon 18:00 P2

Probing the active state of Cu(111) for plasma-catalytic CO_2 hydrogenation — •Luka Babić and Roland Bliem — ARCNL, Materials & Surface Science for EUVL, Science Park 106, 1098 XG Amsterdam, The Netherlands

Plasma catalysis combines the concept of heterogeneous catalysis with the activation of reactants by a plasma discharge. The activation of strong molecular bonds is expected to change the kinetics of challenging reactions such as the hydrogenation of CO_2 to methanol. This reaction proceeds in a mixed H_2/CO_2 plasma, which consists of a multitude of species, including radicals, atoms, and ions with energy stored in various states and degrees of freedom. The state of surfaces interacting with this complex mixture is poorly understood, even for well-defined single-crystalline model catalysts.

Here, we use in situ X-ray photoelectron spectroscopy (XPS) and residual gas analysis to disentangle reaction pathways and the evolution of a Cu(111) model catalyst surface during exposure to radicals generated in plasma. Optical emission spectroscopy (OES) is used to characterize plasma and to assess the species hitting the surface during the exposure. XPS reveals the formation of adsorbed oxygen, followed by Cu(I) and finally Cu(II) oxides. Carbon is fully absent during the reaction with neutral activated CO_2 species. Upon reduction by plasma-activated hydrogen, hydroxides are formed. Depending on the operating conditions, we thus expect the active surface of a Cu plasma catalyst to be either Cu hydroxide or Cu metal.

O 23.9 Mon 18:00 P2

Size selected Pt clusters on a CeO_2(111) support: mobility, reactivity and dimensionality — •Fabian Heisinger, Johanna Reich, Mina Soltanmohammadi, Rasmus Bischoff, Friedrich Esch, and Barbara A.J. Lechner — TU Munich, Germany

Ceria is a renowned material for its exceptional oxygen storage capacity with applications in catalysis. Central to this functionality are oxygen vacancies and their mobility. In interaction with metal catalyst particles, this reducible oxide is highly versatile, as we demonstrate for size-selected Pt clusters on a single-crystalline ceria film. We study oxidation reactions as a function of cluster size, dimensionality, support reduction, and gas environment. With conventional and fast STM, we directly observe the dynamics of surface vacancies and supported clusters to determine cluster shape changes related to defect density and sintering. We combine this cluster height and coverage monitoring with LEED and XPS to characterize the CeO_2 films in crystallinity, thickness, oxidation state, and Pt coverage. We demonstrate that the Pt cluster dimensionality during sintering can be steered by controlling the oxygen vacancy coverage on the support[1]. Through STM, we track the mobility of O vacancies in an effort to correlate their dynamics with cluster properties, and the cluster dynamics to unravel the influence of their shape on stability and catalytic activity. These dimensionality-tuned, size-selected clusters provide an ideal platform to study the structural dynamics of small metal clusters during an ongoing oxidation reaction.

[1] Reich, Johanna, et al. ACS catalysis 15 (2025): 18369-18382.

O 23.10 Mon 18:00 P2

Metal clusters on rutile TiO_2(110) as model catalysts: Stability and reactivity under near-ambient pressure conditions — •Jonathan Paul, Marina Isabel de la Higuera Domingo, Lorenz Falling, Florian Kraushofer, Matthias Krinninger, and Barbara A. J. Lechner — Technical University of Munich, TUM School of Natural Sciences, Department of Chemistry, 85748 Garching, Germany

Clusters frequently exhibit strongly size-dependent catalytic properties and have discrete electronic states, often leading to a particularly high activity in heterogeneous catalysis. However, at the elevated temperatures typically employed in industrial applications, clusters tend to sinter into larger particles, which can lead to a decrease in catalytic activity. Reducible oxide supports, such as titania (TiO_2), are effective materials for stabilizing clusters and can further modify their catalytic behavior through encapsulation effects induced by the strong metal-support interaction (SMSI).

Here, we employ near-ambient-pressure scanning tunneling microscopy (NAP-STM) to investigate how reducing, oxidizing and reaction atmospheres influence the stability, structural dynamics and geometry of Pt and Ni clusters supported on rutile TiO_2(110).[1] Structural insights obtained from microscopy are complemented by a highly sensitive sniffer setup for activity measurements, investigation of reaction mechanisms and determination of turnover frequencies.[2]

[1] F. Kraushofer, et al. J. Am. Chem. Soc. 2025, 39846-39859.
[2] J. Reich, et al. Top. Catal. 2024, 880-891.

O 24: Solid-liquid interfaces: Reactions and electrochemistry – Poster

Time: Monday 18:00–20:00 Location: P2

O 24.1 Mon 18:00 P2

Real-Time Electrochemical AFM Observation of Lithium Plating and Dissolution on HOPG: Surface Morphology and Mechanistic Insights — •Luca Kaufer[1,2], Daniel Ebeling[1], André Schirmeisen[1], and Jürgen Janek[2] — [1]Institute of Applied Physics, Justus-Liebig-University, Gießen, Germany — [2]Institute of Physical Chemistry, Justus-Liebig-University, Gießen, Germany

This investigation demonstrates the utilisation of atomic force microscopy (AFM) to examine the interactions between liquid electrolytes and Highly Ordered Pyrolytic Graphite (HOPG) electrodes. In particular, the focus is on the deposition of lithium on HOPG surfaces, a crucial process in lithium batteries. Atomic force microscopy measurements facilitate precise analysis of the surface structure, topog raphy, and mechanical properties. In addition, they permit observation of dynamic changes during lithium deposition. This, in turn, provides a deeper insight into the mechanisms of electrode surface reactions and the quality of the electrode surface. Such measurements are of great importance to improve the efficiency and lifetime of batteries by helping to understand and control processes such as dendritic growth or non-uniform deposition.[1,2] We will demonstrate the use of Asylum Research's Fast Force Mapping mode in relation to the mechanical changes in HOPG during lithium deposition. [1] J. Phys. Chem. C 2011, 115, 25484*25489. [2] ACS Appl. Mater.Interfaces 2015, 7, 25441*25447

O 24.2 Mon 18:00 P2

Influence of electrolyte and electrode parameters on the current voltage characteristics during high voltage and plasma electrolysis — •Benjamin Schilling, Lukas Forschner, Justus Leist, Timo Jacob, and Albert K. Engstfled — Ulm University, Ulm, Germany

Electrolysis at gas evolving electrodes at high voltages, up to several hundreds of volts, leads to vivid bubble formation at the electrode, which ultimately leads to the ignition of a plasma in a gas sheath forming around the significantly smaller driving electrode. [1] Depending on the applied voltage, the approach can be used to tailor the electrodes structural properties or to modify the electrolyte, to form nanoparticles or generate H2O2. Systematic studies to elucidate the fundamental physical properties are still scarce [2], which are, however, highly relevant to understand the aforementioned changes on the electrode and electrolyte. In this work we focus on the influence of the electrolyte concentration and composition, voltage scan rate, working electrode geometry and material, electrode distance and electrolyte convection. The electrode structural properties are studied by SEM imaging, the dynamics of the gas film around the electrode are monitored using a high-speed camera and the temperature is proved locally by multiple temperature probes. By correlating these results, we discuss the parameters influencing the temporal changes of the system's properties and their consequences for the application of high-voltage electrolysis. [1] Yerokhin et al., *SURF COAT TECH* **122** (1999) 73-93. [2] Forschner et al., *J. Phys. D: Appl. Phys* **58** (2025) 215204.

O 24.3 Mon 18:00 P2

Predicting Potential-Dependent Binding Energies at the Electrified Metal/Water Interface — •Ann Kathrin Tran, Elias Diesen, Karsten Reuter, and Vanessa J. Bukas — Fritz-Haber-Institut der MPG, Berlin

Density-functional theory studies of electrified metal/water interfaces present many challenges and uncertainties. Even the methodology for computing the thermodynamics of adsorption is not yet well-established, albeit crucial to e.g. heterogeneous electrocatalysis. Here, we discuss common approaches and approximations in a systematic study of electrochemical binding energies. We choose Au(111) as our model system and focus on the adsorption of key intermediates during O_2 electro-reduction. Firstly, we benchmark predictions from three increasingly advanced models of the double layer: an applied sawtooth potential in vacuum, an implicit solvent model, and explicitly modelled H_2O via *ab initio* molecular dynamics (AIMD). This comparison disentangles the purely electrostatic energy contribution from stabilization due to explicit H-bonding with the solvent. The latter contribution can be sizeable, yet is only captured by atomistic H_2O in expensive AIMD. We next address the issue of predicting grand-canonical energetics, that is, energies under realistic constant-potential conditions. In this context, we present workfunction information within constant-charge AIMD data, the emerging workfunction-charge relation, as well as different transformation techniques toward constant-potential results. This analysis reveals notable caveats for each approach and highlights the need for further systematic benchmark studies.

O 24.4 Mon 18:00 P2

molecular dynamics simulations of belite-water interac tions using HDNNPs — •Usman Tafida[1,2], Maite Böhm[1,2], Henry Wang[1,2], Bernadeta Prus[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

Advances in the development of machine learning potentials (MLPs), such as High-Dimensional Neural Network Potentials (HDNNPs), have enabled *ab initio*-level accuracy for molecular dynamics (MD) simulations of high dimensional systems at greatly reduced computational cost. In this work, HDNNPs are trained on DFT-D3 energies and forces data of beta-belite (Ca_2SiO_4) clusters in water, which serve as model systems for complex oxide-water interfaces. Here, we present the dataset construction scheme, training and validation of the potential. Moreover, MD simulations have been performed to study the structural and dynamical properties of interfacial water at these clusters.

O 24.5 Mon 18:00 P2

High-Dimensional Neural Network Potentials for Molecular Dynamics Simulations of Mineral-Water Interfaces — •Maite Böhm[1,2], Bernadeta Prus[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

In recent years, High-Dimensional Neural Network Potentials (HDNNP) have emerged as a popular tool for atomistic simulations of complex systems such as mineral-water interfaces. In this work, we present the construction of an HDNNP based on density functional theory energies and forces for tricalcium aluminate (C_3A)-water interfaces. We discuss the development of a dataset that includes the relevant solid-liquid interface interactions by active learning and propose approaches for an accelerated extension of the dataset. The trained potential is applied in Molecular Dynamics simulations of the (100) surface of C_3A in contact with water, which are further investigated with respect to the structure and dynamics of water on the surface.

O 24.6 Mon 18:00 P2

Developing High-Dimensional Neural Network Potentials for Studying Tricalcium Silicate-Water Interfaces — •Henry Wang[1,2], Bernadeta Prus[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

The emergence of machine learning potentials (MLP) trained on energies and forces from electronic structure calculations has revolutionized the simulation of solid-liquid interfaces by molecular dynamics (MD). For instance, High-Dimensional Neural Network Potentials (HDNNP) have shown excellent accuracy for describing the interaction of water with several solid minerals. In this study, we investigate interfaces of liquid water with alite (Ca_3SiO_5), a calcium silicate forming several polymorphs, which is characterized by a particularly high reactivity with water. Insights into the behavior of water at calcium silicate surfaces at an atomistic level are crucial to reach a better understanding of general hydration reactions of this class of materials. An approach for realizing high-accuracy, large-scale MD simulations is presented.

O 24.7 Mon 18:00 P2

Exploration of the Pt(111)-water interface by high-dimensional neural network potentials — •Daniel Trzewik[1,2], Moritz R. Schäfer[1,2], Alexander L. Knoll[1,2], and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

In-depth knowledge of solid-liquid interfaces is essential for understanding numerous catalytic and electrochemical processes. However, accurately describing these interfaces with first-principles methods is computationally demanding, limiting the system sizes and complexities that can be explored. Modern machine learning potentials offer a powerful alternative, delivering near-first-principles accuracy at a fraction of the cost. In this work, we use high-dimensional neural network potentials (HDNNPs) to examine the Pt(111)-water interface in detail. Trained on DFT reference data, these models enable molecular dynamics simulations which reveal the structural and dynamical behavior of water molecules at the interface.

O 25: Solid-liquid interfaces: Structure, spectroscopy – Poster

Time: Monday 18:00–20:00 Location: P2

O 25.1 Mon 18:00 P2

Role of Interfacial Water for CO_2 Reduction Reactions in Ionic Liquid/Acetonitrile Electrolytes — •Björn Ratschmeier[1], Arik Geringswald[1], Alisa Kamaric[1], Angel Cuesta[2], and Björn Braunschweig[1] — [1]University of Münster, Institute of Physical Chemistry, Münster, Germany — [2]Advanced Centre for Energy and Sustainability (ACES), School of Natural and Computing Sciences, University of Aberdeen, UK

Room-temperature ionic liquids (RTILs) such as 1-butyl-3-methyl-imidazolium bis(trifluoromethanesulfonyl)imide ([BMIM][NTf_2]) are promising electrolytes for CO_2 reduction reaction (CO_2RR), where the availability of water at the electrode/electrolyte interface is known to play a decisive role in the reaction mechanism. We find that the addition of acetonitrile (ACN) to [BMIM][NTf_2] with 1.5 M H_2O markedly increases the CO yield, while the onset potential for CO formation remains essentially unchanged. *In situ* IRAS of bulk intermediates formed during CO_2RR are indicative for a reaction pathway [1] via a [BMIM]-COOH intermediate that requires the presence of interfacial H_2O as shown in previous work. In contrast, *in situ* ATR-SEIRAS reveals ACN-induced modifications of the electrode/electrolyte interface. OH vibrational bands increase significantly at cathodic potentials, indicating enhanced water accumulation at the interface, thus, causing larger availability of water for CO_2RR. Ref.: [1] Ratschmeier et al. ACS Catalysis 14, 1773 (2024).

O 25.2 Mon 18:00 P2

Capacitance of Nanoconfined Salt Solutions: Interplay between Concentration and Temperature — •Caterina Sartori, Haoyuan Quan, Louis Lehmann, and Roland Netz — FU Berlin, Fachbereich Physik, Arnimallee 14 14195 Berlin, Germany

The capacitance of confined aqueous salt solutions is important for a variety of applications, including thermal energy conversion, but remains poorly understood. Performing Molecular Dynamics simulations and treating bulk electrolytes as a reservoir, we determine the temperature and bulk-concentration dependent density, slit concentration and capacitance of confined salt solutions. On a microscopic level, the capacitance is determined by the inverse dielectric profile, which we also present. Our results constitute a crucial step towards understanding the electrostatic behavior of confined electrolytes.

O 26: Plasmonics and nanooptics: Fabrication, characterization and applications – Poster

Time: Monday 18:00–20:00 Location: P2

O 26.1 Mon 18:00 P2

Extending multiphysics crystallization models for phase-change materials with parameters derived from machine learning — •Luis Schüler[1,2], José Moreira[2], Andrei Lupuleasa[2], Wenjing Lei[2], Keerthika Kalavalapudi[2], Matthias Wuttig[2], Thomas Taubner[2], and Dmitry Chigrin[1,2] — [1]AMO GmbH, Aachen — [2]I. Institute of Physics (IA), RWTH Aachen

Optical metasurfaces based on dielectric or metallic scatterers such as nanoantennas provide advanced control over light-matter interactions. Dynamic tuning can be realized with phase-change materials (PCMs), which can be reversibly switched between amorphous and crystalline states with a strong difference in refractive index. Especially metallic nanostructures can significantly influence the crystallization dynamics of PCMs, resulting in deviations from the expected spectral behavior of the metasurface. Therefore, Multiphysics simulations that couple electrodynamics, heat transport, and crystallization kinetics are essential for understanding these effects and optimizing device geometry. However, it is experimentally challenging to obtain key crystallization parameters, such as viscosity or free energy density, over the relevant temperature range. Here, we use machine-learned interatomic potentials trained molecular dynamics data to compute the required material parameters. Furthermore, we use machine learning to predict the viscosity of chalcogenide-based PCMs using data from related glasses. This approach broadens the range of phase-change materials that can be reliably simulated and provides a pathway toward the systematic design of dynamically tunable metasurfaces.

O 26.2 Mon 18:00 P2

Toward Plasmonic Pump-Probe Spectroscopy of a Hot-Electron-Driven Reduction Reaction — •Marcel Schalling, Lukas Schmidt, Ferdinand Bauer, Thorsten Schumacher, and Markus Lippitz — University of Bayreuth

Plasmon-induced hot electrons offer a promising way to drive surface-catalytic chemical reactions with enhanced efficiency and selectivity. We want to follow the dynamics of the hot carriers by pump-probe spectroscopy.

In our approach, an initial laser pulse excites surface plasmons in the gold taper, generating hot electrons. These subsequently reduce adsorbed metal complexes on the taper's surface. This reduction is expected to locally modify the refractive index, which we probe by a second laser pulse. We show our first steps towards this goal. We start from the opto-electrochemical model system of methylene blue, and gradually add plasmonics and hot-electron generation towards the full implementation of the plasmonic pump-probe concept.

O 26.3 Mon 18:00 P2

Dissipation engineered plasmonic ratchet — •Anna Sidorenko[1], Jan Mathis Giesen[2], Sebastian Eggert[2], and Stefan Linden[1] — [1]Physikalisches Institut, Rheinische Friedrich-Wilhelms-Universität Bonn, 53115 Bonn, Germany — [2]Physics Department and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, D-67663 Kaiserslautern, Germany

This joint theoretical and experimental study presents a new design of a plasmonic ratchet, where directional transport is implemented purely by dissipation. Using Floquet theory, we identify resonant driving regimes depending on driving frequency and dissipation rates. An experimental observation of the ratchet effect in arrays of evanescently coupled plasmonic waveguides is provided by utilizing leakage radiation microscopy. Remarkably, we find that on resonance the transmitted signal shows lower losses for stronger local dissipation.

O 26.4 Mon 18:00 P2

Is the linkng number a topological invariant? — •Maja Manten[1], Alexander Neuhaus[1], Pascal Dreher[1], Phillip Gessler[1], Bettina Frank[2], Tim Davis[1,2,3], Harald Giessen[2], Michael Horn-von Hoegen[1], Karin Everschor-Sitte[1], and Frank Meyer zu Heringdorf[1] — [1]Faculty of Physics and Center for Nanointegration, Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47048 Duisburg, Germany. — [2]4th Physics Institute, Research Center SCoPE, and Integrated Quantum Science and Technology Center, University of Stuttgart, Germany. — [3]School of Physics, University of Melbourne, Parkville, Victoria 3010 Australia

Optical near fields, like they occur in surface plasmon polaritons, exhibit a wide range of topological textures, including skyrmions, merons, and optical vortices carrying orbital angular momentum. Near fields that carry a fractional orbital angular momentum rather than integer orbital angular momentum, however, pose a challenge: they form a complex phase-vortex landscape and break the simple picture of a single vortex carrying the topological charge. When the fields become distorted, the situation becomes more complicated as more and more vortices appear. The sequence of vortices and antivortices can extend to infinity and evade global topological classification in real space. Here we show that a global topological invariant, the linking number, can be found in Fourier space. We show how the linking number of a plasmonic field can be determined from a time resolved polarimetric photoemission microscopy experiment and demonstrate the robustness of the linking number against deformation of the excitation structure.

O 26.5 Mon 18:00 P2

Reconfiguring resonator shapes optically to tailor the resonator modes of phonon polaritons in hBN using In_3SbTe_2 — •Arvid Schick, Lina Jäckering, Lukas Conrads, Matthias Wuttig, and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University

The van der Waals material hexagonal boron nitride (hBN) hosts hyperbolic Phonon Polaritons (HPPs) with high volume confinement and low losses, suitable for nanophotonic devices [1]. Restricting the HPPs to resonators enables ultra-confined resonances [2]. Conventionally, resonator fabrication requires cumbersome lithography processes. Instead, resonators can be fabricated via optical programming of the phase-change material In_3SbTe_2 (IST), as IST can reversibly be switched between a metallic and a dielectric phase in the infrared [3]. Optical programming of reconfigurable, circular resonators for HPPs in hBN has been demonstrated and allowed for tailoring the field confinement [4]. We investigate square, rectangular and triangular resonators. We reconfigure resonator shape and aspect ratio to tailor the resonator modes that we investigate with scattering-type scanning near-field optical microscopy (s-SNOM). By decreasing the resonator size, we find confinement of up to $\lambda/69$ and a Q-factor of 49. Our results pave the way for rapid and reconfigurable prototyping of confined polariton resonators of arbitrary shape for various 2D materials. [1] Dai et al. *Science* **343**, 1125-1129 (2014); [2] Sheinfux et al. *Nat. Mat.* **23**, 499-505 (2024); [3] Conrads et al. *Opt. Mater. Express* **15**, 2664-2687 (2025); [4] Jaeckering et al. *Nano Lett.* **25**, 15809, (2025)

O 27: Plasmonics and nanooptics: Light-matter interaction, spectroscopy – Poster

Time: Monday 18:00–20:00 Location: P2

O 27.1 Mon 18:00 P2

Charge reservoir as a design concept for plasmonic antennas — •Rostislav Řepa, Michal Horák, Tomáš Šikola, and Vlastimil Křápek — Brno University of Technology, Brno, Czechia

Plasmonic antennas exploit localized surface plasmons to shape, confine, and enhance electromagnetic fields with subwavelength resolution. The field enhancement is contributed to by various effects, such as the inherent surface localization of plasmons or the plasmonic lightning-rod effect [1]. Inspired by nanofocusing observed for propagating plasmons [2], we test the hypothesis that plasmonic antennas with a large crosssection represent a large charge reservoir, enabling large induced charge and field enhancement. Our study reveals that a large charge reservoir is accompanied by large radiative losses, which are the dominant factor, resulting in a low field enhancement.

[1] Křápek et al., arXiv:2407.09454.
[2] Babadjanyan et al., J. Appl. Phys. **87**, 3785-3788 (2000).

O 27.2 Mon 18:00 P2

Distinct Multiphoton Orders in Photoelectron Spectra of Individual Silver Nanoparticles — Waqas Pervez[1], •Frithjof Harmsen[1], Kevin Oldenburg[2], Moha Naeimi[1], Sylvia Speller[1], and Ingo Barke[1] — [1]Institute of Physics, University of Rostock, Germany — [2]Department of Life, Light & Matter, University of Rostock, Germany

We investigate how the multiphoton photoemission process of individual metal clusters deposited on a non-metallic substrate is affected by the particle shape and its local environment. Here we present photoelectron spectra acquired by time-of-flight spectroscopy using a photoemission electron microscope (PEEM). Size-selected particles produced in a magnetron cluster source are deposited in-situ onto silicon substrates. The cluster source can produce single particles as well as agglomerates with characteristic plasmon modes [1], as revealed by transmission electron microscopy (TEM). Photoelectron spectra are obtained using illumination by a femtosecond laser at wavelengths around 800 nm, where at least 3 photons are required to overcome the work function. In addition, we observe well-separated above-threshold processes (ATP / ATI) of 4th order and up to 7th order for agglomerates. No noticeable resonances are observed across the spectral range, in contrast to illumination around 400 nm [2], i.e., at the plasmon energy. Mechanisms are discussed in view of symmetry properties and dipole selection rules.

[1] K. Oldenburg et al., Phys. Rev. Research 7, 023267 (2025)
[2] K. Oldenburg et al., J. Phys. Chem. C 123, 1379 (2019)

O 27.3 Mon 18:00 P2

Plasma-assisted defect modification in hBN studied with cathodoluminescence spectroscopy — •Bharti Garg, Masoud Taleb, and Nahid Talebi — Institute of Experimental and Applied Physics, Kiel University, Germany

In this work, we study exfoliated hexagonal boron nitride (hBN) flakes treated with argon plasma for different durations and compare their optical response using cathodoluminescence (CL) spectroscopy. Emission spectra collected before and after plasma exposure allow us to isolate the effects of the treatment. hBN is known for defect-dependent optical emission, and plasma processing is a commonly used method to introduce or modify the density and the atomic structure of defects. We observe that longer plasma exposure leads to stronger defect-related emission and broader CL features, indicating an increase in defect density. The emission though occurs at the same wavelength before and after the plasma treatment, allowing us to conclude that the atomic structure of the defects remains similar even after the plasma interaction with the surface of hBN. These results clarify the influence of plasma treatment on defect formation in hBN and highlight the role of exposure time in tuning its optical properties.

O 27.4 Mon 18:00 P2

Tunable Stokes-shifted photoluminescence and defect emission from hBN excited with a supercontinuum laser — •Prabhdeep Singh, Bharti Garg, Maximilian Black, Masoud Taleb, and Nahid Talebi — Institute of Experimental and Applied Physics, Kiel University, Kiel, Germany

We investigate the photoluminescence (PL) of hexagonal boron nitride (hBN) flakes placed on holey carbon grids under tunable supercontinuum excitation from 460 to 650 nm. The spectra consistently show a fixed defect emission around 537 nm together with a stokes-shifted peak that moves linearly with the excitation wavelength. The excitation emission energy differences cluster around 0.17 eV and 0.20 eV, matching the in-plane E_1u and E_2g phonon modes of hBN. Cathodoluminescence measurements on the same flakes exhibit only the defect line, along with phonon sidebands. On a gold substrate, we additionally observe a weak third moving peak at the sum of the two phonon energies, arising from surface enhanced Raman spectroscopy scattering (SERS). Spatial PL maps, intensity variations, and measurements with different optical density filters further allow us to evaluate the local emission characteristics and estimate the down-conversion efficiency. The results provide a consistent picture of phonon-mediated optical processes in hBN. Using tunable supercontinuum excitation, we reveal phonon-assisted stokes emission in hBN and a SERS phonon-combination peak on gold an excitation scheme not previously explored for Raman-type processes in this material.

O 27.5 Mon 18:00 P2

Energy and momentum distribution of surface plasmon-induced hot carriers — •Ellen Brennfleck[1], Christopher Weiss[1], Jannis Lessmeister[1], Laurenz Rettig[1], Tobias Eul[2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, Germany — [2]Institute of Physics, University of Augsburg, Germany

Are the spectroscopic properties of plasmon- and photon-induced carriers fundamentally different? This question is crucial for advancing plasmonic energy conversion. Initial studies have suggested characteristic energy and momentum distributions for the photoemission of both bulk plasmon resonances and surface plasmons. For surface plasmons, however, the separation of plasmon and photon-induced emission patterns by their inherent spatial and temporal dynamics remains challenging [1].

To further characterize the electron emission pattern of surface plasmons, we combine a femtosecond laser system with a spatial light modulator to generate a vector vortex beam to excite surface plasmon polaritons at an annular structure. Our photoemission electron microscope enables us to compare the spectroscopic properties of photoemitted electrons and those generated by plasmonic emission at the center of the structure, providing valuable insights into the distinct emission mechanisms.

[1] Hartelt et al., ACS Nano 15, 12 (2021), 19559–19569

O 27.6 Mon 18:00 P2

Hot electron generation in tapered plasmonic waveguides — •Ferdinand Bauer, Valentin Dichtl, Marcell Schalling, Thorsten Schumacher, and Markus Lippitz — University of Bayreuth, Germany

The efficient generation of hot electrons is important for applications such as photochemical catalysis. Hot electron-hole pairs are created by Landau damping of surface plasmon polariton (SPP) and decay through electron-electron scattering.

A symmetric taper in a waveguide enhances the generation of hot electrons. At one end the waveguide is excited by a laser pulse. The emission at the other end is then used as a metric for the transmission and thus the creation of hot electrons.

Numerical simulations (COMSOL) are used to find a high energy density at the hot spot. Within the simulations, Beer's law holds for a broad range of taper lengths and can be used to make geometry optimisation more efficient.

We demonstrate how to maximize energy density in the waveguide hot spot by using numerical simulations and experimental data, thereby optimising the production of hot electrons.

O 27.7 Mon 18:00 P2

Optical Response of Noble Metals based on Metal Boltzmann-Bloch Equations — •Robert Lemke, Andreas Knorr, and Jonas Grumm — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Berlin, Germany

The optical response of plasmonic noble metals can be attributed to the interplay of electronic intra- and interband processes. These processes are addressed by coupled metal Boltzmann-Bloch equations derived from microscopic many-body theory. The specific properties of noble metals are caused by an anisotropic band structure in the vicinities of the X and L high symmetry points.

In order to analyse the line broadening of intra- and interband excitations we consider linearised electron-phonon and electron-electron scattering. Our approach allows to connect spectroscopic signatures directly to microscopic processes, not possible with phenomenological Drude-Lorentz models.

O 28: Oxide and insulator surfaces: Structure, epitaxy and growth – Poster

Time: Monday 18:00–20:00 Location: P2

O 28.1 Mon 18:00 P2

Probing Reactions at the Plasma-Catalyst Interface — •Maarten van Dorp and Roland Bliem — ARCNL, Amsterdam, The Netherlands

Efficient conversion of CO2 into value-added chemicals is a major step towards tackling climate change. However, chemical activation of CO2 by conventional catalysis requires exceedingly high reaction temperatures, straining energy efficiency and consequently industrial viability. Plasma-assisted catalytic conversion (PLAC) circumvents this by activating CO2 dissociation through the repeated impact of *hot* electrons from a non-thermal plasma, lowering the reaction barrier while selectively heating chemically activated CO2 species. However, to rationally design new PLAC catalysts, and therefore unlock the full potential of PLAC, crucial information about the short-lived intermediates is still unknown.

Here, a NiAl(110) substrate with an epitaxially grown alumina layer (Al10O13) was selected as well-defined support for carrying Cu-nanoparticles as a model system for the hydrogenation of CO2 with PLACIn this model system, a complete characterization of transient intermediates * both within the ECR microwave plasma and on the catalyst surface * requires a combination of complementary spectroscopic techniques, such as XPS, in-situ IRAS, LEED, and OES. . We establish the model system for plasma applications by synthesizing different alumina thicknesses, characterizing them with LEED, and testing their stability during exposure to plasma-activated species using in situ XPS.

O 28.2 Mon 18:00 P2

Influence of sample temperature on electron-beam-induced modifications in ultrathin CaF_2 films on Si(111) — •Luis Witte, Chris Schröder und Joachim Wollschläger — Institute of Physics, University of Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

The development of modern transistor technologies based on 2D materials requires gate dielectrics with low defect densities and high chemical stability. CaF_2 layers on Si(111) are well suited for this purpose due to their low lattice mismatch and large band gap. However, a crucial aspect is their stability under electron irradiation, e.g. during LEED analysis of the layers, which can lead to structural and chemical changes.

In this study, ultrathin CaF_2 layers were deposited on Si(111) using molecular beam epitaxy. First, a growth temperature study was carried out at substrate temperatures between 400 °C and 700 °C. In a second step, the influence of the sample temperature during LEED measurements on the structural stability of the layers was studied. The electron beam of the LEED served both as a source of excitation for structural changes and as a probe for detecting these modifications. The measurements were conducted at sample temperatures from −150 °C to 600 °C in order to systematically investigate temperature-related effects. The results show that modifications induced by the electron beam exhibit a pronounced temperature dependence. In addition, ex-situ XPS measurements were performed to analyse chemical changes.

O 28.3 Mon 18:00 P2

Growth of MgO on Ag(100) for promoting charge transfer of organic molecules — •Christian Haberland, Felix Otto, Maximilian Schaal, Jonas Brandhoff, Leon Bojunga, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Integer charge transfer between metal substrates and adsorbed organic molecules is a central mechanism governing interfacial electronic structure and thus the functionality of molecular devices. To control this process, ultrathin insulating films offer a powerful strategy by decoupling molecular orbitals from metallic states while still enabling quantized charge exchange. In this work, we report the successful preparation of MgO monolayer films on Ag(100) using controlled deposition of Mg and annealing procedures in an oxygen atmosphere. The resulting MgO/Ag(100) system provides a reliable platform for studying charge-transfer phenomena at oxide-supported interfaces. Comprehensive characterization was performed using photoelectron spectroscopy (UPS, XPS, XPD), revealing the electronic structure and stoichiometry, while scanning tunneling microscopy confirmed atomic-scale order and film continuity. The established growth of MgO serves as a robust model system for investigating integer charge transfer in metal/organic hybrid interfaces.

O 28.4 Mon 18:00 P2

Epitaxy of ultrathin α-Fe_2O_3(0001) and Fe_3O_4(111) on α-Al_2O_3(0001) — •Hanna Laguta, Tobias Pollenske, Chris Schröder, Luis Witte, Felix Johannsmann, and Joachim Wollschläger — Inst. of Physics, Univ. Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

Iron oxides have a lot of technological applications and occur in magnetic, catalytic or electronic devices. Fe_3O_4 (magetite) and α-Fe_2O_3 (hematite) belong to the most stable iron oxides which can be found in nature.

Hematite is antiferromagnetic and has a lot of potential to be used for magnetic data storage. Thus it is of interest to study ultrathin hematite films. In this work, on the one hand α-Fe_2O_3 was grown directly onto the α-Al_2O_3(0001)-substrate using MBE. On the other hand Fe_3O_4 was deposited first to be oxidised to hematite in a second step. The magnetite films underwent exposures of oxygen between $6 \cdot 10^{-3}$ mbar·s and $180 \cdot 10^{-3}$ mbar·s, one sample was oxidised step-by-step.

The samples were respectively investigated using Soft and Hard X-ray Photoelectron Spectroscopy to determine the stoichiometries of near-surface and subsurface regions. Low Energy Electron Diffraction is used to determine the surface structure of the ultrathin oxide films and to distinguish hematite (α-Fe_2O_3) from maghemite (γ-Fe_2O_3) films. Additional measurements using SQUID provide insight into the magnetic properties of the samples.

O 28.5 Mon 18:00 P2

STM and LEED studies on the stabilization of two-dimensional scandium oxides on Pt(111) by Ba and Ti incorporation — •Selina Schmechel, Muriel Wegner, Stefan Förster, and Wolf Widdra — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

The formation of two-dimensional oxides on metal support crucially depends on a charge transfer between the film and the substrate. For the particular case of M_2O_3 transition metal oxide honeycomb (HC) structures, it was found that potentially di- and quadrivalent metal cations form HC structures by charge exchange with the support [1]. This is not possible for trivalent metals and, therefore, they do not form 2D oxides.

Here we study the growth of submonolayer scandium oxide films. We confirm the 3D growth for the binary Sc_2O_3 compound with the bulk lattice parameter of 3.2Å. However, when incorporating Ti an immediate transition into a 2D layer is observed. For different compositions, these mixed Sc-Ti-O films develop long-range ordered 2D wagonwheel structures. By incorporating Ba into Sc_2O_3 we succeed in the formation of a HC structure. In this case, all HC pores are filled with Ba ions, which donate their valence electrons to the substrate. This HC posses a lattice parameter of 6.1Å as determined from LEED. This points to an increased Sc-Sc distance as compared to bulk conditions. This host atom-assisted HC stabilization will be applied to the preparation of lanthanide HC oxides in the future.

[1] J. Goniakowski et al., J. Phys. Chem. C **123**, 9272 (2019)

O 28.6 Mon 18:00 P2

Oxidation behaviour of nickel on magnesium oxide (001): An in situ study of structural development. — •Tobias Pollenske, Laurenz Hüffmeier, Hannah Hilmer, and Joachim Wollschläger — Inst. of Physics, Univ. Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

Precise control of nickel oxidation on magnesium oxide (MgO)(001) surfaces under ultra-high vacuum (UHV) conditions is of fundamental importance for understanding metal/oxide interfaces and developing novel materials with tailored magnetic, electronic or catalytic properties. In this study, an approximately 15 nm thick Ni layer was deposited on MgO(001) using molecular beam epitaxy (MBE) and oxidised in situ at 250°C, 300°C and 400°C under 1×10^{-5} mbar O_2. The structural changes during oxidation were monitored by X-ray diffraction

(XRD) near the MgO(002) Bragg reflection. In addition, GIXRD, XRR and soft XPS measurements were performed between the oxidation steps. The results show that structured NiO formation only occurs at 400°C, while lower temperatures only lead to surface-limited oxidation. The soft XPS data confirm that the Ni surface oxidises almost immediately once a sufficient temperature is reached, with longer exposure to oxygen having little additional effect. Furthermore, the diffraction data show that annealing above 250°C improves the crystalline order of the Ni film. These combined in situ measurements provide a detailed picture of the oxidation kinetics and temperature-dependent structure development at the Ni/MgO(001) interface.

O 28.7 Mon 18:00 P2

Initial stages of gold nanoparticle growth on sapphire — •Hannah Hilmer[1], Chris Schröder[1], Tobias Pollenske[1], Timo Kuschel[2,4], Arno Jeromin[3], and Joachim Wollschläger[1] — [1]Institute of Physics, Univ. Osnabrück, 49076 Osnabrück, Germany — [2]Faculty of Physics, Univ. Bielefeld, 33615 Bielefeld, Germany — [3]Centre for X-ray and Nano Science CXNS, Deutsches Elektronen-Sychrotron DESY, 22607 Hamburg, Germany — [4]Institute of Physics, Johannes Gutenberg Univ. Mainz, 55128 Mainz, Germany

Gold nanoparticles are of great interest for applications in catalysis, sensor technology, and electronics due to their shape- and size-dependent optical, electrical, and chemical properties. Their morphological and electronic properties depend heavily on the growth conditions. $Al_2O_3(0001)$ is particularly well suited as a substrate due to its chemical stability and well-defined surface structure.

For this purpose, gold was deposited in ultra-high vacuum using thermal molecular beam evaporation at different deposition durations and varying substrate temperatures. In addition, thermal post annealing was carried out at different temperatures.

The growth processes of Au on $Al_2O_3(0001)$ substrates were characterized using XRR, XPS and LEED. The results show that gold grows on sapphire in the initial stage according to Volmer-Weber growth as discontinuous islands. SEM and EDX analyses show clearly defined gold particles whose size and distribution depend strongly on the substrate temperature, the evaporation time per interval, and annealing temperature.

O 28.8 Mon 18:00 P2

Local Characterization of Structural and Electronic Properties of the ZnO(0001) Surface — •Yuyang Zhang and Martin Wenderoth — IV Physical Institute, University of Göttingen

Zinc oxide (ZnO) serves as a key model system for understanding Proton-Coupled Electron Transfer (PCET) at interfaces.[1] To unravel electron dynamics on hydrated and doped surfaces, a profound understanding of the pristine surface is the indispensable baseline. Here, high-quality single-crystalline ZnO (0001) surface were prepared under ultra-high vacuum (UHV) conditions. The desired reconstruction was achieved by optimizing cycles of Ar+ sputtering and annealing. The structural properties were characterized by Low-Energy Electron Diffraction (LEED), confirming the long-range order and the intrinsic hexagonal surface symmetry. Similar to [2], Scanning Tunneling Microscopy (STM) revealed an ordered morphology dominated by atomically flat terraces with a high concentration of defects characteristic of polar face. Complementary atomic force microscopy (AFM) measurements provided additional information on the mesoscale morphology. Tunneling current measurements were utilized to probe the local electronic properties, providing insight into the surface band structure. This work was financially supported by the DFG through the CRC1633.
[1] Hammes-Schiffer et al, ACS Nano 2017, 11, 10295-10302 [2] Diebold et al, Surf. Sci. 2002, 519, 201-217

O 29: Oxides and insulators: Adsorption and reaction of small molecules – Poster

Time: Monday 18:00–20:00 Location: P2

O 29.1 Mon 18:00 P2

Impact of atomic oxygen on alumina surfaces investigated by molecular dynamics simulations — •Stephen Hocker, Hansjörg Lipp, and Johannes Roth — FMQ, University of Stuttgart, Germany

Oxygen atoms impinging on satellite surfaces in very low earth orbit (VLEO) transfer momentum and energy leading to material degradation as well as drag forces which result in orbital decay of the satellite. The first step in finding solutions to counteract significant drag is to gain understanding of the interaction of atomic oxygen (AO) with material surfaces. We investigate the angular and velocity distributions of reflected AO on crystalline and amorphous alumina surfaces using molecular dynamics simulations. Adsorption processes are evaluated and their influence on the surface structure and resulting changes regarding AO reflection is revealed. A strong dependence on the angle of incidence and the initial velocity is found. A high ratio of specular reflection can be obtained for grazing angles of incidence and hyperthermal initial velocities.

O 29.2 Mon 18:00 P2

First Principles investigation of the electronic properties and OER activity of (sub)stoichiometric WO_{3-x} (x =0.0, 0.1) — •Jeel Swami and Rossitza Pentcheva — Department of Physics, University of Duisburg-Essen

Tungsten trioxide (WO_3) exhibits a rich sequence of temperature and defect-driven structural phase transitions. Using density functional theory (DFT) calculations with the SCAN0 (with and without a Hubbard U term) and HSE06 functionals, we explore the influence of oxygen defects on the electronic properties of WO_{3-x}. For substoichiometric Magnéli phase $WO_{2.9}$ our results show partial localization of charge at the interface exhibiting weak magnetisation and n-type conductivity. We further investigate the application of WO_3 as anode material for the oxygen evolution reaction. At the (001) facet we consider various surface terminations. Gibbs free energy plot reveal that *OOH formation is the potential determining step for WO_3(001) facet.

We acknowledge computation time at the MagnitUDE and AmplitUDE HPC systems at the University of Duisburg-Essen.

O 29.3 Mon 18:00 P2

Interaction of atomic Oxygen with Silica Surfaces — •Ahmad Kassem Arrak, Stephen Hocker, Hansjoerg Lipp, and Johannes Roth — FMQ, University of Stuttgart, Germany

In order to increase the lifetime of VLEO (very low earth orbit) satellites, the drag forces on the satellite and the degradation of the surface material must be reduced. Both arise mainly from atomic oxygen (AO) impinging on the satellite surfaces at hyperthermal velocities. We investigate the influence of AO impact on silica surfaces using molecular dynamics simulations (LAMMPS). A focus is on adsorption, reflection and chemical reactions. Three interaction potentials were used, one from Vashishta, a Tersoff potential and a PACE machine learning potential. We prepared three (001) surface structures of alpha silica differing by their surface layers. The oxygen impact simulations revealed that the interaction processes occurring at the surface depend strongly on the chemical composition of the surface layers. At the oxygen-rich surface the formation and desorption of O2 can be observed while reflection or adsorption of AO is favored at other surfaces.

O 30: Metal & Semiconductor substrates: Structure, epitaxy and growth – Poster

Time: Monday 18:00–20:00 Location: P2

O 30.1 Mon 18:00 P2

Structural analyses for S and Te on transition metal chain-like phases on the Ir(100) substrate — •Eric Engel, Alexander Wegerich, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

The magnetic properties of one-dimensional transition metal oxide chains Ir(100)-(3×1)-MO_2 (M = Mn, Fe) [1,2] may in the case of Mn be tuned by changing the number of oxygen atoms in the chain structure [3]. Here, we present our attempts to replace O by S and Te and the quantitative LEED-IV analyses of the resulting structures.

Dosing H_2S to the MnO_2 or FeO_2 chains leads to the formation of a dominant $c(2\times2)$ superstructure. The structural analyses reveal with Pendry R-factors $R_P < 0.11$, that reduced transition metal chains remain as ordered (3×1) structures in the surface layer. The true unit cell of the system is hence a $c(6\times2)$ but with only little deviations in the S adsorbate layer from a $c(2\times2)$.

For Te, MO_2 chains were reduced in H_2 first, followed by Te deposition. In the case of 1/6 ML Te on the Ir(100)-(3×1)-$FeIr_2$ a (3×2)-Te superstructure emerges, where the Te atoms take positions on pure Ir hollow sites between the Fe-chains (R_P = 0.123). For 1/2 ML Te a dominant $c(2\times2)$ superstructure appears, again with only slight influences of the metal chains in the Ir(100) surface adsorbate positions.

[1] P. Ferstl et al., Phys. Rev. Lett. **117**, 046101 (2016)
[2] M. Schmitt et al., Phys. Rev. B **100**, 054431 (2019)
[3] J. Qi et al., Phys. Rev. B **107**, 060409 (2023)

O 30.2 Mon 18:00 P2

Structure of Standing Tetracyanoethylene Molecules on Cu(111) and Cu(100) — •Lorenz Brill[1], Jonas Brandhoff[1], Christoph Wachter[2], Roman Forker[1], Oliver T. Hofmann[2], and Torsten Fritz[1] — [1]Friedrich Schiller University Jena, Germany — [2]Graz Universtiy of Technology, Austria

Tetracyanoethylene (TCNE) has been predicted to go through a standing-lying transition on Cu(111) depending on the deposition conditions. However, only disordered growth with a mix of standing and lying molecules has been observed in the past. Here, we present the first evidence of well ordered structures of standing TCNE molecules grown on Cu(111) and Cu(100), observed by low energy electron diffraction and scanning tunneling microscopy. We compare the obtained structures to predictions calculated in thermodynamic equilibrium.

O 30.3 Mon 18:00 P2

Quantitative sputter depth profiling: LEIS measurements and SDTrimSP simulations on silicon oxide — •Julian Pichler, Camil Bocaniciu, Alper Tunga Celebi, and Markus Valtiner — Technische Universität Wien, Wiedner Hauptstr. 8-10, Vienna, 1040, Austria

Precise surface characterization is crucial in semiconductor devices, to guarantee highest quality and optimal device fabrication.

This involves identifying defects, accurate handling of layers and surface contaminations, as well as determining elemental concentrations. This study focuses on a combined interpretation of Low Energy Ion Scattering Spectroscopy (LEIS) measurements on silicon oxide by quantification with references and Monte Carlo simulations with the SDTrimSP code [1]. We calculate surface erosion rates from simulations to deduce layer thicknesses in target materials, under consideration of atomic intermixing effects induced by sputtering.

For silicon oxide on pure silicon we find good quantitative agreement in sputtering depth profiles between LEIS measurements and SDTrimSP simulations for oxide layer thicknesses around 2 nm. We provide an estimation of layer thicknesses within a few Ångstrom and demonstrate intermixing at the interface induced by sputtering.

References [1] Mutzke et al., SDTrimSP Version 6.00, IPP report (2019)

O 30.4 Mon 18:00 P2

Should Doping be illegal at inorganic/organic Interfaces — •Aleksey Sokolov, Christoph Wachter, and Oliver T. Hofmann — Institute of Solid State Physics, Graz University of Technology, Graz, 8010, Austria

Organic/inorganic-semiconductor interfaces are central to the performance of devices such as organic light-emitting diodes and photovoltaic cells. The geometric arrangements of the molecules at the interface, known as polymorphism, heavily influence the properties of the interface, such as ionization energy, electron affinity, and charge mobility. Which arrangement molecules assume under given deposition conditions is governed by a variety of factors, such as the molecular size and shape, the intermolecular interactions as well as the molecule-substrate interactions, particularly the adsorption-induced charge-transfer. The amount of charge transfer, however, is critically determined by the substrate's doping concentration. Although there are now successful methods in predicting stable polymorphs, the role of the substrate doping for the interface polymorphism is not sufficiently understood. In this work, we use density functional theory in combination with the machine learning-driven structure search method SAMPLE to investigate how doping-induced charge transfer influences the thermodynamically stable phases of the example of F4TCNQ on ZnO. The results give insight into the interplay between doping, charge transfer, and interface structure, which can be used to generalize the effects in similar systems.

O 31: Metal & Semiconductor substrates: Adsorption and reaction of small molecules – Poster

Time: Monday 18:00–20:00 Location: P2

O 31.1 Mon 18:00 P2

Investigating the native oxide layer of CoCrFeNi(100) by co-adsorption of O_2 and H_2: an XPS study — •Peter Richter, Kavya Harsha Kumar, Susanne Wolff, and Thomas Seyller — Technische Universität Chemnitz, Chemnitz, Deutschland

High-entropy alloys (HEAs) are a relatively new class of materials with potential applications under ambient conditions. Hence, understanding the formation and the properties of their native oxides is essential. In this study, we use X-ray photoelectron spectroscopy to investigate the native oxide layer present on CoCrFeNi(100) as well as on the clean surface subjected to controlled exposures of O_2 and H_2.

To evaluate the stability of the native oxide layer, samples were annealed in ultra-high vacuum at temperatures in the range of 350 to 1100 °C. Oxide reduction increased significantly at 700 °C and was complete at 1100 °C. The exposure of clean CoCrFeNi(100) surfaces to 1 to 1000 L of O_2 leads to controlled oxidation, with Cr contributing most to oxide formation, followed by Co and Fe. The subsequent introduction of H_2 at sample temperatures of up to 500 °C leads to systematic changes in the surface chemistry.

Experimentally, the information of the bonding configuration is best observed in the 2p core levels of Co, Cr, Fe and Ni. However, when using the Al K_α line, several Auger peaks overlap with the Co2p and Fe2p core levels. In addition, multiplet splitting and satellite features further complicate the evaluation of the XPS data. To improve this, we performed reference measurements and developed fitting models for the Auger lines using pure metal foils.

O 31.2 Mon 18:00 P2

Molecular bottom up: Site-selective adsorption of cyclooctyne on partially passivated Si(001) — Jannick A. Peters[1], •Sophie Göbel[1], Dominik Scharf[2], Ulrich Koert[2], and Michael Dürr[1] — [1]Institut für Angewandte Physik and Zentrum für Materialforschung, Justus-Liebig-Universität Giessen, Germany — [2]Fachbereich Chemie, Philipps-Universität Marburg, Germany

Organic molecular structures on the technologically most important Si(001) surface are of great potential for future applications in terms of "more than Moore". The synthesis of organic structures on semiconductor surfaces requires several aspects to be considered, such as precise choice of adsorbates and their functional groups, as well as a well-prepared surface where the reaction sites can be controlled. For a lateral ordering of the organic layer, pre-patterned substrates are seen as promising starting point; e.g., alternating passivated and non-passivated surface areas are generated by means of STM in hydrogen desorption lithography. A self-organized approach might be based on ethylene on Si(001) which is known to show a well-ordered adsorbate structure on Si(001) in the submonolayer regime due to nearest-neigh-bor interactions. The reaction of cyclooctyne and its derivatives on the Si(001) surface pre-passivated with ethylene was studied by means of XPS and STM. Whereas C_2H_4 shows strongly reduced reactivity at the remaining, unreacted silicon dimers, cyclooctyne with its direct reaction channel on clean Si(001) shows high reactivity also at these strongly hindered sites. Furthermore, the reaction of bifunctional cyclooctynes was observed to be more selective than on clean Si(001).

O 31.3 Mon 18:00 P2

Quantitative imaging of surface potential of PTCDA molecules on Ag(111) and Pb(111) — •Sandhya Anchamkudy[1], Janine Lorenz[1,2], Amin Karimi[1], Christian Wagner[1,2], Ruslan Temirov[1,3], Henry Thake[4], Reinhard Maurer[4], Stefan Tautz[1,2], and Felix Lüpke[1,3] — [1]Peter Grünberg Institut (PGI 3), Forschungszentrum Jülich, Germany — [2]Institut für Experimentalphysik IV A, RWTH Aachen, Germany — [3]Institute of Physics II, Universität zu Köln, Germany — [4]Department of Chemistry, University of Warwick, United Kingdom

Scanning Quantum Dot Microscopy (SQDM) enables quantitative imaging of surface dipoles with unprecedented energy and spatial resolution. In the past, SQDM has been applied to molecular adsorbates, adatoms, defects, and atomic assemblies on silver [Phys. Rev. Lett. 115, 026101 (2015), Nat. Mater. 18, 853 (2019)] - and provided valuable benchmarks for theory where metal-organic hybrid systems are particularly challenging. Here, we investigate the adsorption geometry dependent effects of isolated perylene tetracarboxylic dianhydride (PTCDA) molecules on Ag(111). We identified two preferred orientations of PTCDA molecules: along the <1-10> and <11-2> directions of the Ag(111) surface. In SQDM measurements, the two orientations yield distinct dipole moments of -0.51 D and -0.65 D, respectively. In addition, we carried out SQDM of a single PTCDA molecule on superconducting Pb(111) and found that the dipole is seven times larger compared to PTCDA on Ag(111). This difference can be attributed to a significantly higher charge transfer and adsorption height on Pb(111).

O 31.4 Mon 18:00 P2

Redox Molecules on Gold Surfaces: Insights into Triboelectric Behavior through Simulations — •Zohreh Izadi[1,2], Michael Moseler[1,2,3], Michael Walter[1,2,3], and Leonhard Mayrhofer[3] — [1]Cluster of Excellence livMatS @Freiburg Center for Interactive Materials and Bioinspired Technologies(FIT), University of Freiburg, Freiburg, Germany — [2]Institute of Physics, University of Freiburg, Freiburg, Germany — [3]Fraunhofer IWM, MikroTribologie Centrum μTC, Freiburg, Germany

Triboelectricity, the electrostatic charge generated during the contact and separation of materials, remains poorly understood at the microscopic level. Redox-active molecules on metal surfaces provide a controlled platform to probe these charge-transfer processes. We studied donor and acceptor molecules adsorbed on Au(111) and evaluated their adsorption geometries and binding energies, as well as the electronic signatures associated with interfacial charge transfer. We

also considered different environments and found that humidity was a key factor facilitating charge transfer between the molecules and the surface. Our results are in very good agreement with the experimental findings from our joint study, offering insight into how redox-driven charge transfer at metal-molecule interfaces contributes to triboelectric behavior.

Reference: N. Ranjan, Z. Izadi et al., Contact Electrification via Redox-Active Molecules, Angewandte Chemie International Edition, 2025, e10031. DOI: 10.1002/anie.202510031.

O 31.5 Mon 18:00 P2

TPD Studies of Metal-Substrate Interactions in LOHCs and Polyfluorinated Compounds — Kassandra Zoltner, •Evelyn Versok, Leonard Neuhaus, Stefan R. Kachel, and J. Michael Gottfried — Fachbereich Chemie und mar.quest, Philipps-Universität Marburg, Germany.

Metal-substrate interactions critically govern catalytic reaction pathways and degradation mechanisms. Here, we investigate two chemically contrasting classes of adsorbates - hydrogen-rich liquid organic hydrogen carriers (LOHCs) and fluorocarbons - to clarify their stability and reactivity on metal surfaces. LOHCs such as decalin and tetralin are attractive hydrogen-storage materials but are prone to side reactions and catalyst-induced decomposition. In contrast, fluorocarbons including all-cis-hexafluorocyclohexane and perfluoromethylcyclohexane exhibit exceptional thermal and chemical stability, which is technologically valuable yet contributes to unwanted environmental persistence. Understanding molecule-metal interactions is therefore important for both hydrogen-storage chemistry and fluorocarbon degradation strategies. We employ temperature-programmed desorption (TPD) to determine adsorption energies, reaction kinetics, and product distributions. Systematic analysis of the selected LOHCs and fluorinated compounds on Au(111), complemented by comparison with partially dehydrogenated and defluorinated analogues, reveals detailed metal-induced transformation pathways. These insights advance the mechanistic understanding of hydrocarbon and fluorocarbon degradation on metal surfaces and support catalyst development.

O 31.6 Mon 18:00 P2

Orientation-dependent Adsorption and Manipulation of a Boron-doped Polycyclic Aromatic Hydrocarbon — •Elishka Vaz[1], Matthias Schnitzlein[2], Frank Würthner[2], Matthias Bode[1], and Jing Qi[1] — [1]Physikalisches Institut, Experimentelle Physik 2, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institut für Organische Chemie, Organische Chemie II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The incorporation of boron atoms into polycyclic aromatic hydrocarbons (PAHs) alters their electronic properties since the boron centres act as π-acceptors [1]. In this contribution, we present a novel boron-centered PAH with terminal bromine-substituents. Upon adsorption on the Cu(111) surface, the B-PAHs adopt twelve distinct azimuthal orientations: six aligned with the crystallographic directions of the (111) surface, and six rotated by 30°. Differential-conductance spectroscopy and apparent-height analyses reveal a pronounced influence of the substrate on both the topographic appearance and electronic structure. Atomic-resolution imaging enables assignment of adsorption sites via interpolation of the surface atomic rows. Moreover, lateral tip-induced manipulation demonstrates controlled stacking along the molecular short axis. Finally, we identify a double-chain arrangement, likely composed of intact molecules, which exhibits a notable spectral shift in the differential-conductance signature relative to isolated adsorbates.

[1] M. Schnitzlein *et al.*, ChemistryEurope **3**, e202500135 (2025)

O 32: Topical Talk Witte

Time: Tuesday 9:30–10:15 Location: TRE/PHYS

Topical Talk O 32.1 Tue 9:30 TRE/PHYS

Excitons in molecular solids: from unitary films to donor-acceptor co-crystals — •Gregor Witte — Renthof 7, 35032 Marburg

Their strong light-matter interaction makes organic semiconductors (OSCs) promising candidates for optoelectronic devices. However, the microscopic picture of photophysical excitations and their properties is still incomplete. Reasons for this are the different nature of excitons in inorganic and organic SCs and the frequently used simplified description of excitons in OSCs within the framework of H- and J- aggregates, which disregards high-energy states and the delocalization of wave functions. Optical transmission-absorption measurements on single crystals or films with large crystalline domains enable the spectroscopy of higher energy excitons and, by means of polarization- and direction-resolved measurements, also a correlation with the molecular packing motif. Among OSCs, acenes represent an ideal platform for exciton studies, as they allow both polymorph-selective crystallization and versatile modification of the molecular electronic structure through chemical substitutions. Furthermore, also highly ordered acene-perfluoroacene cocrystals can be produced, which enable detailed characterizations of heteromolecular charge transfer excitons in molecular donor-acceptor systems with well-defined internal interfaces. In this talk I will present some of our recent exciton studies on various acenes, which combine polarization-resolved optical spectroscopy with modern ab initio calculations based on density functional theory and many-body perturbation theory.

O 33: Graphene: Growth, structure and substrate interaction (joint session O/HL)

Time: Tuesday 10:30–12:30 Location: HSZ/0201

Invited Talk O 33.1 Tue 10:30 HSZ/0201

During-synthesis functionalization of graphene layers — •Cristina Africh — CNR-IOM, Trieste, Italy

Introducing heteroatoms into graphene is a powerful way to modulate its catalytic, electronic, and magnetic properties. During the last decade, we developed a clean and scalable functionalization strategy that exploits the sponge-like properties of nickel substrates as well as the catalytic role played by transition metal (TM) single atoms at graphene edges during Chemical Vapor Deposition synthesis [1]. Following this route, it is possible to grow N-doped, B-doped and TM-doped graphene as well as co-doped layers [2,3,4]. The potential of the functionalized networks for sensing and, as a perspective, for catalysis, was evaluated by monitoring their response upon gas exposure [5,6].

[1] C. Africh, M. Peressi and G. Comelli, Surf. Sci. 753, 122652 (2025). [2] S. Fiori et al., Carbon 171, 704-710 (2021). [3] S. Patil et al., Surf. Interfaces 51, 104700 (2024). [4] V. Chesnyak et al., Sci. Adv. 10, eado8956 (2024). [5] D. Perilli, S. Fiori et al., J. Phys. Chem. Lett. 11 8887-8892 (2020). [6] D. Perilli, V. Chesnyak et al., Angew. Chem. Int. Ed. 64, e202421757 (2025).

O 33.2 Tue 11:00 HSZ/0201

Heterotriangulene Kagome Graphene Films: Growth and Effect of Kinetic Reaction Parameters — •Wyatt Behn[1], Simon Briesenick[1], Chang Wan Kang[2], Manuel González-Lastre[3], Pablo Pou[3], Rubén Pérez[3], Dmytro Perepichka[2], and Peter Grutter[1] — [1]Dept. of Physics, McGill — [2]Dept. of Chemistry, McGill — [3]Universidad Autónoma de Madrid

Nanoporous graphenes featuring Kagome lattices formed by heterotriangulene units continue to attract interest for their correlated electronic properties. Their symmetry gives rise to flat bands and Dirac cones [1,2]. Covalent organic frameworks (COFs) like these are often synthesized by surface-assisted Ullmann coupling, and are susceptible to defects such as voids, irregular-sided linkages, and limited grain sizes of around 100 nm [3,4]. We perform a series of polymerizations over a range of sample temperatures (180-250 C) for tribromo- and triiodotrioxaazatriangulene precursors on the Au(111) surface. Using scanning tunneling microscopy (STM) and non-contact atomic force microscopy (nc-AFM) we interrogate how deposition conditions and choice of halogen affect the final polymer film quality, which we quantify using minimum spanning tree and persistent homology approaches. We also investigate the prevalence of halogenated edge terminations and of undesired organometallic intermediates. Experimental results are complemented by simulated STM and nc-AFM analyses.

[1] C. Steiner, et al. Nat. Commun. 8, 14765 (2017). [2] G. Galeotti, et al. Nat. Mater. 19 (2020). [3] M. Lackinger, Chem. Commun. 53 7872 (2017). [4] T. Qin, et al. Commun. Chem. 7 154 (2024).

O 33.3 Tue 11:15 HSZ/0201

Defect-Driven Formation of Distinct 2D-Ag Phases at the Graphene/SiC Interface — •Sawani Datta[1], Boyang Zheng[2], Arpit Jain[2], Vibha Reddy[1], Kathrin Küster[1], Joshua A. Robinson[2], Vincent H. Crespi[2] und Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]Pennsylvania State University, State College, USA

Intercalation of two-dimensional (2D) materials at the graphene/SiC interface is important for improving environmental stability of the intercalant and tuning graphene's electronic properties. However, the underlying mechanisms remain complex and are still not fully understood. In this study, we show that by modify-

ing the intercalation process, specifically through defect engineering, it is possible to selectively stabilize two distinct phases of intercalated silver (Ag). The previously established phase (Ag_1) aligns with nearly (1×1) registry of SiC [1, 2], while the second phase (Ag_2) develops a denser $(3\sqrt{3}\times3\sqrt{3})R30^\circ$ superstructure on a (5×5) SiC unit cell, producing a 6.25×6.25 Moiré pattern with respect to graphene, as seen in the low energy diffraction (LEED) pattern [2]. Angle-resolved photoemission spectroscopy (ARPES) reveals a striking kaleidoscopic modulation of the Ag_2 and graphene bands, absent in Ag_1, along with notable differences in charge transfer between the two phases. These results demonstrate that defect-controlled, phase-selective intercalation offers a promising pathway to design and explore exotic 2D electronic states at graphene/SiC interfaces. [1] PRB 101, 201407(R) (2020). [2] arXiv:2511.07151v1 (2025).

O 33.4 Tue 11:30 HSZ/0201

Strain-Induced 2D Pb phases confined between graphene and SiC — •Sergii Sologub[1,2], Markus Gruschwitz[1], Zamin Mamiev[1], Chitran Ghosal[1], and Christoph Tegenkamp[1] — [1]Institut für Physik, TU Chemnitz, Reichenhainer Str. 70, 09126 Chemnitz — [2]Institute of Physics, NAS of Ukraine, Nauki avenue 46, 03028 Kyiv

The intercalation of metals beneath graphene offers a powerful route to stabilizing and protecting novel 2D phases. We performed a detailed intercalation study of Pb beneath the ZLG on SiC(0001) using low-energy electron diffraction (at the temperatures from 70 to 600° C) as well as scanning electron and tunneling microscopy [1]. Our analysis reveals the formation of different 2D Pb monolayer phases, such as stripes and hexagons, which emerge due to the interplay between substrate pinning and strain within the Pb layer, depending on local coverage. The interface reconstruction of Pb was shown can be tuned by varying the details of the intercalation protocol. Based on our experiments combined with recent simulations [2], an intercalation model, accounting for the different periodicities observed in the interface layer, was proposed. These findings provide new insights into the strain-driven stabilization of intercalated metal layers and highlight the potential of graphene as a versatile platform for engineering low-dimensional materials.

[1] Adv. Mater. Interfaces 12, no. 21: e00617 (2025); [2] Appl. Surf. Sci. 681, 161572 (2025).

O 33.5 Tue 11:45 HSZ/0201

Strain engineering in graphene on Ru(0001) — Paula García-Mochales[1] and •Antonio J. Martínez-Galera[1,2,3] — [1]Departamento de Física de Materiales, Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [2]Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, E-28049 Madrid, Spain — [3]Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

The ability to induce and characterize strain in the atomic lattice of 2D materials, localized within only a few nanometers around specific positions, is a major challenge for the development of straintronics. In this work, the interaction between Si nanoparticles and the surface of graphene/Ru(0001) is employed to induce local strain in the latter. The strain field has been mapped at the nanoscale by scanning tunneling microscopy (STM), using the moiré pattern intrinsic to graphene/Ru(0001) surfaces as a magnifying lens. The induced strain is found to be confined within only a few nanometers around each nanoparticle. To achieve more accurate control, strain engineering at the nanometer scale was successfully performed by manipulating nanoparticles through the STM tip. This approach to controlled strain could provide a key tool for exploring new physics arising by strain in 2D materials.

P. García-Mochales and A. J. Martínez-Galera, Nano Lett. 25, 16097-16103 (2025).

O 33.6 Tue 12:00 HSZ/0201

Subsurface carbon controls graphene growth on Ir(111) — •Smruti Ranjan Mohanty, Lothar Brendel, Marko Kriegel, Niels Ganser, Frank-Joachim Meyer zu Heringdorf, and Michael Horn-von Hoegen — Faculty of Physics, University of Duisburg-Essen, 47057 Duisburg, Germany

The CVD growth of 2D materials is governed by a balance between adsorption, surface diffusion, and nucleation. For transition metal substrates, dissolution into the bulk acts as an additional parameter. By employing in-operando low-energy electron microscopy (LEEM) to monitor graphene growth on Ir(111), the effect of the growth temperature and the precursor pressure on the nucleation behavior is studied. The island nucleation density exhibits two distinct regimes, described as separate cases within Venables nucleation theory [1]. For a critical nucleus size i* = 5, low dosing pressures yield a low nucleation density that is governed by incomplete condensation with a scaling exponent of 2.5. At higher-dosing pressures, adsorptions at island edges dominate over the adatoms loss into the substrate, resulting in a higher nucleation density and a strongly reduced scaling exponent. Kinetic Monte Carlo simulations that incorporate bulk dissolution reveal both nucleation regimes and find a universal, temperature-independent scaling law. The results indicate a universal nucleation behavior for 2D materials with finite, non-negligible solubility in the supporting metal substrate.

[1] J A Venables et al 1984 Rep. Prog. Phys. 47 399

O 33.7 Tue 12:15 HSZ/0201

Thermodynamics of heteroatom-doped graphene: Brute forcing the partition function — •Lukas Hörmann[1,2], Benedict Saunders[1], and Reinhard J. Maurer[1,2] — [1]University of Warwick, United Kingdom — [2]University of Vienna, Austria

The introduction of dopants into graphene can be used to tune material properties for specific applications, such as electronics, sensors, or catalysis. Achieving such tunability requires precise control over the composition and concentration of dopants within the lattice. This demands a fundamental understanding of the thermodynamics that govern the phase space of heteroatom superstructures in the two-dimensional graphene framework. We present a comprehensive approach to determining dopant structures that enables the near-exhaustive enumeration of all relevant heteroatom superstructures. The approach combines Density Functional Theory and machine learning to build a transferable energy model for dopant formation. Our method's efficient data handling and fast inference enable the evaluation of more than 150 million possible structures, allowing us to effectively brute force the partition function and derive all thermodynamic properties from it. We show the capabilities of our approach for free-standing graphene doped with nitrogen atoms, establishing a thermodynamic model to investigate how temperature affects the configuration space of doped graphene. Our analysis yields physical insights into defect interactions. We observe a characteristic peak in the heat capacity, indicating an order-to-disorder transition, and present a mechanistic understanding of how this peak arises.

O 34: Catalysis and surface reactions I

Time: Tuesday 10:30–12:30 Location: HSZ/0204

O 34.1 Tue 10:30 HSZ/0204

From Global Optimization to Transition State Search: Automatic Workflow for Surface Reaction Kinetics — •Hyunwook Jung[1], Emanuel Colombi Manzi[1], Johannes T. Margraf[1,2], Hendrik H. Heenen[1], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Universität Bayreuth

Reaction-barrier calculations present the major bottleneck in the systematic exploration of surface reaction networks via atomistic simulations. Each involved transition-state search introduces a high-dimensional configuration space, comprised of many initial and final state combinations, that must be explored to identify the minimum-energy pathway with the lowest activation barrier. Typically, this task is delegated to human chemical intuition as user-input to e.g. a nudged elastic band (NEB) calculation, since its automation remains a significant challenge. Here, we introduce a fully automated workflow for transition-state optimization that does not require any human intervention. Initial and final geometries are generated through global optimization and subsequent alignment, followed by an atom-mapping and index permutation to arrive at the nonequivalent transition pathways. This process still leads to a large combinatorial number of possible interpolations from which we select a tractable subset using heuristic reaction-distance metrics. We demonstrate the workflow across a range of reactions and surface combinations from the OC20NEB database and discuss its overall performance.

O 34.2 Tue 10:45 HSZ/0204

Machine-learning Driven Approach of Surface Adsorption Energy Prediction — •Karlo Sovic and Johannes Margraf — University Bayreuth, Bayreuth, Germany

Heterogeneous catalysis is a cornerstone technology across industrial chemistry, materials science, and environmental engineering, effectively promoting and redirecting key chemical reactions in various applications. In these processes, control of surface adsorption energies is paramount for designing efficient catalysts. However, in the case of large adsorbates, the high computational cost of accurate DFT calculations limits comprehensive exploration of the corresponding potential energy surface. Machine-learning interatomic potentials offer a promising solution to this challenge. Leveraging recently reported pre-trained models, the complex interactions crucial for accurate surface chemistry can be captured with effectively via fine-tuning.

Here, a data-efficient workflow for describing the glycerol hydrodeoxygenation mechanisms leading to propanediols on M(111) and M(211) surfaces (M=Pt, Cu, Ni) is reported. With our approach, the fine-tuned model yields high-fidelity adsorption energies with near-DFT accuracy at low computational cost. Furthermore, analysis of thermodynamic properties was carried out to accurately determine the overall Gibbs free energetics of investigated reaction pathways. Based on these comprehensive insights, we propose a versatile work-

flow for the accelerated screening of catalytic systems, enabling the rapid construction of adsorption energy databases and exploring relevant reaction mechanisms.

O 34.3 Tue 11:00 HSZ/0204

Modeling Solvothermal Reactions at Surfaces with Machine Learning Interatomic Potentials — •Maciej Baradyn[1], Nils Gönnheimer[1,2], and Johannes T. Margraf[1] — [1]University of Bayreuth, Bayreuth, Germany — [2]Fritz-Haber Institute, Berlin, Germany

Dynamical processes such as adsorption, desorption and diffusion are vital elementary reactions involved in heterogeneous catalytic reactions. In solvothermal reactions, the presence of solvent molecules has significant effects on the dynamics of the adsorbates, which must displace hydration layers to diffuse or adsorb on the surface and undergo resolvation during desorption. The presence of solvent molecules also affects the interactions between surfaces and adsorbates, and can contribute to the (de-)stabilization of the adsorbed species.

In this contribution, we explore the robustness of machine learning potentials based on the MACE-MP-0 foundation model for describing dynamical processes under these conditions. This is demonstrated on a representative system of a glycerol molecule interacting with the Cu(111) surface in explicit water. Enhanced sampling methods are used to compute free energy profiles of the studied processes, and to reflect the experimental reaction conditions under which they occur in industrial applications.

O 34.4 Tue 11:15 HSZ/0204

Converting MoS_2 to MoO_2 by Thermal Treatment Under Dilute O_2 — •Armin Sahinovic[1], Jixi Zhang[2], Osamah Kharsah[1], Marika Schleberger[1], Rossitza Pentcheva[1], and Rodney Smith[2] — [1]Department of Physics and Center for Nanointegration, University of Duisburg-Essen, 47057 Duisburg, Germany — [2]Department of Chemistry, University of Waterloo, ON N2L 3G1 Waterloo, Canada

The reaction of MoS_2 with O_2 at elevated temperatures introduces the risk of structural and functional degradation that decrease the lifespan of MoS_2-based devices [1]. In experiment, variable-temperature Raman measurements indicate that depending on the O_2 concentration in the environment the MoS_2 is converted into either MoO_3 or MoO_2. To elucidate the specific mechanism of this reaction, density functional theory (DFT) calculations were performed including the van der Walls dispersion correction. We show that the S-vacancy formation energy as well as O substitution energy are lowered with increasing O content. DFT calculations show that at high O contents in $MoS_{2-x}O_x$ the $P2_1/c$ phase is energetically preferred over the 2H-MoS_2 structure. A *P-T* phase diagram of the Gibbs free energy obtained from DFT shows that the partial O pressure tunes whether MoO_3 or MoO_2 is the dominant product of the reaction. We explored the band structure of multiple vacancies in MoS_2 and find additional in-gap states compared to the monovacancy. Our results offer insight into the conditions that control the degradation of MoS_2-based devices.

[1] J. Gao, et al., ACS Nano, 10 (2), 2628 (2016)

O 34.5 Tue 11:30 HSZ/0204

2D TiS2 Nanoparticles in reductive and oxidative Atmospheres as Model (Photo-)Catalysts — •Niko Kruse[1], Justin Klimek[1], Aaron von Seggern[1], Martin Hedevang[2], Sergi Camposs Jara[2], Jeppe Vang Lauritsen[2], and Lars Morhusen[1] — [1]Carl von Ossietzky Universität Oldenburg, Oldenburg, Germany — [2]iNano Center, Aarhus University, Aarhus, Denmark

Sustainable materials for the thermal and photochemical utilization of (waste) carbon dioxide (CCU) become more and more demanded.[1] Titanium-based 2D materials such as TiS2 can directly harvest sunlight and have demonstrated high CO2 conversion activity.[2] To illuminate atomistic structure-property relationships of such catalytic systems, we present a model system consisting of 2D TiS2 nanoparticles on Au(111) and TiO2 (110) surfaces, rendering it suitable for atomic-level microscopy and spectroscopy. A direct synthesis route was developed by Ti metal evaporation in the presence of benign organic S precursors.[3] The resulting materials were characterized by combined STM, XPS, and NEXAFS experiments, along with DFT calculations.[4] We demonstrate the substrate-dependent structure and compositional detail of the nanoparticles and highlight the chemical potential of S as the relevant shape descriptor. In addition, the surface chemistry of 2D TiS2 nanoparticles in reactive atmospheres will be presented, highlighting the strong stability even in oxidative & reductive conditions. [1] R. Guil-López, N. M. et al., Materials 2019, 12. 3902. [2] A. Aljabour, et al, ACS Catal. 2020, 10, 66. [3] F. Besenbacher et al., J. Catal. 2021, 403, 4. [4] N. Kruse et al., Small 2025, 21, e06023.

O 34.6 Tue 11:45 HSZ/0204

In situ X-ray Imaging of PtPd Core-Shell Nanoparticles under Methane Oxidation Conditions — •Lydia J. Bachmann[1,2], Thomas F. Keller[1,2], Ivan A. Vartanyants[1], and Andreas Stierle[1,2] — [1]Deutsches Elektronen-Synchrotron DESY — [2]University of Hamburg

Due to the high global warming potential of methane, the release of any methane into the atmosphere needs to be avoided. Therefore, catalysts are used for the emission control. Common catalyst nanoparticles (NPs) for methane oxidation consist of Pd or Pt. Combining them allows to build more stable NPs. Since the surface chemical composition is crucial for the activity, segregation and mixing processes need to be taken into account. In this study we successfully tuned the initial chemical composition of one core-shell and one partially alloyed NP. We confirmed these elemental distribution by Bragg coherent diffraction imaging (BCDI). During in situ BCDI measurements under methane oxidation at temperatures between 320°C and 560°C, Pt segregated to the {111} oriented facets of the initial core-shell NP. Conversely, the initially partially alloyed NP did not exhibit such facet-dependent segregation, but rather observed the formation of a Pd core, Pt shell structure at 680°C. Since the initial Pt core, Pd shell NP showed Pd-Pt mixing at 620°C, we hypothesize that this NP would form such an inverted core-shell structure under higher temperatures as well. These results demonstrate opportunities for systematically investigating promising core-shell NPs and their catalytic activity, offering valuable insights for the design of advanced catalysts.

O 34.7 Tue 12:00 HSZ/0204

The mechanism and Rate-Determining Step of Catalytic Ammonia Oxidation on Pd(332) at High Temperatures — •Jan Fingerhut[1], Jessalyn DeVine[2], Rongrong Yin[3], Mark Bernard[2], Alice Bremer[4], Dmitriy Borodin[2], Kai Golibrzuch[2], Theofanis Kitsopoulos[5], Daniel Auerbach[2], Hua Guo[3], and Alec Wodtke[2] — [1]Leiden Institute of Chemistry, Leiden, the Netherlands — [2]Max-Planck-Institute for Multidisciplinary Science, Göttingen, Germany — [3]University of New Mexico, Albuquerque, USA — [4]Georg-August-Universität, Göttingen, Germany — [5]University of Southern Mississippi

Despite its immense practical importance in industrial production of nitric acid, the mechanisms of catalytic ammonia oxidation on platinum group metals remain controversial. In this work, we employ velocity-resolved kinetics to study ammonia oxidation on a model Pd(332) catalyst between 600 and 700 K. We obtain the temporal evolution of gas-phase reactants (NH_3), products (NO, H_2O) and - with the help of femtosecond laser-induced desorption - of a reaction intermediate, N^*. The reaction exhibits the prompt appearance of H_2O and the delayed formation of NO; the rate-determining step is the reaction $N^* + O^* \rightarrow N^*O$ occurring at step sites. This means that N^* is the longest-lived reaction intermediate, an insight that helps explain formation of byproducts like N_2 and N_2O. We present a mechanism that explains all experimental observations, based on transition-state theory calculations and using input from density functional theory. We also show that N^*O desorption is accelerated by coadsorbed oxygen.

O 34.8 Tue 12:15 HSZ/0204

Promoting Role of Isolated Surface Hydroxyls on Selective Dehydrogenation of 2-Propanol over Co3O4 Catalyst — •Jan Smyczek[1], Patrick Hubert[1], Hauke Scheele[2], Carsten Schröder[1], Sharif Najafishirtari[2], Paul Kohlmorgen[1], Malte Behrens[2], and Swetlana Schauermann[1] — [1]Institute of Physical Chemistry, Christian-Albrechts-University Kiel, Max-Eyth-Str. 1, 24118 Kiel, Germany — [2]Institute of Inorganic Chemistry, Christian-Albrechts-University Kiel, Max-Eyth-Str. 2, 24118 Kiel, Germany

This study investigates the catalytic decomposition of 2-propanol to acetone over Co_3O_4 catalysts, examining both powdered materials under ambient pressure and model Co_3O_4(111) surfaces in ultrahigh vacuum. Water pretreatment at elevated temperatures substantially enhanced acetone formation rates. Scanning tunneling microscopy and infrared spectroscopy revealed that high-temperature water pretreatment creates isolated hydroxyl groups (O_sH) involving lattice oxygen atoms, whereas low-temperature deposition forms an extended, partly dissociated OH/H_2O network layer. The role of isolated O_sH groups can most likely be attributed to their function as hydrogen acceptors for H atoms leaving from either 2-propanol or the propoxy intermediate. Critically, dissociation occurs only with isolated O_sH species, not within the extended OH/H_2O network, which nearly completely suppresses both abstraction steps. The isolated O_sH groups function as efficient hydrogen acceptors, proving substantially more effective than adsorbate-free lattice oxygen.

O 35: Organic molecules on inorganic substrates: Adsorption and growth II

Time: Tuesday 10:30–12:15 Location: HSZ/0401

O 35.1 Tue 10:30 HSZ/0401

Phophangulenes on Au(111): comparing the influence of the environment on single molecule rotation — •Wyatt Highland[1], Sajjan Mohammad[1], Paul Philip Schmidt[1], Roberto Robles[2], Milan Kivala[3], Nicolas Lorente[2], Meike Stöhr[1,4], and Sabine Maier[1] — [1]Department Physik, FAU Erlangen-Nürnberg, Erlangen, Germany — [2]CFM/MPC (CSIC-UPV/EHU), Donostia-San Sebastian, Spain — [3]Institute of Organic Chemistry, Heidelberg University, Heidelberg, Germany — [4]University of Applied Sciences of the Grisons, Switzerland

Bowl-shaped phosphangulenes represent a promising class of rotor molecules for molecular energy-storage applications on surfaces, owing to their fixed rotational axis defined by the central phosphorus atom, which simultaneously serves as the anchoring group on gold substrates. For low coverge, the phosphangulenes stay isolated on Au(111). We examined their adsorption configurations and subsequently, the possibility for rotational motion using both the STM tip and thermal activation as external triggers. At higher coverage, phosphangulenes form compact self-assemblies that suppress their rotational motion. To overcome this, we employ porous, hydrogen-bonded trimesic-acid networks to isolate individual phosphangulenes at the surface. Comparing their rotational dynamics inside and outside the pores allowed to directly reveal the influence of the immediate surroundings on the rotational motion.

O 35.2 Tue 10:45 HSZ/0401

Self-assembly and electronic properties of functionalized norbornadiene photoswitches on Au(111) and graphene/Ir(111) — •Shreya Garg[1], Roberto Robles[2], Pedro Ferreira[3], Kasper Moth-Poulsen[3], Nicolas Lorente[2], Meike Stöhr[1,4], and Sabine Maier[1] — [1]Department of Physics, Friedrich Alexander University Erlangen-Nürnberg, Germany — [2]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), Donostia-San Sebastián 20018, Spain, SanSebastián, Spain — [3]Universitat Politecnica de Catalunya, Barcelona, CT, Spain — [4]University of Applied Sciences of the Grisons, Switzerland

The norbornadiene/quadricyclane (NBD/QC) system represents a notable class of photoswitches, in which the low-energy NBD isomer can be transformed into its metastable QC isomer upon exposure to external energy. Here, we investigate the self-assembly and electronic properties of a benzoic acid-functionalized NBD on Au(111) using STM, STS, and DFT. Two distinct adsorption conformations are identified; nevertheless, the overall structure of the self-assembled layers remains governed by hydrogen bonding between the carboxyl groups. To further elucidate molecule-substrate coupling effects, we examined NBD derivatives on graphene/Ir(111), which offers a reduced density of states near the molecular levels, thereby providing partial electronic decoupling. This approach revealed differences in electronic properties compared to Au(111), emphasizing the critical influence of the substrate and contributing to the optimization of their switching performance in future electronic systems.

O 35.3 Tue 11:00 HSZ/0401

Validation of the Rotational Degrees of Freedom in Azobenzene Subphthalocyanine — •Dominik Volavka[1], Wyatt Highland[1], Bartosz Szczefanowicz[1], Rebecci Samuele[1], Roberto Robles[2], Nicolas Lorente[2], Meike Stöhr[1,3], and Sabine Maier[1] — [1]Department of Physics, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany — [2]Centro de Física de Materiales (CSIC-UPV/EHU), Donostia-San Sebastián, Spain — [3]University of Applied Sciences of the Grisons, Switzerland

Azobenzene mounted on Subphthalocyanine (Azo-SubPC) via a single covalent oxygen bond is predicted to exhibit interesting rotational and switching properties due to the single bonding character of the boron-oxygen-carbon. Recent attempts at observing these rotational actions through scanning tunneling microscopy were hindered because of the self-assembling nature of Azo-SubPC when deposited on Au(111) and Ag(111). In each case, one-dimensional arrangements of Azo-SubPC formed, wherein molecules were neighbored by additional Azo-SubPC molecules on both sides. The resulting configuration of the molecules thusly led to a high steric hindrance and ultimate restriction of Azo-SubPC's anticipated rotational degree of freedom. Alternative preparation methods of Azo-SubPC are herein proposed and evaluated in the attempt of depositing and identifying isolated Azo-SubPC molecules with preserved rotational freedom. Isolated Azo-SubPC molecules can give insight into the underlying principles dictating the mechanisms of rotation in rotor molecules.

O 35.4 Tue 11:15 HSZ/0401

TPD/R Investigations of Metal-Substrate Interactions of Polyfluorinated Molecules on Au(111) — •Stefan R. Kachel, Evelyn Versok, Leonard Neuhaus, Kassandra Zoltner, and J. Michael Gottfried — Fachbereich Chemie und mar.quest, Philipps-Universität Marburg, Germany.

Interfaces between organic molecules and metal surfaces are crucial in heterogeneous catalysis, organic electronics, and related nanotechnological and sensing applications. Molecules with large dipole moments are particularly relevant, as dipole enhancement through tailored fluorination can strongly influence adsorption geometries, adsorbate-substrate interactions, and thus the electronic properties of molecule-metal interfaces. Among nonionic, saturated compounds, all-cis-hexafluorocyclohexane (HFCH) exhibits the highest known polarity (μ = 6.2 D). Here, we use temperature-programmed desorption and reaction (TPD/R) to investigate the desorption kinetics and energetics of HFCH and two reference compounds, perfluoromethylcyclohexane and cyclohexane, on Au(111). The polar HFCH shows markedly stronger interactions with the substrate than the two reference compounds, and all systems display desorption behavior that deviates substantially from structurally related aromatic species. The pronounced polarity and stacked packing motif of HFCH render it a promising model system for studies in supramolecular chemistry and organic materials research, including potential applications in organic ion-conducting materials.

O 35.5 Tue 11:30 HSZ/0401

TPD Studies on LOHC-relevant Cycloalkanes and Aromatics on Au(111) — •Kassandra Zoltner, Leonard Neuhaus, Stefan R. Kachel, and J. Michael Gottfried — Fachbereich Chemie and mar.quest, Philipps-Universität Marburg, Germany

Liquid organic hydrogen carriers (LOHCs), such as the decalin/tetralin pair, are promising compounds for hydrogen storage, yet their (de)hydrogenation cycles are limited by catalyst-induced side reactions. In this context, molecule–surface interactions fundamentally determine adsorption strength and reactivity, thereby controlling catalytic selectivity and activity. This work presents surface analytical studies using temperature-programmed desorption (TPD) to investigate the desorption kinetics and energetics of decalin, perhydroazulene, and (partially) dehydrogenated analogues on Au(111). The study focuses on how the degree of hydrogenation, structural motifs including ring connectivity, and configurational isomerism as well as electronic properties influence substrate and intermolecular interaction strengths. The results reveal distinct differences in desorption characteristics: aromatic molecules (naphthalene, azulene, tetralin) exhibit stronger adsorption to the metal substrate and repulsive intermolecular interactions, arising from their π-electron system, whereas saturated hydrocarbons (decalin, perhydroazulene) show weaker substrate binding and intermolecular attraction. The findings provide molecular-level insights into LOHC adsorption properties on metal surfaces and contribute to the development of improved hydrogen storage–catalysis systems.

O 35.6 Tue 11:45 HSZ/0401

MAD-SURF: a general Machine-Learning Potential for molecular adsorption on metal surfaces — •Manuel González Lastre[1], Joakim S. Jestilä[2], Rubén Pérez[1], and Adam S. Foster[2] — [1]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Spain — [2]Department of Applied Physics, Aalto University, 00076, Espoo, Finland.

Predicting how organic molecules adsorb, assemble and interact on metal surfaces is central to surface chemistry, molecular electronics and scanning probe microscopy. Yet, the application of first-principles simulations to interfaces is hampered by the computational cost for evaluating the electronic structure for the large number of atoms typically involved. Here we present MAD-SURF, a general Machine-Learning Interatomic Potential tailored for molecular adsorption on metal surfaces. Trained on a broad dataset spanning diverse molecules, adsorption motifs, surfaces, molecular dynamics and non-covalent aggregates, MAD-SURF achieves near quantum-mechanical accuracy while enabling simulations that are orders of magnitude faster than Density Functional Theory. The model reliably reproduces energies, forces and adsorption geometries across different surfaces. We demonstrate its versatility by capturing experimentally observed systems, ranging from organic monolayers and polycyclic aggregates to flexible biomolecules and long-range metal surface reconstructions. By combining accuracy, speed, and generalizability, MAD-SURF offers a practical framework for accelerating atomistic simulations in surface science.

O 35.7 Tue 12:00 HSZ/0401

Using Machine Learning to predict molecular conformations from STM images — •Tim J. Seifert[1], Dhaneesh Kumar[2], Stephan Rauschenbach[3], Klaus Kern[2], Markus Etzkorn[1,4], Kelvin Anggara[2], and Uta Schlickum[1,4] — [1]Institute of Applied Physics, TU Braunschweig, Braunschweig — [2]Max Planck Institute for Solid State Research, Stuttgart — [3]Department of Chemistry, Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, United Kingdom — [4]Laboratory for Emerging Nanometrology LENA, Braunschweig

Single-molecule imaging of biologically essential building blocks such as saccharides and peptides by scanning tunneling microscopy (STM) holds immense promise, enabling key insights into their structure and biological functions. However, automatic structural analysis remains bottlenecked by the lack of

available experimental training data. We overcome this fundamental limitation through a novel workflow that rapidly generates vast datasets of high-fidelity synthetic STM images from geometric molecular models. We train a custom Machine Learning architecture on this synthetic data to predict atomic coordinates directly from STM images, enabling fully automated reconstruction of molecular conformations. Validated on two distinct organic systems - glycans and polypeptides - the method achieves atomic positional accuracies below 4 Å and 2 Å, respectively, with unsupervised conformer classification of polypeptides exceeding 97% accuracy. The trained models transfer robustly to experimental STM data, delivering visually convincing structural predictions.

O 36: Focus Session: Mineral-water interfaces II

The Focus Session discusses recent advances in the understanding of mineral-water interfaces. These interfaces are ubiquitous in nature, host of many geological and biological processes, intimately linked to the global carbon cycle, and therefore highly relevant for Earth*s climate. For example, silicate weathering removes carbon dioxide from the atmosphere on geological timescales, acting as a stabilizing feedback mechanism since weathering rates increase with temperature. In the oceans, carbonates dissolve and precipitate in response to changing atmospheric carbon dioxide concentrations, thus far mitigating part of the anthropogenic impact of CO_2 emissions. In addition, numerous industrial and technological processes involve mineral-water interfaces, including seawater desalination, scaling and incrustation prevention, as well as various biochemical applications. However, and despite their importance, many fundamental aspects of mineral-water interfaces remain poorly understood, including water binding and diffusion, structure formation, ice nucleation, growth, or desorption.

This DPG Focus Session will address these aspects at the molecular level, elucidating fundamental processes involving both single water molecules and bulk water in contact with mineral surfaces. The session brings together scientists investigating mineral-water systems under ultrahigh vacuum conditions as well as at mineral-water interfaces in bulk aqueous environments. We aim for a balanced Session with contribution from both renowned experts and young investigators active in the field.

Organized by Philipp Rahe (U Osnabrück), Angelika Kühnle (U Bielefeld), Jan Balajka (TU Vienna), Wolf Gero Schmidt (U Paderborn).

Time: Tuesday 10:30–12:30 Location: HSZ/0403

Invited Talk O 36.1 Tue 10:30 HSZ/0403

Acidity in nanoconfinement from ab initio and NNPs simulations — Anthony Baldo[2], Muhammad Saleh[1], Kevin Leung[2], and •Marialore Sulpizi[1] — [1]Department of Physics and Astronomy, Ruhr-University Bochum, Universitätsstraße 150, 44801 Bochum, Germany — [2]Geochemistry Department, Sandia National Laboratories, Albuquerque, New Mexico, USA

Chemical and physical properties in nanoconfined systems may substantially differ from bulk, a phenomenon that can be exploited for the development of new industrial processes for energy generation and storage. Here we consider the specific behavior of acids within silica nanopores, a topic of relevance to the geochemistry and the nanofluids communities.

Starting from ab initio molecular dynamics simulations we develop neural network potentials (NNPs) capable of describing the solid/liquid interfaces and the nanoconfined liquids* behavior over a wide range of temperatures. These NNPs can capture the change in acidity constants when e,g acetic acid is confined in nanoscale slit or when it approaches the interface. Our approach can be further extended to more complex geometries and solution compositions.

O 36.2 Tue 11:00 HSZ/0403

Ab initio exploration of water clusters on CaF_2 — •Isaac Azahel Ruiz Alvarado[1], Wolf Gero Schmidt[1], Paul Laubrock[2], Jonas Heggemann[2], and Philipp Rahe[2] — [1]Lehrstuhl für Theoretische Materialphysik, Universität Paderborn, Paderborn, Germany — [2]Institut für Physik, Universität Osnabrück, Osnabrück, Germany

The electronic and structural properties of the CaF_2(111) surface-water interface are investigated from first-principles calculations. The energetic landscape for single molecular adsorption is calculated using standard DFT with London dispersion forces corrections. Single water molecules are found to preferentially adsorb on surface Ca atoms while large diffusion energy barriers are determined that restrict lateral movement of the water molecules. Additionally, the adsorption energies for the intact water molecule are compared to dissociative adsorption.

Multiple water molecules are included in the calculations to simulate the ice-like clusters observed experimentally by high-resolution AFM data acquired with CO-terminated tips. In order to understand the formation of these clusters, hexagonal rings similar to the ice I_h motif are modeled on top of the CaF_2 surface slab. The ice-surface incommensurability coupled with large diffusion barriers and preferred adsorption sites is suspected to limit the formation of a closed water monolayer. Complete water overlayers and additional structures are also calculated using molecular dynamics aided by machine learning force fields trained from ab initio calculations.

O 36.3 Tue 11:15 HSZ/0403

Surface Structure of Polar Silver Iodide (0001) in Various Liquids: No Indication for a Surface Reconstruction — •Kim Noelle Dreier, Annamaria Latus, Ralf Bechstein, and Angelika Kühnle — Physical Chemistry I, Department of Chemistry, Bielefeld University, Universitätsstraße 25, 33615 Bielefeld, Germany

Silver iodide (AgI) has long been known as a material that induces precipitation in clouds. The superior ice nucleation ability is commonly explained by the close lattice match between β-AgI(0001) and the basal plane of ice. However, this surface is polar, indicating that a stabilization mechanism should be present. Here, we investigate the Ag-terminated β-AgI(0001) and the I-terminated β-AgI(000-1) surfaces in water and compare the results with images recorded in n-dodecane, 0.1 M NaCl and 0.1 M KI aqueous solutions. Strikingly, high-resolution images consistently reveal a bulk-truncated structure. These findings align with observations at a larger scale, which neither indicate any surface reconstruction. Although the observed structures reveal a variety of features and depend on the surface termination, some general conclusions can be drawn. Firstly, in solvents with poor AgI solubility, only minor changes are observed. Secondly, the images taken in KI solution exhibit patterns that are characteristic of mineral dissolution and growth. Thus, even in a situation where AgI can and does dissolve, no indication for a surface reconstruction can be found. These results shed new light onto the surface structure of β-AgI(0001), challenging the expectation that a surface reconstruction is present under ambient conditions.

Invited Talk O 36.4 Tue 11:30 HSZ/0403

Living Interfaces: Dissolution and Precipitation Processes at Mineral-Brine Interfaces Revealed by AFM — •Igor Siretanu, Vincenzo Alagia, Saravana Kumar, Shilpa Mohanakumar, Max Nederstigt, Chinmay Shukla, Michel Duits, and Frieder Mugele — Physics of Complex Fluids Group and MESA+ Institute, Faculty of Science and Technology, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands

Mineral-brine interfaces are dynamic systems where dissolution and precipitation govern reactivity and morphology. Using in-situ Atomic Force Microscopy (AFM), we examine olivine ([Mg,Fe]2SiO4) and calcite. Olivine, a candidate for carbon mineralization, shows etch-pit-mediated surface retraction with morphology strongly dependent on solution chemistry. In H2SO4, pits are larger and deeper than in HCl, while oxalic acid induces anisotropic complexation, forming rectangular pits and stepped terraces aligned with crystallographic directions. These changes accelerate step retreat and Mg release, offering mechanistic insight into dissolution kinetics relevant for CO2 sequestration. At calcite-water interfaces near equilibrium, AFM force spectroscopy reveals two regimes: (A) DLVO-type forces with low surface potentials (<5 mV) and (B) long-range viscoelastic repulsion from a soft interfacial layer formed by coupled dissolution-precipitation. This dynamic interphase explains inconsistencies in reported

surface forces and highlights how solution composition, crystallography, and transient phases control mineral reactivity, with implications for geochemistry, biomineralization, and carbon capture.

O 36.5 Tue 12:00 HSZ/0403

Water Organization and Speciation at the Calcite (10.4)-Water Interface at High pH — •Tobias Dickbreder[1], Frank Heberling[2], and Ellen H. G. Backus[1] — [1]Institute of Physical Chemistry, Faculty of Chemistry, University of Vienna, Vienna, Austria. — [2]Institute for Nuclear Waste Disposal, Karlsruhe Institute of Technology, Eggenstein-Leopoldshafen, Germany

Calcite dissolution and precipitation are central for various environmental processes including the geological carbonate-silicate cycle, buffering of sea- and freshwater pH values and biomineralization. Since these processes take place at the calcite-water interface, the structure and properties of the interface between water and the most stable calcite (10.4) surface have been well studied. Despite this effort the protonation state of surface-bound water and interfacial carbonate groups remains poorly understood, because dissolution and carbonate buffering complicate studying calcite de-/protonation experimentally.

Here, we apply vibrational sum frequency generation (SFG) spectroscopy to directly assess the water species present at the calcite-water interface. As reported previously, the SFG spectrum at neutral pH is almost featureless due to the opposite orientation of the first two water layers [1]. At very high pH, however, we observe the emergence of spectral features suggesting surface charging and the presence of interfacial hydroxyl groups. Our study, thus, confirms the presence of hydroxyl groups at the calcite-water interface, facilitating the development of more-accurate models of the calcite-water interface.

[1] Söngen et al., J. Phys. Chem. Lett. 12 (2021), 7605 - 7611.

O 36.6 Tue 12:15 HSZ/0403

The mechanism of selenite incorporation into the calcite surface revealed by atomic-scale imaging — •Marie Luigs, Ralf Bechstein, and Angelika Kühnle — University of Bielefeld, Bielefeld, Germany

Selenium is an essential trace element for human health. However, the margin between its required and toxic intake is very narrow, making its distribution in soils and waters an important subject of research. Moreover, the interaction between the nuclear waste component 79Se and minerals in the Earth's crust is relevant for the selection of nuclear waste disposal sites. Selenium in the form of selenite can be incorporated into the mineral calcite by substituting for carbonate ions. However, the mechanism of selenite incorporation into calcite remains unknown. Here we demonstrate that selenite incorporation occurs at step edges during calcite crystal growth. Atomic-scale atomic force microscopy (AFM) images of the calcite surface exposed to a selenite-rich calcium carbonate growth solution shows that calcite layers grown in the presence of selenite displayed a significantly higher defect density than layers that were exposed to selenite only after their formation. These observations indicate that significant selenite incorporation into calcite, reflected by an increased defect density, does not occur via ion exchange on terraces but via step edge growth. Our results give further insights into the conditions required for selenite incorporation into calcite and present the first atomic-scale AFM images of a selenite-rich calcite surface.

O 37: Electronic structure theory I

Time: Tuesday 10:30–12:30 Location: TRE/PHYS

Invited Talk O 37.1 Tue 10:30 TRE/PHYS

Calculations of excited electronic states by converging on saddle points on the electronic energy surface — •Hannes Jonsson — University of Iceland, Reykjavik, Iceland

Calculations of excited electronic states are important in various contexts, e.g. photocatalysis and molecular motors. They are challenging as commonly used optimization methods are based on minimization and thereby converge on the ground state. A time-dependent formulation of density functional theory (TD-DFT), especially within the linear response and adiabatic approximations, is therefore often used to estimate excited states, but can fail especially when significant charge transfer occurs and when states are close in energy. Alternatively, by converging on a saddle point on the electronic energy surface, the orbitals can be optimised for an excited state to provide a solution of the underlying Kohn-Sham equations with higher energy than the ground state. This turns out to a give more robust estimate of the excitation energy than TD-DFT with computational effort similar to that of a ground state calculation. Several applications of this approach with commonly used density functionals will be presented, as well as calculations using a self-interaction corrected functional giving improved results. In particular, excited states involving twisting of a C=C bond, e.g. in molecular motors, and Rydberg states have been analysed. As a solid state application, the various states involved in the optical preparation of a pure spin state in nitrogen/vacancy defect in diamond will be presented. The results show close agreement with more computationally demanding calculations as well as experiments.

O 37.2 Tue 11:00 TRE/PHYS

Probing quantum coherence with free electrons — •Hebrew Crispin and Nahid Talebi — Christian-Albrechts-Universität, Kiel, Germany

Advances in ultrafast electron microscopy have enabled the study of coherent interactions between free electrons and quantum systems with high spatial resolution. Recent works have examined the coupling of free electrons to two-level systems, including the use of coherently shaped electron wavefunctions to probe coherence in individual or collective quantum emitters. Coherence can also be accessed through sequential time-resolved cathodoluminescence spectroscopy, which has demonstrated the ability to measure ultrafast radiative decay and dephasing in single emitters with femtosecond resolution. In addition, there is increasing interest in time-resolved electron energy-loss spectroscopy (EELS) techniques capable of tracking system dynamics.

Here, we present a general theoretical framework for coherent interactions between free electrons and quantum emitters prepared in arbitrary initial superposition states. We employ a fully quantum, time-dependent description of both the propagating electron wavepacket and the emitter. Quantum coherence manifests as transient oscillations in both the emitter populations and in the zero-loss peak of the spectral energy-loss probability density, even for an unmodulated electron wavepacket. Our work reveals novel coherent dynamics in the interactions between free electrons and quantum systems.

O 37.3 Tue 11:15 TRE/PHYS

Phonons in polar materials: a DFPT extension in the FLAPW method *FLEUR* — •Friedrich Hanrath[1,2], Thomas Bornhake[1,2], Gustav Bihlmayer[1], Gregor Michalicek[1], Daniel Wortmann[1], and Stefan Blügel[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Institute for Theoretical Physics, RWTH Aachen University, D-52074 Aachen, Germany

Phonons play a pivotal role in determining many essential properties of solids. Using Density Functional Perturbation Theory (DFPT), a state-of-the-art approach for computing fundamental physical response properties from first principles, phonon calculations have previously been realized [1] within the full-potential linearized augmented plane-wave (FLAPW) method *FLEUR* [2]. In polar materials, zone-center vibrations are altered by their interaction with long-range electric fields, giving rise to the characteristic LO-TO splitting in the long-wavelength limit. In this talk, we present the extension of the DFPT framework in *FLEUR* to a macroscopic electric-field perturbation, enabling the calculation of high-frequency dielectric tensors and Born effective charges, quantities required to describe LO-TO splitting, and compare our results with experiments. This work was supported by the CoE-MaX (EuroHPC Joint Undertaking, Grant 101093374) and DFG through CRC 1238 (Project C01).

[1] C.-R. Gerhorst *et al.*, Electron. Struct. **6**, 017001 (2024).
[2] D. Wortmann *et al.*, 10.5281/zenodo.7576163; www.flapw.de

Invited Talk O 37.4 Tue 11:30 TRE/PHYS

Many-Body Theory meets Electrochemistry: Electronic Structure of Cathode Materials — •Silke Biermann — Centre de Physique Théorique, UMR7644, Ecole Polytechnique, Institut Polytechnique de Paris, 91128 Palaiseau, France

Progress in dynamical mean field-based electronic structure methods over the last years has provided us with precious tools allowing for a microscopic understanding of electronic mechanisms at work in correlated materials, including functional materials. In this talk, we will focus on layered transition metal compounds studied for battery applications. Analysing the electronic structure, energetics and intercalation voltage, we find that Hund's exchange coupling plays a crucial role for the electrochemistry of these compounds. We identify the battery charging process as a transition from a high-spin Mott insulator to a low-spin correlated metal. We argue that a deeper understanding of the microscopic mechanisms at work in such materials might contribute to paving the way to better battery materials in the future.

O 37.5 Tue 12:00 TRE/PHYS

Massively parallel and GPU-accelerated evaluation of three-center integrals for numerical atomic orbitals (NAOs) — •Moritz Leucke, Antonio F. Delesma, and Dorothea Golze — Julius-Maximilians-Universität Würzburg, Germany

Four-center electron repulsion integrals appear in many electronic structure methods, such as many-body perturbation methods like the Random-Phase-Approximation or GW and others. To reduce their computational cost, the

resolution-of-the-identity (RI) approximation is commonly employed. RI refactors the four-center integrals into three- and two-center integrals, among which the three-center integrals remain a computational bottleneck, particularly when using NAOs.

We present a global RI scheme combined with a local metric (attenuated Coulomb) within an all-electron NAO framework, treating molecules and solids on equal footing. Central to the approach is a novel GPU-accelerated algorithm for computing 3-center integrals that relies on domain decomposition to improve load balancing and strong scaling.

We demonstrate that our RI implementation achieves linear scaling with system size and maintains meV-level accuracy for GW energies. Performance benchmarks show scalability across thousands of CPU cores and substantial speedups with GPU support.

[1] Delesma et al., NIC Symposium Proceedings, 52(2025), 113-123.

O 37.6 Tue 12:15 TRE/PHYS

Efficient all-electron implementation of the Bethe-Salpeter method using crystal symmetries — Jörn Stöhler, Stefan Blügel, and •Christoph Friedrich — Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany

We describe an implementation of the Bethe-Salpeter equation (BSE) method in the full-potential linearized augmented-plane-wave (FLAPW) method. As in most implementations, the BSE is solved by the diagonalization of a two-particle Hamiltonian matrix, whose dimension is proportional to the number of **k** points. Due to the large number of **k** points required to converge the spectra, the resulting matrix becomes large even for small unit cells. We describe a method that exploits the crystal symmetries to accelerate the construction and diagonalization of the two-particle Hamiltonian. In particular, we employ group theoretical tools to bring the Hamiltonian into block-diagonal form. It is shown that, in many cases, only one of the blocks needs to be taken into account, which leads to a considerable speedup of the diagonalization step. In the case of Si, for example, the dimension of the Hamiltonian is reduced by a factor of five, giving rise to a speedup factor of 125 in its diagonalization. The optical absorption spectrum calculated with a 60×60×60 **k** mesh is very close to the experimental spectrum. The code allows for the inclusion of spin-orbit coupling and is parallelized with the possibility of storing the Hamiltonian in distributed memory over many nodes. We also show results for LiF and the MoS_2 monolayer.

O 38: Ultrafast electron dynamics at surface and interfaces II

Time: Tuesday 10:30–12:30 Location: TRE/MATH

O 38.1 Tue 10:30 TRE/MATH

Ultrafast momentum microscopy of exciton dynamics at ZnO surfaces — •Hashima Marukara, Paul Werner, Jan Philipp Bange, G S Matthijs Jansen, Wiebke Bennecke, Junde Liu, and Stefan Mathias — Georg-August-Universität Göttingen, I. Physikalisches Institut, Germany

ZnO is a prototypical wide-band-gap material with long-lived excitons, making it a central platform for modern optoelectronic and catalytic technologies, especially for investigating exciton-related phenomena [1]. Excitons*bound electron*hole pairs that can exist in various forms near the surface, significantly shape the material*s optical and electronic response and play an essential role in interfacial energy-conversion processes [2]. However, studies that directly characterize these excitons, particularly if they are defect-mediated, localized or mobile, or predominantly Frenkel- or Wannier-type, remain limited.

Here we address these questions using time-resolved momentum microscopy to map the fingerprints of excitons in energy, momentum and time [3]. We present first experimental momentum-space maps of the ZnO(10-10) surface exciton states and track their real-time evolution following photoexcitation. We observe clear signatures of surface exciton formation, including their emergence in the unoccupied band structure and their subsequent relaxation dynamics on ultrafast timescales.

[1] Gierster *et al.*, Nat Commun 12, 978 (2021) [2] Deinert *et al.*, Phys. Rev. Lett. 113 057602 (2014) [3] Bennecke *et al.*, Nature Phys. (2025), https://doi.org/10.1038/s41567-025-03075-5

O 38.2 Tue 10:45 TRE/MATH

Investigating the light-induced metallization of ZnO through time-resolved photoemission spectroscopy — Gian Marco Pierantozzi[1], Federico Motti[1], Matteo Gatti[2], •Monika Schied[1], Alice Crosato[3], Thomas Sartori[3], Riccardo Cucini[1], Giorgio Rossi[1,4], Fausto Sirotti[2], and Giancarlo Panaccione[1] — [1]CNR – Istituto Officina dei Materiali (IOM), Trieste, Italy — [2]École polytechnique, Paris, France — [3]Università Ca' Foscari Venezia, Italy — [4]Università degli Studi di Milano, Italy

With a direct bandgap of ~3.4 eV and a high exciton binding energy (~60 meV), ZnO is ideal for optoelectronics and excitonic studies. Under optical excitation, the system shows ultrafast metallization with several relaxation timescales [1,2]. The relevance of defects in stabilizing the photoinduced metallic state is known, but many aspects of the processes remain unclear. Here we investigate the ultrafast dynamics of the optically populated conduction band and the Zn 3d core level with time- and angle-resolved photoemission spectroscopy after resonantly pumping, in order to disentangle the excitations of defect levels. Our experiments cover the whole metallization process in ZnO. We observe a fast rise in the conduction band population within 100 fs, a slower temperature-dependent rise, probably due to carrier transport and redistribution, a decay on the ns timescale and a long-lasting metastable state. All these dynamics occur also pumping below resonance, albeit to a lower extent, highlighting the role of the defect levels.

[1] L. Gierster et al. Nat. Comm. 12:978 (2021);
[2] L. Gierster et al., Far. Disc. 237, 58 (2022)

O 38.3 Tue 11:00 TRE/MATH

Ultrafast electron dynamics in charge-transfer insulators $LaFeO_3$(001) and $BiFeO_3$(001) — •Friederike Wührl, Antonia Rieche, Anne Oelschläger, Kathrin Dörr, and Wolf Widdra — MLU Halle-Wittenberg

The electron dynamics in strongly correlated systems, where electron-electron correlation leads to band gap opening, are highly unexplored. One example is the prototypical charge transfer insulator NiO, which shows a remarkable short lifetime of <10 fs at the conduction band minimum, relaxing in a many-body in-gap state, which couples to the antiferromagnetic spin system [1]. Here we are extending our time-resolved studies to the unoccupied states of epitaxial antiferromagnetic $LaFeO_3$(001) and ferroelectric $BiFeO_3$(001) thin films grown on $SrRuO_3/DyScO_3$(001) substrates. We use two-photon photoemission in a UV-UV pump-probe experiment, exciting electrons across the band gap, which opens between strongly hybridized oxygen 2p/Fe 3d and Fe minority states for both perovskites. We find in both sytems a broad state at ~ 1.3 eV above E_F with a short lifetime of 20 fs, whereas the conduction band minimum shows a multiexponential decay with timescales in the femtosecond to picosecond range. The different decay channels show an energy dependent increase of lifetimes towards the Fermi level. Comparing $BiFeO_3$ and $LaFeO_3$, the decay channels differ solely in their amplitudes, with a higher probability for the fast decay channel in $LaFeO_3$.

[1] Gillmeister *et al.* Nat. Commun. **11**, 4095 (2020).

O 38.4 Tue 11:15 TRE/MATH

Ultrafast Formation and Annihilation of Strongly Bound Anisotropic Excitons in CrSBr — •Lawson T. Lloyd[1], Tommaso Pincelli[1,2], Mohamed A. Wahada[1], Alessandro De Vita[1,2], Ferdinand Menzel[3], Kseniia Mosina[4], Túlio H. L. G. Castro[1], Alexander Neef[1,2], Andreas V. Stier[3], Nathan P. Wilson[3], Zdeněk Sofer[4], Jonathan J. Finley[3], Martin Wolf[1], Laurenz Rettig[1], and Ralph Ernstorfer[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Technische Universität Berlin, Berlin, Germany — [3]Technische Universität München, Garching, Germany — [4]University of Chemistry and Technology Prague, Prague, Czech Republic

Excitons dominate the optical response and determine the functionality of atomically thin semiconductors. In the van der Waals magnetic semiconductor CrSBr, strongly bound, anisotropic excitons couple to the underlying spin order, which could be leveraged in next-generation opto-spintronics. However, mechanisms of exciton formation, dissociation, and interaction with free carriers remain largely unexplored. Employing time- and angle-resolved photoemission spectroscopy, we probe the nature of the exciton in CrSBr by directly imaging the nonequilibrium electronic states, extracting fundamental properties of the excitonic wavefunction and revealing the driving mechanisms of exciton relaxation on ultrafast timescales. Notably, we observe an excitation-density-dependent interconversion between bound excitons and quasi-free carriers, indicating that many-body effects govern the excited state dynamics during the initial stages of relaxation.

O 38.5 Tue 11:30 TRE/MATH

Large relative delays for photoemission final states less than 1 eV apart — •Tillmann Schabbehard, Andreas Gebauer, Walter Enns, Luis Maschmann, and Walter Pfeiffer — Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld

The reconstruction of attosecond beating by interference of two-photon transitions (RABBITT) allows probing photoemission dynamics in atoms, molecules and solids. However, the interpretation of retrieved relative delays between different emission channels in particular for emission from solids is controversial.

Here we employ spin-orbit delays in GaSe by RABBITT, i.e., relative delays for emission from the different initial states of the spin-orbit doublet, to investigate the relative photoelectron kinetics in emission channels, which differ less than 1 eV in their final state energy (E_{final}). Despite the small spin-orbit splitting for both Ga3d and Se3d the extraction of relative delays for the two spin-orbit doublets yields 180±53 as and 94±45 as. These unexpectedly large delays can neither be attributed to intraatomic delay mechanisms nor to kinetic propagation effects in the final state continuum. This challenges common concepts about photoelectron emission dynamics, which predict much smaller delays for E_{final} differences below 1 eV. Notably, the Se3d spin-orbit delay in GaSe agrees well with those observed in Bi_2Se_3 and WSe_2 indicating a general high variability of emission dynamics as function of the E_{final}. Predictions based on the one step model, which take into account transport via propagating and evanescent states match observations much better, while modelling based on propagation effects in the final state alone fail.

O 38.6 Tue 11:45 TRE/MATH

Lightwave-driven flat bands in a van der Waals crystal — •Changhua Bao[1], Vincent Eggers[1], Manuel Meierhofer[1], Jakob Helml[1], Lasse Münster[1], Suguru Ito[2], Leon Machtl[1], Sarah Zajusch[2], Giacomo Inzani[1], Ludwig Wittmann[1], Marlene Liebich[1], Robert Wallauer[2], Ulrich Höfer[1,2], and Rupert Huber[1] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Department of Physics, Philipps-University of Marburg, Marburg, Germany

Flat bands lead to an extremely high density of states and suppressed kinetic energy, thereby increasing electronic correlations and leading to intriguing light-matter interaction. Here, we reveal the band structure of the van der Waals crystal $NbOCl_2$ using photoelectron momentum microscopy. We directly map out an electronic band that is flat throughout the entire Brillouin zone and well isolated from both the conduction and remote valence bands. By utilizing subcycle photoemission spectroscopy [1,2], the dynamics of the flat band under atomically strong mid-infrared light fields are explored. Intriguingly, the carrier field of light induces long-lived collective modes, which are resolved with subcycle precision. These collective modes not only accelerate the electrons but also renormalize the energy of the flat band. We investigate the microscopic mechanisms of these dynamics, highlighting novel possibilities of flat bands in strong-field physics.

[1] Reimann *et al.,* Nature **562**, 396 (2018); [2] Ito *et al.,* Nature **616**, 696 (2023)

O 38.7 Tue 12:00 TRE/MATH

Spin-orbit entangled exciton formation in a 2D correlated semiconductor — •Tania Mukherjee[1,2], Lawson T. Lloyd[1], Alessandro De Vita[1,2], Martin Wolf[1], Laurenz Rettig[1], Ralph Ernstorfer[1,2], and Tommaso Pincelli[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Technische Universität Berlin, Berlin, Germany

Excitons govern the magneto-optical properties in spin-ordered 2D materials. $NiPS_3$, a layered antiferromagnetic semiconductor, has recently gained significant attention because of its unconventional excitonic behaviour. Previous literature suggests that excitons are composed of bound electron and holes pairs in a highly spin and orbitally entangled Zhang-Rice-singlet state, resulting in strong coupling with the underlying magnetic ordering.However, the microscopic mechanism that governs the exciton formation remains elusive and unexplored. Using time- and angle-resolved photoemission spectroscopy, we map the electronic structure and the excited state dynamics of $NiPS_3$ across the magnetic phase transition and, for the first time, observe directly the long-lived exciton footprint below the Néel temperature. This paves the way for exploring similarly complex excitonic behavior in other layered correlated materials.

O 38.8 Tue 12:15 TRE/MATH

Understanding resonantly enhanced light-induced superconductivity in K3C60 — •Michael A. Sentef[1,2], Juan I. Aranzadi[1], Paul Fadler[1], and Joseph Tindall[3] — [1]Institute for Theoretical Physics, University of Bremen — [2]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg — [3]Center for Computational Quantum Physics, The Flatiron Institute, New York

Light-induced superconducting-like responses have been observed in K3C60 when driving with mid-infrared laser pulses [1], with a pronounced 10 THz resonance reported more recently [2]. Here we address the microscopic origin of this resonance. Using numerical calculations on finite clusters for a realistic multi-orbital model of K3C60 we simulate the effect of a periodic drive on the strongly correlated system. We find a sharp enhancement of pairing correlations when the drive frequency is tuned close to 10 THz, in agreement with experiment. The microscopic origin of this enhancement and its potential implications for a light-induced hidden phase [3] will be discussed. Our results thus provide a microscopic explanation for the resonantly enhanced light-induced superconducting-like state in K3C60 and strengthen its interpretation as being closely connected to superconducting pairing rather than to purely optical or nonthermal population effects.

[1] Mitrano et al., Nature 530, 461-464 (2016). [2] Rowe et al., Nature Physics 19, 1821-1826 (2023). [3] Budden et al., Nature Physics 17, 611-618 (2021).

O 39: Focus Session: Structure and Dynamics of Solvent at Electrochemical Interfaces I

Understanding how solvent molecules organize and move at electrochemical interfaces is central to catalysis, energy conversion, and electrochemical materials science. This Focus Session will bring together experimental and theoretical leaders using complementary surface specific spectroscopies as vibrational sum frequency generation, advanced X ray/electron techniques, and multiscale simulations to reveal intermolecular structure, hydrogen bond networks, ion-solvent coupling, and field driven dynamics from single crystal electrodes to complex battery interfaces. By highlighting recent breakthroughs in time-resolved measurements and operando platforms, the session aims to connect fundamental interfacial physics with macroscopic performance in electrocatalysis, corrosion, and electrochemical energy storage.

Organized by Yujin Tong (U Duisburg-Essen) and Angelika Kühnle (U Bielefeld).

Time: Tuesday 10:30–12:30 Location: WILL/A317

O 39.1 Tue 10:30 WILL/A317

Influence of Tip Apex Modification on Force Microscopy at the Solid-Liquid Interface — •Lucas Andreas Scheibel and Andrea Auer — Institute of Physical Chemistry, Innsbruck, Austria

Recent advances in electrochemical atomic force microscopy (EC-AFM) at the electrified solid-liquid interface using stiff, self-sensing quartz cantilevers (qPlus sensors [1]) have enabled high-resolution imaging of both electrode surfaces and interfacial solvent structures.[2,3] This interfacial region plays a decisive role in determining the performance of electrocatalysts, fuel cells, and electrochemical processes. In this work, we introduce chemically modified Si tips functionalized with charge-neutral hydrophobic or hydrophilic groups to identify how charge buildup at the tip apex influences the ability to resolve solvent structures and distinguish water from ion layering at the Au(111)-electrolyte interfaces across a range of pH values. These strategies provide new insight into atomic-scale contrast mechanisms of liquid AFM and highlight the role of tip-apex chemistry[2] in resolving the interfacial organization of solvent molecules at well-defined electrified solid-liquid interface.

[1] F. J. Giessibl, Rev. Sci. Instrum. 90, 011101 (2019)

[2] A. Auer, F. J. Giessibl, J. Kunze-Liebhäuser, ACS Nano, 19, 9, 8401-8410 (2025)

[3] A. Auer, X. Ding, A. S. Bandarenka, J. Kunze-Liebhäuser, J. Phys. Chem. C, 125, 9, 5020-5028 (2021)

O 39.2 Tue 10:45 WILL/A317

High-Resolution Hydration Layer Mapping: Does a Hydration Structure above Gold Imply a Clean Surface? — •Antonia Köhler[1], Ralf Bechstein[1], Michael Reichling[2], and Angelika Kühnle[1] — [1]Bielefeld University, Bielefeld, Germany — [2]Institut für Physik, Osnabrück, Germany

Solid-liquid interfaces are pivotal in a broad range of fields, including electrochemistry, catalysis and geochemistry. In electrochemistry, the molecular structure of the electrode-water interface is decisive for understanding and improving electrochemical reactions. In this context, the Au(111) surface constitutes a prototypical model system as gold is believed to be a relatively inert and well-characterized sample material. So far, however, little is known about the hydration structure at the Au(111)-water interface at the molecular level. Here, we present atomic force microscopy data on a gold sample carefully cleaned according to standard electrochemistry preparation recipes. Our three-dimensional atomic force microscopy data reveal a vertically ordered hydration structure with layer-to-layer distances of 0.36 nm as expected for water. Strikingly, despite our extensive cleaning efforts (validated by cyclic voltammetry measurements), our

two-dimensional data reveal stripe-like structures at the Au(111)-water interface. The dimensions of these structures differ from the well-known herringbone reconstruction of the gold surface, which is why we interpret them as surface contamination. Our work, hence, demonstrates that the presence of a hydration structure is no evidence for a clean gold surface.

Invited Talk O 39.3 Tue 11:00 WILL/A317

Electric double layer of platinum electrodes — •Marc Koper — Leiden University

Platinum is the most studied electrode material in electrocatalysis, but its electric double layer properties are still incompletely understood. Only Pt(111) has a true double layer window, which charges purely electrostatically. However, the properties of the electric double layer of Pt(111) do not follow the classic Gouy-Chapman-Stern theory. Lower coordination sites and facets on platinum are always covered by either hydrogen or hydroxyl adsorbates, which have an important influence on its double layer properties, as will be illustrated by recent results of double-layer measurements on stepped Pt single-crystal electrodes combined with ab initio molecular dynamics simulations and mean-field modeling. In addition, we show that at low electrolyte concentrations, which are often necessary for double-layer measurements, Pt(111) displays strong constant-phase element behavior, which complicates the accurate measurement of its double layer capacitance. The possible origin of this nonideality will be discussed. Finally, the effect of adsorbates on the electric double layer of platinum will be discussed on the basis on hydrogen-covered Pt(111).

O 39.4 Tue 11:30 WILL/A317

Nonequilibrium density-potential functional theoretical approach of electrochemical plasmonics — •Lulu Zhang[1,2], Michael Eikerling[1,2], and Jun Huang[1,2] — [1]Forschungszentrum Juelich GmbH, Juelich, Germany — [2]RWTH Aachen University, Aachen, Germany

Electrochemical plasmonics enables in-situ optical probing and modulation of electrochemical interfaces. Experiments have revealed that localized surface plasmon resonance (LSPR) in metal nanoparticle-solution systems is sensitive to surface charge, morphology, electrolyte composition and chemisorption. However, resolving nanoscale interfacial structures from the measured LSPR is rarely practiced; all existing theoretical methods fall in short of simulating the electrochemical plasmonics of nanoparticles under realistic conditions, namely, at a constant electrode potential for a particle with a diameter above 10 nm immersed in an electrolyte solution with a moderate concentration below 100 mM. We are developing a nonequilibrium density-potential functional theoretical (DPFT) approach to enable LSPR simulations under realistic conditions, considering coupled electron-ion-solvent interactions under a terahertz electromagnetic perturbation and on the mesoscale. It ensures constant-potential simulations, scalability to realistic systems, consistency for electronic effects under equilibrium and nonequilibrium, and systematic analysis under working conditions. The fundamental insights into coupled light-electron interactions at electrochemical interfaces are provided, including the extinction spectra, enhanced electric fields and perturbed electron densities.

O 39.5 Tue 11:45 WILL/A317

Insights into the Structure and Dynamics of Co_3O_4–Water Interfaces Using a High-Dimensional Neural Network Potential — •Amir Omranpour[1,2] and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

Co_3O_4 is an important catalyst for the oxygen evolution reaction and for the oxidation of organic molecules in the liquid phase. Therefore, understanding the Co_3O_4–water interface is essential for understanding the mechanistic aspects of those catalytic processes. The interactions at such complex interfaces, including hydrogen-bond fluctuations, hydroxylation, proton transfer, and solvent structuring, are inherently reactive atomistic processes that cannot be fully described by continuum or implicit-solvent models. On the other hand, *ab initio* molecular dynamics with explicit solvent remain restricted to only a few picoseconds and a few hundred atoms. In this work, we overcome these limitations by training a high-dimensional neural network potential (HDNNP) on density functional theory data, which enables us to greatly extend the accessible time and length scales. Using this HDNNP, we carry out simulations that uncover the structure, dynamics, and reactivity of Co_3O_4–water interfaces in detail. Our simulations show that different surface terminations give rise to significantly different hydration structures. They also reveal how each termination templates the interfacial water network, affects hydroxylation, and determines the degree of structural ordering at the interface.

Invited Talk O 39.6 Tue 12:00 WILL/A317

First-principles modelling of electrochemical interfaces — •Axel Gross — Institute of Theoretical Chemistry, Ulm University, 89069 Ulm

Electrochemical processes occur at the interface between an electron conductor, the electrode, and an ion conductor, the electrolyte. From an atomistic point of view, the liquid nature of electrolytes requires appropriate statistical averages which can be numerically rather demanding. Still it has become possible to model these interfaces using using first-principles quantum chemical methods [1,2]. In this talk I will present which insights can be gained from such studies, but I will also identify limititations of this approach and discuss how they can be overcome, contrasting the cases of solvated cations and anions [3, 4] as one example.

[1] A. Groß and S. Sakong, Chem. Rev. **122**, 10746 (2022).
[2] A. Groß, Curr. Opin. Electrochem. **40**, 101345 (2023).
[3] F. Gossenberger, F. Juarez, A. Groß, Front. Chem. **8**, 634 (2020).
[4] F. Dominguez-Flores, A. Groß, W. Schmickler, J. Phys. Chem. C **129**, 9179 (2025).

O 40: Ultrafast electron dynamics at surface and interfaces – Poster (joint session O/TT)

Time: Tuesday 14:00–16:00 Location: P2

O 40.1 Tue 14:00 P2

Nonequilibrium phonon dynamics after laser-excitation — Tobias Held, Christopher Seibel, Markus Uehlein, •Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau

Electron-phonon coupling is a fundamental process governing the energy relaxation dynamics of solids excited by ultrafast laser pulses. While this coupling is often described in terms of an effective electron temperature, recent works have highlighted the important roles of both nonequilibrium electronic distributions and detailed phononic properties.

In this study, we investigate how nonequilibrium electron occupations, phonon stiffness, and wavenumber-resolved coupling collectively shape the energy exchange between electrons and the lattice in metals. We find that deviations from thermal electronic distributions can substantially modify the coupling parameter, challenging the conventional assumption that electron temperature alone determines the coupling strength. We further identify a roughly quadratic scaling of the coupling parameter with phonon stiffness, with high-wavenumber phonon modes consistently dominating the interaction. Finally, we demonstrate that this preferential coupling leads to the emergence of hot phonons near the Brillouin-zone boundary, which in turn induces a collapse of the overall energy transfer rate and significantly delays electron-phonon equilibration.

O 40.2 Tue 14:00 P2

Comparing temperature change during light-matter interaction of thermal and athermal electron systems — •Fabio A. Müller, Tobias Held, Christopher Seibel, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau

When an ultrashort laser pulse irradiates a metal, the electronic system initially absorbs energy and is driven far from equilibrium. This transient nonequilibrium distribution modifies the light-matter interaction, in part through changes in Pauli blocking, while electron-electron scattering concurrently drives the system toward a hot Fermi-Dirac distribution. Consequently, ultrashort laser pulses of the same fluence but different duration lead to different absorption, even in the linear regime.

Here, we investigate how the capability of an electron ensemble to absorb photons depends on its instantaneous energy distribution. Specifically, we compare the absorption arising from nonequilibrium electron distributions with that of Fermi-Dirac distributions carrying the same energy density. Our results show that, for realistic materials, the relative absorption is highly sensitive to the photon energy, a behavior that can be traced back to distinct features in the electronic density of states.

O 40.3 Tue 14:00 P2

Role of non-thermal electrons on energy dissipation and phase transition in laser excited metals — •Lukas Jonda, Tobias Held, Markus Uehlein, Christopher Seibel, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics andResearch Center OPTIMAS, RPTU Kaiserslautern-Landau

The influence of non-equilibrium electrons on energy dissipation and phase transitions is not well understood. It is known that during femtosecond laser irradiation of a surface, electrons are excited to a state of non-equilibrium in space and energy. These highly excited electrons then transport energy ballistically into the bulk. On a picosecond timescale, electrons transfer energy to the lattice via electron-phonon collisions. If the transferred energy is large enough to reach the melting point, the crystal lattice can undergo a phase transition.

We developed a hybrid model that combines a kinetic Monte Carlo simulation and a two-temperature model. The latter describes diffusive transport as well as electron-phonon equilibration, and the former describes primary electron excitation by the laser pulse, transport of non-equilibrium electrons, and secondary electron generation.

We present results for gold, where the influence of non-equilibrium electrons on energy transport is expected to be significant, due to the long mean free path of its electrons. Finally, we are interested in the influence of non-equilibrium electrons on the melting process.

O 40.4 Tue 14:00 P2

Capturing thermalization through electron-electron scattering with machine learning — •David L. Kaiser, Tobias Held, Christopher Seibel, Markus Uehlein, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau

Ultrafast excitation of metals by optical laser pulses induces nonequilibrium energy distributions in the electron system. This nonequilibrium gives rise to complex electron-electron scattering processes, which typically restore a Fermi-Dirac distribution on a femtosecond timescale. Accurately modelling the thermalization requires evaluating the full electron-electron collision integral, which is however computationally costly.

In this study, we explore the possibility to use machine learning to emulate the dynamics generated by the full collision integral. Our goal is to significantly accelerate these calculations, enabling efficient simulations of bulk and multilayer systems. This approach opens the door to uncovering new relaxation pathways and predicting the response of complex material systems to ultrafast excitation.

O 40.5 Tue 14:00 P2

Studies of laser ablation of band-gap materials — •Markus Bonifer[1,2], Sebastian T. Weber[1], Nils Cremer[2,3], Gabriel Schaumann[2,3], and Baerbel Rethfeld[1] — [1]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, Germany — [2]Focused Energy GmbH, Im Tiefen See 45, 64293, Darmstadt, Hessen, Germany — [3]Institute of nuclear physics (IKP), Technische Universität Darmstadt, Darmstadt, Germany

We aim to explore laser ablation as a possible approach for creating clean, well-defined microholes in polymers used for laser fusion targets where symmetry and control of surface roughness are important. Because polymers differ widely in their properties, general insights into laser material interaction are sought through modeling of density-dependent excitation in band-gap materials.

The theoretical models used are based on the density-dependent two-temperature model (nTTM) and extended multiple rate equations (EMRE). These calculations are intended to guide experimental studies carried out in collaboration with Focused Energy to identify suitable processing conditions and improve overall feature quality.

O 40.6 Tue 14:00 P2

Thermalization of optically excited electrons in metals: electron-electron scattering dynamics — •Stephanie Roden, Christopher Seibel, Tobias Held, Markus Uehlein, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau

When a metal is irradiated with a short-pulsed optical laser, the electron distribution is disturbed into a state far from equilibrium. On a femtosecond timescale, the non-thermal electrons thermalize by collisions with each other, which drives the electrons towards a hot Fermi distribution.

In this work, we present a derivation of the full electron-electron Boltzmann collision integral within the random-$\boldsymbol{k}$ approximation. Building on this approach, we trace the temporal evolution of the electron energy distribution in metals after ultrafast excitation. Furthermore, we examine to which extent the resulting dynamics can be captured by the numerically simpler relaxation time approach, applying a constant and an energy-dependent relaxation time derived from Fermi-liquid theory.

We find a better agreement with the latter, while specific features caused by the balance of scattering and reoccupation can only be captured with a full collision integral.

O 40.7 Tue 14:00 P2

Time-resolved PEEM and μARPES using a 100 kHz ToF momentum microscope — •Isabella Alexandra Hofmeister[1,2], Michael Herb[1,2], Maria Federl[1], Franz Seitz[1], and Isabella Gierz[1,2] — [1]University of Regensburg, Regensburg, Germany — [2]Regensburg Center for Ultrafast Nanoscopy - RUN, Regensburg, Germany

Momentum microscopy provides energy-resolved imaging in real and reciprocal space with < 100 meV resolution, combining PEEM (Δx < 40 nm lateral resolution) and μARPES (Δk < 0.02 Å^{-1}) capabilities. We implemented an ultrafast setup with a time-of-flight momentum microscope and a 100 kHz laser system delivering 6 eV probe pulses and pump pulses tunable from the mid-infrared to visible range. Procedures for converting time-of-flight to kinetic energy and for establishing spatial and temporal pump-probe overlap are discussed. Proof-of-principle time-resolved PEEM and μARPES experiments on the topological insulator Bi_2Se_3 demonstrate femtosecond-resolved carrier dynamics with high spatial and momentum precision.

O 40.8 Tue 14:00 P2

First steps with a qPlus-based MIR AFM — •Furkan Özyigit, Lukas Böhm, Leonie Weiss, Jay Weymouth, Rupert Huber, and Franz Giessibl — University of Regensburg, 93053 Regensburg

We report initial progress in an ultrafast non-contact atomic force microscope/scanning tunneling microscope (NC-AFM/STM) platform based on qPlus sensors, integrated with a CEP-stabilized mid-infrared (MIR) pump-probe system and tunable optical parametric amplifier (OPA) for versatile excitation. In first experiments, we successfully induced transient tunneling currents on Cu(111) using MIR pulses, demonstrating precise control of ultrafast electronic excitation at the atomic scale via laser-coupled tunneling. While the tunneling cur- rent reflects the ultrafast electronic excitation dynamics, the qPlus sensor permits complementary force detection to monitor subsequent structural or electrostatic interaction changes, such as those resulting from induced charge redistribution or lattice relaxation. This enables simultaneous probing of electronic and mechanical dynamics with fem- tosecond time and sub-nanometer spatial resolution. Beyond investi- gations of transient electrostatic forces, this versatile system facilitates a broad class of ultrafast nanoscale experiments, including scattering- type scanning near-field optical microscopy (s-SNOM) for imaging car- rier and phase dynamics, time-resolved tip-enhanced spectroscopy for molecular states, and pump-probe tunneling spectroscopy.

O 40.9 Tue 14:00 P2

Image potential states of oxide quasicrytals — •Barbara Drobinski[1], Friederike Wührl[1], Richard Kraska[1], Konrad Gillmeister[1], Stefan Förster[1], Cheng-Tien Chiang[2], and Wolf Widdra[1] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany — [2]Institute of Atomic and Molecular Sciences , Academia Sinica, Taipeh, Taiwan

Quasicrystals are aperiodically ordered materials that lack translational symmetry. Their aperiodic potentials give rise to an infinitely dense set of Fourier components, which can induce gaps and mini-gaps in the electronic band structure. Here, we investigate this phenomenon for nearly free-electron-like image-potential surface states, where electrons propagate in front of the surface while experiencing the aperiodic potential. Using momentum-resolved two-photon photoemission, we determine both the electronic dispersion and relaxation dynamics of oxide quasicrystals (OQCs) based on Ba-Ti-O/Pt(111) [1] and Eu-Ti-O/Pt(111). The latter is obtained via Eu decoration of a Ti_2O_3 honeycomb precursor [2]. In both systems, we observe n=1 and n=2 image potential states, located 340 meV (360 meV) and 150 meV (190 meV) below the vacuum level for Ba-Ti-O (Eu-Ti-O), respectively. The states exhibit parabolic dispersions without apparent gap openings. We discuss the momentum-dependent electron lifetimes in the context of possible mini-gaps in the underlying aperiodic potential.

[1] S. Förster *et al.*, Nature **502**, 215 (2013)
[2] M. Haller *et al.*, http://arxiv.org/abs/2510.11426

O 40.10 Tue 14:00 P2

Ultrafast Electron Diffraction Study of Lattice Dynamics in Elemental Chromium — •Justus Richter[1,2], Victoria Taylor[1], Hyein Jung[1,2], Ralph Ernstofer[1,2], and Yoav William Windsor[1,2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Institut für Physik und Astronomie, Technische Universität Berlin

Femtosecond electron diffraction (FED) allows to quantitively study ultrafast atomic motion. Here we use FED to study photoinduced atomic motion in Cr. We saw that measurements taken above- and below T_N exhibit qualitatively different responses from the lattice, hinting to the effect of the spin-induced periodic lattice distortion within the antiferromagnetic Cr phase, though further investigation is required. A two temperature model (TTM) was used to model the energy flow between the electronic and lattice subsystems by which we extract an estimate for the electron-phonon coupling constant $G_{ep} = (4.8 \pm 0.6) \times 10^{17}$ Jm^{-3}K^{-1}, which fits into the wide range of values reported in literature. Finally, we measured Cr side-by-side with Pt and demonstrate qualitative differences in their temporal responses, including a significantly faster thermalization of the Cr lattice and differences in the shape of their temporal response.

O 40.11 Tue 14:00 P2

Ultrafast electron dynamics in the valence-fluctuating intermetallic $EuIr_2Si_2$ — •Abeer Arora[1], Túlio de Castro[1], Amine Wahada[1], Lawson Lloyd[1], Tommaso Pincelli[2], Kristin Kliemt[3], Cornelius Krellner[3], Denis V. Vyalikh[4,5], Yoav Will Windsor[2], Martin Wolf[1], Ralph Ernstorfer[1,2], and Laurenz Rettig[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Institut für Physik und Astronomie, TU Berlin, Germany — [3]Physikalisches Institut, Göthe-Universität Frankfurt, Germany — [4]Donostia International Physics Center, San Sebastián, Spain — [5]Ikerbasque, Basque Foundation for Science, Bilbao, Spain

$EuIr_2Si_2$ is a valence-fluctuating intermetallic compound that, despite its non-magnetic bulk, develops 2D ferromagnetic order below 48 K in the topmost Eu

layer due to a stable Eu^{2+} configuration. Its heavy Ir ions generate strong Rashba spin-orbit coupling, which interacts with magnetic exchange and influences the surface electronic states. Probing the non-equilibrium dynamics of the 2D electrons in the Si-Ir-Si surface layer offers a direct way to study the coupling of the spin-orbit and surface magnetic interaction. Using femtosecond XUV time- and angle-resolved photoemission spectroscopy, we investigate how the surface states evolve following photoexcitation with a 1.55 eV pulsed laser. Our preliminary results show an ultrafast quenching of the surface-state splitting, which we discuss in terms of demagnetization of the Eu 4f moments and modified spin-orbit coupling.

O 40.12 Tue 14:00 P2

Ultrafast STEM locked to GHz sample excitation — •Andreas Wendeln[1], Alexander Schröder[1], Sakal Singla[1], and Sascha Schäfer[1,2] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Regensburg Center for Ultrafast Nanoscopy (RUN), Regensburg, Germany

Ultrafast transmission electron microscopy (UTEM) has been an established method for investigating nanoscale dynamics for several years, combining the nanometer spatial resolution of TEM with the femtosecond temporal resolution of a pump-probe approach. In recent years, there have been numerous advances in the development of new femtosecond electron sources, such as laser-driven Schottky [1] or cold-field emitters [2]. A combination of these sources with advanced electron optical elements, such as a probe aberration corrector, is expected to deliver even smaller electron spot sizes and to increase the available pulsed current but was not yet demonstrated. Here, we present a measurement scheme for ultrafast STEM with a focus on magnetic imaging, utilizing an aberration corrector and a laser-driven cold-field emitter. In initial measurements using a continuous photoelectron beam, the measurement method is characterized regarding experimental parameters, such as probe currents, focal spot sizes, and stability. Subsequently, we report the locking of femtosecond electron pulse train at repetition rates between 100 kHz up to 80 MHz to GHz radiofrequency currents which we aim to employ for DPC and ptychography imaging schemes of current-driven magnetic dynamics. [1] Feist et al., Ultramicroscopy, 2017. [2] Schröder et al., Ultramicroscopy, 2025.

O 40.13 Tue 14:00 P2

Probing Ultrafast Structural Dynamics in Multilayer Graphene Using ULEEM — •Simon Briesenick[1,2,4], Johannes Otto[1,2,4], Leon Brauns[1,2], Philip Schädlich[3], and Claus Ropers[1,2] — [1]Department of Ultrafast Dynamics, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Göttingen, Germany — [3]Institute of Physics, TU Chemnitz, Chemnitz, Germany — [4]authors contributed equally

Multilayers of graphene (MLG) exhibit electronic and structural properties that vary strongly with, e.g., layer number and stacking order, making MLG a suitable model platform for studying ultrafast phenomena in two-dimensional materials [1]. We investigate the behavior of MLG after excitation with ultrashort light pulses using our newly developed ultrafast low-energy electron microscope (ULEEM) [2]. The instrument allows for the investigation of surface structural dynamics with sub-picosecond and nanometer spatial resolution, utilizing low-energy ($\leq$ 100 eV) ultrashort probe electron pulses. We present first data on the light-induced Debye-Waller effect in MLG, demonstrating the potential of ULEEM studies for resolving ultrafast structural behavior in MLG.

[1] K. V. Emtsev, et al. Phys Rev B. 77, 155303 (2008) [2] J. Otto et al. (in preparation)

O 40.14 Tue 14:00 P2

Hot-electron dynamics in moiré structures studied with resonant scanning tunneling spectroscopy — •Martin Lülff, Marta Przychodnia, Maciej Bazarnik, and Anika Schlenhoff — Institute of Physics, University of Münster, Germany

To study hot-electron dynamics in Gr-metal heterostructures, image-potential states (IPSs) serve as ideal model system. While their energies are known to be highly sensitive to the respective Gr-metal distance variation within the moiré unit cell [1, 2], recent two-photon photoemission experiments suggest moiré-site dependent lifetimes [3].

Here, utilizing the high spatial resolution of resonant scanning tunneling microscopy (STM) and spectroscopy (STS) we study the moiré-site dependent IPSs' lifetimes for highly corrugated Gr/Fe/Ir(111) and Gr/Ir(111), respectively. Comparing these resonant STS data with those recorded on bare Fe/Ir(111) and Ir(111), respectively, enables the influence of the varying Gr-metal distance on the lifetimes to be distinguished from that of the underlying metal substrate. We analyse the IPSs' lifetimes for a Stark shift in their energies by applying various electric field strengths in current-dependent STS series, and discuss the results in terms of their resulting energetic positions with respect to the underlying unoccupied electronic band structure. Our work contributes to an in-depth understanding of electron transfer processes at Gr-metal interfaces.

[1] M. Bazarnik and A. Schlenhoff, ACS Nano **19**, 25812 (2025)
[2] N. Armbrust *et al.*, New J. Phys. **17**, 103043 (2015)
[3] N. Armbrust *et al.*, Phys. Rev. Lett. **108**, 056801 (2012)

O 40.15 Tue 14:00 P2

Photo-induced electron pressure drives THz phonon in Platinum-Copper superlattice — •Jan-Etienne Pudell[1], Maximilian Mattern[2,3], Marc Herzog[2], Alexander von Reppert[2], Daniel Schick[3], Chandan Singh[4], Peter M. Oppeneer[4], Michel Hehn[5], Ulrike Boesenberg[1], Angel Rodriguez-Fernandez[1], Roman Shayduk[1], Wonhyuk Jo[1], Johannes Möller[1], Jörg Hallmann[1], James Wrigley[1], Matias Bargheer[2,6], and Anders Madsen[1] — [1]European XFEL — [2]University Potsdam — [3]MBI, Berlin — [4]Uppsala University — [5]IJL, Université Lorraine — [6]HZB Berlin

Using ultrafast X-ray diffraction (UXRD) at the MID end-station at the European XFEL, we investigate the ultrafast lattice dynamics of metal-metal superlattice (SL) with few atomic layers of Pt and Cu upon femtosecond photoexcitation. Our results reveal that the absorbed optical energy is rapidly localizes within the Pt layers, driving the excitation of a coherent artificial THz phonon mode defined by the superlattice period. The signal's amplitude and phase modulation of the SL Bragg peaks induced by the lattice excitation i.e. the artificial THz phonon, are predominantly driven by electron pressure within the first picosecond. This response is faster than the Debye-Waller effect, which is limited by the electron-phonon coupling time.

O 40.16 Tue 14:00 P2

Experimental realization of an interferometric XUV-trARPES experiment with phase-stabilized IR pulses — •Antonius Naujok[1], Gregor Zinke[1,2], Franz Spartz[1], Sebastian Hedwig[1], Tobias Eul[2], Martin Aeschlimann[1], and Benjamin Stadtmüller[2] — [1]Department of Physics and Re search Center OPTIMAS, RPTU University Kaiserslautern- Landau, 67663 Kaiserslautern, Germany — [2]Experimental Physics II, Institute for Physics, University of Augsburg, 86159 Augsburg

Layered 2D van der Waals materials, such as TMDCs, have been extensively studied for their optical properties and coherent responses. However, exploring coherent excitations and dephasing processes in such materials using time-resolved ARPES is challenging because the key points of the materials' band structure cannot be accessed using phase-stabilized pulses in the visible regime, as has been done in most experiments thus far [1]. To overcome this limitation, we introduce a modified version of coherent multidimensional spectroscopy. This new method is based on time-resolved ARPES and utilizes a pair of phase-stabilized femtosecond infrared (fs-IR) pulses in combination with femtosecond XUV pulses for photoionization. We demonstrate the feasibility of our approach by focusing on the A-exciton excitation and the subsequent carrier dynamics in WSe_2. Through temporal Fourier-analysis of the entire ARPES spectrum, we're able to resolve distinct frequency components within characteristic features of the WSe_2 electronic band structure. [1] M. Aeschlimann et al., Phys. Rev. B. 105, 205415 (2022)

O 40.17 Tue 14:00 P2

Implementation of white light continuum probing for pump-probe spectroscopy — •Joris Wicker, Tim Titze, Maximilian Staabs, Jacob Kutzner, Stefan Mathias, and Daniel Steil — University of Göttingen, 1. Institute of Physics, Göttingen, Germany

We integrated a white-light continuum (WLC) probe together with a prism spectrometer in a conventional two-color femtosecond pump-probe setup. Further, we developed a custom measurement program using Microsoft's .NET Framework and Python, enabling instrument control, automated measurement sequences, and preliminary data analysis. To test the modified setup and software, we investigated the transient evolution of the reflectivity in metallic thin film systems and perovskite oxides using 1030 nm pumping. Spectrally and temporally resolved reflectivity variations were observed, confirming the proper functionality of the system. Furthermore, the stability of the WLC source was characterized. Possible future improvements include integrating a Wollaston prism to enable spectrally and time-resolved magneto-optical Kerr effect (MOKE) measurements.

O 40.18 Tue 14:00 P2

Investigation of the light-dressed bandstructure of graphene — •Lina Segerer[1], Marco Merboldt[1], Mattis Langendorf[1], Paul Werner[1], Jan Philipp Bange[1], Junde Liu[1], Wiebke Bennecke[1], Marcel Reutzel[2], and Stefan Mathias[1] — [1]Georg-August-Universität Göttingen, I. Physikalisches Institut, Germany — [2]Philipps-Universität Marburg, Germany

Time-periodic driving of solids with strong laser fields enables optical control of material properties. Photon-driven systems not only exhibit replicas of their equilibrium band structure, known as Floquet-Bloch states, but can undergo non-trivial topological phase transitions when excited with circularly polarized light. Recent advances in angle-resolved photoemission spectroscopy (ARPES) have shown that Floquet-Bloch states can be generated in graphene using linear polarized laser pulses [1,2]. However, the oblique incidence angle of the pump pulse so far has limited the realization of a purely circularly polarized light field. In this study, we overcome this challenge by integrating an extra beam path in our ultrafast momentum microscopy (MM) setup enabling backside normal-incidence excitation with linearly and strictly circularly polarized IR

pump pulses. We observe light-induced Floquet-Bloch states and investigate the polarization dependence of Floquet-Volkov interference as well as modifications in the light-dressed band structure of epitaxial graphene.

[1] M. Merboldt *et al.*, Nat. Phys. **21**, 1093 (2025).
[2] D. Choi *et al.*, Nat. Phys. **21**, 1100 (2025).

O 40.19 Tue 14:00 P2

Table-top 3D ultrafast momentum microscopy with a time-preserving EUV-monochromator — •Lennart Weinhagen[1], Wiebke Bennecke[1], Jan Philipp Bange[1], David Schmitt[1], Marco Merboldt[1], Bent van Wingerden[1], Thi Lan Dinh[2], Fabio Frasetto[3], Luca Poletto[3], Marcel Reutzel[1], Daniel Steil[1], D. Russel Luke[2], Stefan Mathias[1], and G.S. Matthijs Jansen[1] — [1]1st Institute of Physics, University of Göttingen, Göttingen, Germany — [2]Institute for Numerical and Applied Mathematics, University of Göttingen, Göttingen, Germany — [3]Institute for Photonics and Nanotechnologies CNR-IFN, Padova, Italy

Photoemission momentum microscopy with tunable probe-photon energy gives unique access to electronic and molecular structures, enabling Fermi-surface imaging, photoemission electron diffraction (PED) and 3D orbital tomography (3D-POT). However, such measurements have largely relied on synchrotron radiation, thus limiting their use in femtosecond-resolved experiments. Here, we present a table-top EUV source with a time-preserving monochromator driven by a 1030 nm femtosecond laser, using an off-plane grating at grazing incidence to reduce spatial chirp. Integrated into our time-resolved momentum microscope [1], it delivers femtosecond, photon-energy-tunable EUV probe pulses. Demonstrated on PTCDA/Ag(110), the setup enabled full 3D reconstruction of the frontier orbitals highlighting the potential of laboratory-scale, energy-selective momentum microscopy [2].

[1] Schmitt *et al.*, Nature 608, 499-503 (2022).
[2] Bennecke *et al.*, arXiv:2502.18269 (2025).

O 40.20 Tue 14:00 P2

Multimode momentum microscopy of cleaved 1T-TaS_2 crystals — •Bent van Wingerden[1], Olena Tkach[2], Hashima Marukara[1], Jan Philipp Bange[1], Wiebke Bennecke[1], Marcel Reutzel[3], Junde Liu[1], Gerd Schönhense[2], and Stefan Mathias[1] — [1]Georg-August-Universität Göttingen, Germany — [2]Johannes Gutenberg-Universität Mainz, Germany — [3]Philipps-Universität Marburg, Germany

Ultrafast momentum microscopy has evolved as one of the most powerful tools to study non-equilibrium electronic structure dynamics of 2D quantum materials [1]. However, the large electric field strength generated by the immersion lens limits its versatility in terms of sample systems. One critical issue is related to vacuum-cleaved van-der-Waals-crystals that often show microscopic protrusions, which are prone to field-induced electron emission and flashovers, both of which can destroy the sample itself as well as the microscope's electronics. In our work, we test the momentum imaging capabilities of a newly designed multi-mode momentum microscope [2,3] in combination with an EUV table-top HHG source. Using vacuum-cleaved bulk crystals of *1T*-TaS_2, we show that operating in modes of reduced electric field strength at the sample position suppresses field emission, while still preserving the field-of-view and imaging quality. We carry out detailed comparisons of different operating modes with the new lens system.

[1] Reutzel, Jansen, Mathias, *Adv. in Phys. X* 9, 2378722 (2024).
[2] Tkach & Schönhense, *Ultramicroscopy* 276, 114167 (2025).
[3] Tkach et al., arXiv:2401.10084 (2024).

O 40.21 Tue 14:00 P2

Towards time-resolved momentum microscopy of plasmon excited quantum materials — •Mattis Langendorf[1], Lina Segerer[1], Paul Werner[1], Marco Merboldt[1], Jonas Pöhls[1], Tobias Meyer[1], Daniel Steil[1], Junde Liu[1], Jan Philipp Bange[1], Wiebke Bennecke[1], G. S. Matthijs Jansen[1], R. Thomas Weitz[1], Marcel Reutzel[2], and Stefan Mathias[1] — [1]Georg-August-Universität Göttingen, Germany — [2]Philipps-Universität Marburg, Germany

For the realization of Floquet*Bloch engineering as well as for the study of formation and propagation of excitons in two-dimensional quantum materials using time- and angle-resolved photoemission spectroscopy (ARPES), a highly localized excitation on a micron scale seems ideal [1]. However, achieving such spatial confinement poses a significant experimental challenge. Surface plasmon polaritons (SPPs) offer a promising solution, as these collective charge-carrier oscillations enable strong electromagnetic field localization and can therefore provide the required tightly focused excitation conditions [2]. In combination with femtosecond momentum microscopy that enables spatiotemporal access to electron and exciton dynamics [3], we investigate the concept of exploiting SPPs as a driving field to excite quantum materials.

[1] Merboldt *et al.*, Nat. Phys. **21**, 1093*1099 (2025).
[2] Dreher *et al.*, Nanophotonics **11**, 3687-3694 (2022).
[3] Reutzel, Jansen, Mathias, Adv. in Phys. X **9**, 2378722 (2024).

O 41: Topology and symmetry protected materials & Topological insulators – Poster (joint session O/TT)

Time: Tuesday 14:00–16:00 Location: P2

O 41.1 Tue 14:00 P2

Manipulation of topological surface states by switchable molecules. — Lukas Staiger[1], Jannis Lessmeister[1], •Ralf Hemm[1], Juliusz Wolny[1], Volker Schünemann[1], Martin Aeschlimann[1], and Benjamin Stadtmüller[2] — [1]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, 67633 Kaiserslautern, Germany — [2]Institute of Physics, University of Augsburg, 86159 Augsburg, Germany

Three-dimensional topological insulators host spin-momentum-locked surface states protected by time-reversal symmetry, giving them potential for spintronic devices. Controlling these states remains challenging but is crucial for opening gaps, shifting the Dirac point and tailoring spin textures for applications. In our work, we utilize a monolayer of the spin-crossover complex $Fe(phen)_2(SCN)_2$ on the topological insulator Bi_2Se_3 to break the time-reversal symmetry of the substrate. Employing angle-resolved photoemission spectroscopy, we trace the evolution of the electronic structure as a function of molecular coverage and temperature. Despite a conspicuous energy shift and modified dispersion, there is no clear evidence for a band gap opening after deposition of a molecular monolayer. Concurrently, additional spectral weight from molecular orbitals emerges, and thermally and optically driven spin-crossover transitions in the $Fe(phen)_2(SCN)_2$ layer induce changes in the Dirac-point energy and spectral weight. Our findings demonstrate that a spin-crossover overlayer can quantitatively alter the dispersion of topological surface states, while allowing them to exist due to strong interactions between molecules and surfaces.

O 41.2 Tue 14:00 P2

Deciphering the complex surface of the topological phase in the polar semiconductor BiTeI — •Adrian Weindl, Christoph Setescak, and Franz J. Giessibl — Faculty of Physics, University of Regensburg, D-93053 Regensburg, Germany

BiTeI is a semiconductor consisting of polar layers that can form Rashba spin-split p-n junctions on its surface due to stacking faults. It has been shown that gentle annealing can transform the surface of BiTeI into a topological insulator with spin-polarized surface modes exhibiting linear dispersion. Previous LEED and RHEED measurements revealed that the surface undergoes a structural change from a non-centrosymmetric triple-layer structure to a quintuple-layer structure. However, the exact surface structure remains elusive. Using scanning tunneling microscopy, atomic force microscopy, and Kelvin probe force spectroscopy we study the surface before and after annealing with atomic resolution. We show that the annealing results in different surface phases that are highly sensitive to the annealing temperature: a chemically homgeneous phase at around 240°C and a inhomogeneous phase with strong charge disorder at 250°C. We determine the termination of each phase and confirm that the surface exhibits the signature of a topological surface state even in the strongly disordered phase.

O 41.3 Tue 14:00 P2

THz-driven nonlinear dynamics studied with high-power THz sources — Atiqa Arshad[1,2], Jan-C Deinert[2], Igor Ilyakov[2], Andreas Gebauer[2], Anjan Kumar N M[1], and •Stefan Kaiser[1] — [1]TU Dresden,Germany — [2]HZDR, Dresden,Germany

THz pump-photoelectron spectroscopy (ARPES) probe is currently being implemented at the THz facility TELBE at Helmholtz-Zentrum Dresden-Rossendorf. This unique combination of high-field terahertz excitation and tr-ARPES probe will enable groundbreaking experiments on solid surfaces and interfaces. To this aim we have set up a high-repetition rate THz source driven by a 180 W laser source yielding > 50 mW THz output power. We report on the THz generation and characterization scheme as well as on first experiments. A highly promising material class to be studied with these light sources is BiTeI, a dual topological insulator that exhibits two different types of surface states on different interfaces. We present our study on the complex nonlinear dynamics, in particular THz harmonic generation in these compounds.

O 41.4 Tue 14:00 P2

The quasi one-dimensional van der Waals material α-Bi_4Br_4 — •Jonathan K. Hofmann[1,2], Serhii Kovalchuk[1,3], Mingqian Zheng[4], Yuqi Zhang[4], Vasily Cherepanov[1], Timofey Balashov[1], Jin-Jian Zhou[4], Zhiwei Wang[4], Yugui Yao[4], Irek Morawski[3], F. Stefan Tautz[1,2], Felix Lüpke[1,5], and Bert Voigtländer[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]Experimentalphysik IV A, RWTH Aachen University, Germany — [3]Institute of Experimental Physics, University of Wrocław, Poland — [4]Key Laboratory of Advanced Optoelectronic Quantum Architecture and Measurement, Beijing Institute of Technology, China — [5]II. Physikalisches Institut, Universität zu Köln, Germany

α-Bi_4Br_4 is a quasi-one-dimensional material: covalently bonded Bi_4Br_4 chains are arranged in parallel, side-by-side and layer-by-layer, with van der Waals gaps in between. Bulk α-Bi_4Br_4 is higher-order topological insulator. At step edges on the (001) surface, quantum spin Hall (QSH) edge states are present. Using a scanning tunneling microscope (STM), we observe a significant shift of the chains, relative to each other, which we attribute to shear stress. Scanning tunneling spectroscopy reveals that the edge states are robust against the strain. Density functional theory confirms that a strained monolayer of Bi_4Br_4 is a QSH insulator with $\mathbb{Z}_2 = 1$. Furthermore, we use a four-tip STM to analyze the electrical transport of α-Bi_4Br_4 *in situ*.

O 42: Electronic structure of surfaces: Spectroscopy, surface states – Poster

Time: Tuesday 14:00–16:00 Location: P2

O 42.1 Tue 14:00 P2

Plasmonic lenses for nano-spectroscopy of Van der Waals materials — •Natalie Lehmann[1], David Huber[2], Daiyu Geng[1], Jiabao Yang[1], Stuart Parkin[1], Wolf Widdra[2], and Niels Schröter[1] — [1]Max Planck Institute of Microstructure Physics, Halle (Saale), DE — [2]Martin-Luther-University Halle-Wittenberg, Halle (Saale), DE

Surface plasmon polaritons excited at the edge of Archimedean spirals carved into a gold (111) surface can be focused to a sub-micrometer spot at the spiral center [1, 2]. We aim to use this nano-focused electric field to spectroscopically investigate 2D materials, which are often only a few micrometers in size. Here we present our measurements on gold/graphene samples. Notably, the plasmonic focus remains intact, and the gold surface is effectively cleaned by the graphene; even without sputtering the gold, its characteristic surface state is observed. Furthermore, the measured k-space spectrum shows replicas of the sp orbitals above the Fermi edge, reflecting the dynamics of an excited electron system. We propose that the laser pulse is pumping the system while the plasmon is probing the excited states. These findings demonstrate the feasibility of ultrafast pumped, nano-focused spectroscopy using a single micrometer-sized laser beam.

O 42.2 Tue 14:00 P2

Hydrogen Plasma Cleaning of Fe_3Sn_2 single crystals for surface-sensitive measurements — •Felix Müller[1], Lu Lyu[1], Lilian Prodan[1], Jannis Lessmeister[2], Tobias Eul[1], Martin Aeschlimann[2], István Kézsmárki[1], and Benjamin Stadtmüller[1] — [1]University of Augsburg — [2]RPTU University Kaiserslautern-Landau

Preparing clean and well-defined surfaces is essential for high-resolution photoemission spectroscopy (PES) and other similarly surface-sensitive studies. Typical preparation methods to realize high-quality surfaces include in situ cleaving under ultrahigh vacuum (UHV) conditions. However, this method cannot be universally applied to all crystal structures. Alternative approaches can rely, for instance, on H_2-based plasma cleaning using H_2 sources integrated into a UHV system. Here, we investigate the effectiveness of this method in preparing Fe_3Sn_2 surfaces for spectroscopy and discuss its potential as a general cleaning technique for other topological bulk materials.

We show that the hydrogen plasma efficiently removes common surface contaminants, particularly oxygen and carbon, while preserving the intrinsic surface structure. This enables the observation of sharp spectroscopic features over the whole energy range and significantly enhances the signal quality of subsequent PES measurements. Our results show that plasma can be a simple and reproducible method for achieving contamination-free surfaces of topological bulk materials for surface-sensitive spectroscopy applications.

O 42.3 Tue 14:00 P2

WTe2: a Cool Look at 330 mK — •Rian A.M. Ligthart, Kevin Hauser, Alexander LaFleur, Gleb Neplyakh, and Fabian D. Natterer — Department of Physics, University of Zurich, Winterthurerstrasse 190, CH-8057 Zurich, Switzerland

As silicon-based electronics reach their size limit, two-dimensional (2D) materials, particularly Transition Metal Dichalcogenides (TMDs), emerge as promising alternatives to enhance efficiency at the same length scale. Among them, WTe2 stands out due to its unique properties including topological states, Weyl semimetal character and graphene-like high electron mobility.

We investigate cleaved bulk WTe2 using a Scanning Tunneling Microscope at 330 mK. With scanning tunneling spectroscopy, the electronic properties and their dependence on vector magnetic fields are studied on the surface of bulk WTe*, as well as at step edges and twin domain boundaries. We scrutinize the topological nature of the edge states and observe a reduced density of states around zero bias in bulk WTe2.

O 42.4 Tue 14:00 P2

Chiral-Induced Spin Selectivity in Thia-Bridged Triarylamine Hetero[4]helicenes SAMs: Structural Insights from XPS and NEXAFS — •Yichen Jin[1], Jan Böhnke[1], Lapo Querci[2], Niccolò Giaconi[2], Cornelius Gahl[1], Dominik Stemer[3], Roberta Sessoli[2], Matteo Mannini[2], and Martin Weinelt[1] — [1]Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]University of Florence, Via della Lastruccia 3-13, Sesto Fiorentino 50019, Italy — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Helicene enantiomers act as efficient spin filters when assembled on metallic surfaces, making them promising candidates for organic spintronic applications. Previous magnetic conductive AFM studies reported spin polarizations of up to ~60% through the respective chiral enantiomers of Thia-Bridged Triarylamine Hetero[4]helicenes (HelSAc) self-assembled monolayers (SAMs) ascribed to the chirality-induced spin selectivity (CISS) effect. To understand the structural origins underlying this behavior, we investigated HelSAc SAMs on Au(111) using XPS and NEXAFS. Angle-dependent XP spectra of sulphur 2p reveal three chemically distinct components assigned to S*C, S*Au, and atomic sulfur. NEXAFS shows pronounced polarization dependences of the σ^* and π^* resonances, demonstrating the parallel alignment of the HelSAc to the Au surface. Together, these results establish a well-defined chemical and structural picture of HelSAc SAMs, providing the essential foundation for interpreting spin-dependent photoelectron spectroscopy and understanding the CISS effect in this chiral system.

O 42.5 Tue 14:00 P2

Structure and Electronic Properties of (Bi, Pb) Atom Layer Structures studied by ARPES and STM — •Lars Konermann[1], Wen Si[2], Hiroko Abe[1], Masaki Imamura[3], Masahiro Haze[2], Kazutoshi Takahashi[3], Yukio Hasegawa[2], and Akari Takayama[1,4] — [1]Waseda Univ., Shinjuku, Japan — [2]ISSP, Univ. of Tokyo, Kashiwa, Japan — [3]SL Center, Saga Univ., Tosu, Japan — [4]IMRAM, Tohoku Univ., Sendai, Japan

In Single-atom layer (SAL) structures comprised of heavy elements on semiconductor substrates, spin-split electronic states occur due to strong spin-orbit interactions and the breaking of the spatial inversion symmetry, known as the Rashba effect. For (Bi, Pb) on Si or Ge, spin-splitting electronic bands have been demonstrated both theoretically and experimentally. Furthermore, the possibility of a superconducting transition is anticipated suggesting spin-triplet superconductivity. Albeit, experimental confirmation has not yet been obtained.

We investigated the atomic and electronic structures of (Bi, Pb)/Si(111) and Ge(111) structures using cryogenic scanning tunneling microscopy (STM) and spectroscopy (STS), as well as angle-resolved photoemission spectroscopy (ARPES) with synchrotron radiation. A series of experiments was conducted to evaluate the sample: observation of the periodic atomic arrangement, determination of the Pb/Bi composition ratio, detailed band dispersion, and investigation of the electronic states at ultra-low temperatures.

In this presentation, we will present these experimental results and discuss the potential for superconductivity with the Rashba effect.

O 42.6 Tue 14:00 P2

Line-Moiré Phases of an Epitaxial Honeycomb Monolayer AgTe/Ag(111) — •Romana Ganser — Exp. Physik VII and Würzburg-Dresden Cluster of Excellence ctd.qmat, Universität Würzburg

Moiré heterostructures offer a versatile platform for engineering electronic band structures by precise control over long-range superlattice potentials that particularly give rise to emergent phenomena [1]. Here, we present angle-resolved photoemission spectroscopy (ARPES) measurements on a highly tunable one-dimensional (1D) epitaxial moiré heterostructure. We show that the electronic structure is strongly altered by the moiré superlattice hosting replica bands and sizable hybridization gaps. From our experimental data, we can trace back to the local, spatially-varying interlayer coupling, shaping the moiré potential. The latter leads to a 1D confinement of the electrons and, interestingly, also gives rise

to Dirac nodal lines, which are robustly protected by the superlattice symmetry.

[1] Balents, L. et al. Nat. Phys. 16, 725-733 (2020).

O 42.7 Tue 14:00 P2

Realization of an Acoustic Kagome lattice — •Louis Müller[1,3], Noah Endres[1,3], Begmuhammet Geldiev[1,3], Simon Widmann[2,3], Maximilian Ünzelmann[1,3], and Friedrich Reinert[1,3] — [1]Exp. Physik VII, JMU Würzburg, Germany — [2]Technische Physik, JMU Würzburg, Germany — [3]Würzburg-Dresden Cluster of Excellence ctd.qmat

Hosting Dirac cones, flat bands, and saddle points in their band structure, Kagome materials have recently attracted great attention. We realize an acoustic Kagome lattice using 3D-printed resonators, enabling direct measurement of amplitude and phase to reconstruct wave functions and extract the band structure. Our experiment resolves the flat band, identifies the sublattice character of the van-Hove singularities, and clearly reproduces the Dirac cones in good agreement with tight-binding calculations. This platform provides a highly flexible and intuitive way to investigate lattice-driven effects that are difficult to isolate in electronic Kagome systems. Finally, we compare this data to angle-resolved photoemission spectroscopy measurements on a prototypical Kagome superconductor.

O 42.8 Tue 14:00 P2

Excitation of spin-polarized electrons by Deep-UV Pulses with Orbital Angular Momentum from Au(111) and Cu(111) — •Ruwen Quenter, Paul valerian Möllers, and Helmut Zacharias — Center for Soft Nanoscience (SoN), University of Münster, Busso-Peus-Str. 10, 48149 Münster, Germany

Photoemission can, depending on the substrate and the circularly polarization of the light, result in a longitudinal spin polarisation of the excited electrons. The angular momentum of the light influences the final state determined by the selection rules in a way that corresponds to a specific total angular momentum. Spin-orbit interactions cause an energetical separation of states with different total angular momenta, resulting in a spin imbalance of the excited electrons. This can be measured by e.g. Mott scattering. Orbital angular momentum light has a helical wavefront that carries its orbital angular momentum as a degree of freedom wich may have an influence on the electron orbital angular momentum in the electron excitation process. Spin-resolved photoemission measurements could determine if this influence could result in a changed photoelectron spin polarization. We present preliminary results from measurements on Au(111) and Cu(111).

O 42.9 Tue 14:00 P2

Wavefunction confinement of deeply buried As δ-layers in Si(001) measured with hard and soft X-ray angle-resolved photoemission spectroscopy — •Emily C. McFarlane[1], Enrico G. Della Valle[2], Procopios C. Constantinou[2], Taylor J. Z. Stock[3], Kieran Spruce[3], Christoph Schlueter[4], Sergii Chernov[4], Thiago R. F. Peixoto[4], Moritz Hoesch[4], Gerd Schönhense[5], Hans-Joachim Elmers[5], Vladimir N. Strocov[2], Neil J. Curson[3], Steven R. Schofield[3], and Niels B. M. Schröter[1] — [1]Max Planck Institute of Microstructure Physics, Halle (Saale), DE — [2]Paul Scherrer Institute, Villigen PSI, CH — [3]London Centre for Nanotechnology, University College London, London, UK — [4]Deutsches Elektronen-Synchrotron (DESY), Hamburg, DE — [5]Johannes Gutenberg University, Mainz, DE

Vertically confined regions of high concentration dopants in silicon, so-called "δ-layers", are potential building blocks of future quantum devices. A momentum-resolved understanding of the wavefunction confinement of the electrons in such systems is required for their future development, which so far has been limited to shallow samples. Here we present both hard and soft X-ray photoelectron spectroscopy studies of shallow (~3nm) and deeper (~7nm) buried As δ-layers measured with a momentum microscope and hemisphere at PETRA-III and the SLS. We find that the deeper buried sample has smaller electron confinement than the shallower δ-layer, and different quantum well states are located at different depths of the sample. In contrast, in shallow δ-layers all quantum well states are located near the surface.

O 43: Scanning probe microscopy: light matter interaction at atomic scales – Poster

Time: Tuesday 14:00–16:00 Location: P2

O 43.1 Tue 14:00 P2

Modelling the near-field enhancement for tip-enhanced photoluminescence on non-conductive layers — •Jinhui Guo and Laerte Patera — Department of Physical Chemistry, University of Innsbruck, 6020 Innsbruck, Austria

While scanning tunnelling microscopy (STM)-based tip-enhanced photoluminescence (TEPL) has been demonstrated for molecules adsorbed on 2-3 monolayers (ML) of NaCl/Ag(111) [1], nonradiative quenching due to charge tunnelling through the insulating layer is expected to affect the exciton lifetime. Employing sufficiently thick insulating layers (> 14 ML) strongly suppresses electron tunnelling [2], potentially preserving the photoexcited state. However, such thick insulating layers are incompatible with STM operation, making atomic force microscopy (AFM) an ideal choice. To elucidate the field enhancement in AFM-based TEPL experiments, we performed three-dimensional finite element method (3D-FEM) simulations [3] for various AFM Cu tip geometries and Cu substrates with and without NaCl layers up to 20 ML. Our results indicate that below the tip, a pronounced electric field enhancement in the plane parallel to the sample surface ($E_{/\!/}$) persists even on a 20 ML-thick NaCl layer. This effect arises mainly from the reduced screening of $E_{/\!/}$ within the NaCl layers compared to the metallic Cu substrate. These findings support the exploitation of non-conductive layers for TEPL experiments.

[1] J. Doležal *et al.*, *Nano Lett.* 2024, 24, 1629-1634. [2] W. Steurer *et al.*, *Nat. Commun.* 2015, 6, 8353. [3] COMSOL Multiphysics® v. 6.3. www.comsol.com. COMSOL AB, Stockholm, Sweden.

O 43.2 Tue 14:00 P2

Sub-nanoscale photochemistry without plasmons: Debromination of dibromoterphenyl on Au(111) — Hao Jiang[1,2], Youngwook Park[1], Adnan Hammud[1], Martin Wolf[1], Qiang Sun[2], and •Akitoshi Shiotari[1] — [1]Fritz Haber Institute of the Max Plank Society, Berlin, Germany — [2]Materials Genome Institute, Shanghai University, Shanghai, China

Local control of light-induced reactions is a crucial process for developing molecule-based optodevices and designing photocatalysis. Nanometer- and angstrom-scale photoreaction controls have been demonstrated using scanning tunneling microscopy (STM) combined with laser irradiation [1,2]; however, so far they rely on localized surface plasmon resonance (LSPR) using plasmonic metal tips. Here we report a novel light-assisted reaction that can be induced locally without LSPR. Using laser-coupled low-temperature STM, we observed 4,4"-dibromo-p-terphenyl (DBTP) on Au(111), which is a representative system undergoing Ullmann coupling by heat or far-field illadiation [3,4]. By tuning both the bias voltage at the STM junction and the wavelength of the incident visible laser, the debromination of DBTP is induced at the sub-nanometer scale using non-plasmonic tips. This research opens up the prospect of performing the single-molecule photochemistry for various non-plasmonic systems.

[1] E. Kazuma et al., Prog. Surf. Sci. 93, 163 (2018). [2] Y. Park et al., Nat. Commun. 15, 6709 (2024). [3] H. Jiang et al., ACS Nano 18, 1118 (2024). [4] H. Jiang et al., Nano Lett. 25, 9597 (2025).

O 43.3 Tue 14:00 P2

Photoisomerization of azobenzene derivatives on Au (111) using various photon energies and polarizations — •Haraprasad Mandal[1], Paul Schöngrundner[1], Stefan Hecht[2], and Leonhard Grill[1] — [1]Department of Chemistry, University of Graz, Austria — [2]Department of Chemistry, Humboldt-Universität zu Berlin, Germany

Azobenzene derivatives continue to serve as model systems for studying photoisomerization at surfaces. Among them, tetra-tert-butyl azobenzene (TBA) is particularly suitable due to its chemical stability, large steric groups, and well-defined trans and cis configurations that can easily be identified in scanning tunnelling microscopy (STM) images. In this work, we systematically studied the photon-energy- and polarization-dependent trans-to-cis isomerization of TBA, using a tunable femtosecond laser in combination with STM (working in ultra-high vacuum and at low temperatures). Illumination is done through an optical port, and STM imaging is used to identify the configuration of individual molecules before and after laser exposure. The switching efficiency was then studied for a variety of wavelengths in the range between 350 nm and 800 nm as well as different (s/p) polarization directions of the incoming light. Our results provide direct insight into the parameters that steer TBA photoisomerization on Au(111) and demonstrate the capability of our laser STM platform for controlled photochemical studies of single molecules.

O 43.4 Tue 14:00 P2

Focal phase evolution of single-cycle THz near-field pulses in a scanning tunneling microscope — •Andrea Rossetti, Vivien Sleziona, Alkisti Vaitsi, Luis Enrique Parra Lopez, Martin Wolf, and Melanie Müller — 1Department of Physical Chemistry, Fritz Haber Institute, 14195 Berlin, Germany

Lightwave scanning tunneling microscopy (LW-STM) employs single-cycle THz pulses as femtosecond bias, enabling imaging at sub-nanometer spatial and sub-picosecond temporal resolution. Control over the polarity and carrier-envelope phase (CEP) of such THz voltage transients is thereby crucial in determining which electronic states contribute to the ultrafast tunneling current. A simple approach for continuous CEP control of the single-cycle THz transients in LW-

STM is via the Gouy phase. In this work, using a spintronic THz emitter, we use photoemission sampling from the point-like apex of the STM tip to monitor the local CEP of the tip-enhanced THz pulses along the focal axis of a focused THz beam. We find that the CEP exhibits a non-trivial evolution through the focus that strongly deviates from the expected Gouy phase shift for a monochromatic beam. Using analytical models and numerical calculations, we discuss the influence of the broad bandwidth of the THz pulses as well as their coupling to the STM tip for the local CEP in LW-STM.

O 43.5 Tue 14:00 P2

Development of Cryogenic Photoinduced Force Microscopy: Introduction and Progression — •Shuxia Chen[1], Claudia Felser[1], Lukas Eng[2], and Fabian Menges[1] — [1]Max Planck Institute for Chemical Physics of Solids — [2]Technische Universität Dresden

Photo-induced Force Microscopy (PiFM) provides access to optical properties at atomic length scales through the detection of near-field optical forces. To date, PiFM experiments have been largely restricted to ambient conditions, with only limited demonstrations in extreme environments such as cryogenic temperatures or high magnetic fields. In this work, we aim to expand PiFM operation to low temperatures and large external magnetic fields. This development opens the door to exploring light matter interactions over an expanded parameter space and in exotic quantum materials.

O 43.6 Tue 14:00 P2

Investigation of atomic defects in quasi-freestanding MoS_2 with THz-STM — •Caroline Firschke, Junyoung Sim, Vibhuti N. Rai, Paul Wiechers, Florian Faaber, Christian Lotze, and Katharina J. Franke — Freie Universität Berlin, Germany

Transition metal dichalcogenides (TMDCs) are an interesting class of materials due to their 2D-like nature and unique band structures. These materials tend to host different types of defects, heavily influencing their optoelectronic properties. THz-driven scanning tunneling microscopy is a unique technique to investigate the nature of these defects on atomic scales with ultrafast time resolution (1).

Here, we grow monolayers of MoS_2 on Au(111) via chemical vapor deposition, which host quasi-freestanding monolayers of MoS_2 with a band gap of around 2.7 eV, the so called "pits" (2). We find structural defects in these pits, which are decoupled from the metal substrate, and show sharp positive ion resonances in the band gap.

These sharp non-linearities of the I-V curve provide favorable conditions for their investigation via THz pulses. We find that these defects show sharp resonances in the light-wave-driven scanning tunneling spectroscopy, which vary depending on the THz field strength, DC bias voltage and tip-sample distance. The THz response of these resonances cannot be modeled with a simple convolution of THz pulses with the static I-V of the junction, suggesting a modulation of the charge state of the defects on ultrafast timescales.

(1) T. L. Cocker et. al. Nature Photon 7, 620-625 (2013)
(2) N. Krane et. al. Nano Letters 2016 16 (8), 5163-5168

O 43.7 Tue 14:00 P2

Photo-switching of azobenzene derivatives on Au(111) — •Matthew J. Timm[1], Robert di Vora[2], Stefan Hecht[3], Birgitta Bernhardt[2], and Leonhard Grill[1] — [1]Institute of Chemistry, University of Graz, Austria — [2]Institute of Experimental Physics, Graz University of Technology, Austria — [3]Department of Chemistry & IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

The light-induced trans-cis isomerization of azobenzene and its derivatives is of great scientific and technological interest as these molecular photo-switches can be used for nano-scale sensing or information storage. Particularly, 3,3',5,5'-tetra-tert-butylazobenzene (mTBA) adsorbed upon Au(111) has seen much interest, being studied at sub-monolayer coverage (around 0.1 ML) by scanning tunneling microscopy (STM) [1,2] and near monolayer (ML) coverage (0.9 ML) by two-photon photoemission [3]. However, missing is a single-molecule level insight into whether photo-switching at low coverage differs from that at higher but still sub-monolayer coverage - does it matter if only small or large areas of the surface are covered? Here, we combine STM with a self-designed computer-vision algorithm to study photoisomerization induced by pulsed laser radiation (λ = 518 nm) at a rather high surface coverage of 0.6 ML. This approach can track the isomerization state of thousands of individual mTBA molecules and enables us to detect subtle variations in switching yields among densely packed, similarly oriented molecules. [1] M. Alemani, et al. JACS 128 (2006) 14446. [2] M. J. Comstock, et al. Phys. Rev. Lett. 99 (2007) 038301. [3] S. Hagen, et al. Chem. Phys. Lett. 444 (2007) 85-90.

O 43.8 Tue 14:00 P2

Sub-10-fs compression of NIR pulses for phase-resolved sampling of MIR lightwave transients — •Justus Hess, Ugaitz Elu, Andrea Rossetti, Martin Wolf, and Melanie Müller — Department of Physical Chemistry, Fritz Haber Institute, 14195 Berlin, Germany

Lightwave scanning tunneling microscopy (LW-STM) employs single-cycle THz pulses as femtosecond bias [1], enabling imaging at sub-nanometer spatial and sub-picosecond temporal resolution. Ultrashort phase-stable mid-infrared (MIR) pulses promise to increase the time resolution in LW-STM. Phase-resolved characterization of the incident and STM tip-enhanced MIR transients requires sampling pulses with a duration of ideally less than 10 fs. For future MIR excitation in our LW-STM, we implement a MIR source and a pulse-compression scheme based on supercontinuum generation in a photonic crystal fiber (PCF) at 2 MHz in our existing LW-STM setup. Near-infrared (NIR) pulses with a duration of ~40 fs at a center wavelength of 1030 nm are spectrally broadened via self-phase modulation in the PCF to a Fourier-limit of 6 fs. Subsequent dispersion control with a transmission-grating compressor yields few-cycle pulses at 30mW average power sufficient for MIR waveform sampling in LW-STM. [1] T. Cocker et al., Nature 539, 263*267 (2016)

O 43.9 Tue 14:00 P2

Excitation of phonons by THz near fields in a quasi-suspended nanoscopic monolayer of MoS2 — •Junyoung Sim, Vibhuti Rai, Caroline Firschke, Christian Lotze, and Katharina J. Franke — Freie Universtiät Berlin, Department of Physics, Arnimallee 14, 14195 Berlin, Germany

Phonons play a central role in describing fundamental physical properties of materials, such as heat capacity and resistivity, and also govern many-body phenomena such as superconductivity and charge-density waves. To resolve ultrafast lattice vibrations at the atomic scale, terahertz scanning tunneling microscopy (THz-STM) has provided important groundworks, where such vibrations are influenced by the presence of atomic-scale defects [1, 2].

In this work, we investigate the phonon dynamics in a monolayer molybdenum disulfide (MoS2) grown on a Au(111) surface. We focus on nanoscopic regions, where the MoS2 layer is suspended and the electronic structure is minimally hybridized with the substrate [3]. We observe an oscillatory behavior in the THz-STM pump-probe spectra on these suspended regions, which we assign to a coherent vibrational mode excited and measured by the tip-enhanced THz near field. To elucidate the excitation mechanism of the phonon modes, we vary the pump/probe field and investigate the influence of defects within the suspended area.

[1] Roelcke et al., Nature Photonics. 18, 595-602 (2024)
[2] Rai et al., arXiv:2506.08219 (2025)
[3] Krane et al., Nano Lett. 2016, 16, 8, 5163-5168 (2016)

O 43.10 Tue 14:00 P2

THz-driven plasmonic STM luminescence — •Alkisti Vaitsi, Luis Enrique Parra López, Vivien Sleziona, Martin Wolf, and Melanie Müller — Fritz Haber Institute of the Max Planck Society, Berlin, Germany

We combine THz scanning tunneling microscopy (THz-STM) with visible light detection to investigate ultrafast STM- luminescence (STML) luminescence from atomic-scale plasmonic junctions. The luminescence is driven by single-cycle THz pulses which act as a quasi-static ultrafast bias. This enables femtosecond gating of ultrafast tunneling currents and the excitation of localized surface plasmon (LSP) modes via ultrafast inelastic tunneling. Our measurements, combined with numerical reconstruction of THz-STML spectra from static STML spectra, show that a quantum cutoff is often absent in THz-STML. In addition, THz-STML spectra frequently exhibit a distinct spectral shape that differs from that predicted from quasi-static, single-electron tunneling-induced luminescence. We discuss the role of overbias emission, hot luminescence, and femtosecond plasmon dynamics in THz-gated STML.

O 43.11 Tue 14:00 P2

Design of a light-coupled high-magnetic-field Scanning Tunneling Microscope — •Colin Geuder[1], Marco Mönnich[1], Kurt Lichtenberg[1], Susanne Baumann[1], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies. — [2]2Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart.

Light-matter interaction at the nanoscale lies at the heart of many fundamental phenomena ranging from light harvesting to ultrafast lightwave electronics. However, accessing magnetic degrees of freedom through light-matter interaction at the atomic scale presents unique challenges. Scanning tunneling microscopy (STM) is the ideal tool, that can locally probe and excite these different interactions at atomic length scales. Here, we present the design of an STM that combines optical access with a large numerical aperture, magnetic fields up to 5 T, and temperatures below 2 K. We mitigate thermal loads introduced by the high-NA optical access through a combination of fiber coupling and radiation blocks at several stages of the cryostat's shields. This instrument enables studies of magnetic degrees of freedom in nanoscale light-matter interaction, such as magnon-photon coupling or exciton-magnon transport in layered materials.

O 43.12 Tue 14:00 P2

strong-field theory model for ultrafast electron transport in laser-assisted STM — •Boyang Ma[1], Melanie Mueller[1], and Michael Krueger[2] — [1]Department of Physical Chemistry, Fritz Haber Institute, 14195 Berlin, Germany — [2]Department of Physics, Technion, Israel Institute of Technology, 32000 Haifa, Israel

In ultrafast scanning tunneling microscopy (USTM), the classification of light-driven currents is usually based on the well-known Keldysh parameter. Similar to the description of strong-field photoemission, it is often used to distinguish photon-driven (weak-field) and field-driven (strong-field) tunneling regimes. Here, we discuss the limitations of the Keldysh parameter in classifying light-induced electron transport in nanoscale gaps, and present a theoretical study of laser-induced electron transport in STM [1,2]. In contrast to strong-field effects in spatially extended systems, we show that the Keldysh parameter alone is insufficient to capture the electron transmission dynamics in a confined nanogap. Instead, it must be complemented by an additional parameter, ζ, defined by the laser field strength, frequency, and junction width [2]. Notably, in the THz-STM, ζ alone becomes the decisive parameter, superseding the role of the Keldysh parameter. This reflects the fact that the Keldysh parameter accounts solely for properties of the driving field and neglects geometric confinement of the tunneling junction.

[1] B. Ma and M. Krüger, Phys. Rev. Lett. 133, 236901 (2024)
[2] B. Ma and M. Krüger, Phys. Rev. A 112, 033104 (2025)

O 43.13 Tue 14:00 P2

Addressing Atomic-scale optical Stark-shift Microscopy — Xabier Arrieta[1,2], Sofia Canola[3], Ruben Esteban[1,4], Javier Aizpurua[2,4,5], and •Tomas Neuman[3] — [1]Centro de Física de Materiales (CFM-MPC), CSIC-UPV/EHU, Donostia- San Sebastián 20018, Spain — [2]Department of Electricity and Electronics, FCT-ZTF, UPV/EHU, Leioa 48940, Spain — [3]Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, Prague, 16200, Czech Republic — [4]Donostia International Physics Center, Donostia-San Sebastián 20018, Spain — [5]IKERBASQUE, Basque Foundation for Science, Euskadi Plaza 5, Bilbao 48009, Spain

An applied external electric field can shift the optical transition energies of molecular emitters through the optical DC Stark effect. Conventional Stark-shift spectroscopy applies spatially homogeneous electric fields, allowing to probe variations in molecular dipole moment and polarizability upon photoexcitation. In contrast, molecules in natural environments experience strongly inhomogeneous internal electric fields, where the Stark effect follows different selection rules. We extend the theory of Stark-shift spectroscopy to account for such nanoscale field. Similar field localization naturally arises in light-assisted scanning tunneling microscopy, which could provide spatially resolved access to the electronic response of individual molecules under optical excitation [1,2]. We demonstrate the potential of this technique to develop into atomic-scale Stark-shift microscopy. [1] Roslawska et al., Phys. Rev. X, 12, 011012 (2022). [2] Imada et al., Science, 373(6550), 95-98 (2021).

O 43.14 Tue 14:00 P2

Light emission from dibenzoterrylene (DBT) molecules studied with STML — •Yannis Hilgers, Andreas Reutter, Markus Etzkorn, and Uta Schlickum — Institute of Applied Physics, LENA - TU Braunschweig, Braunschweig, Germany

Scanning Tunneling Microscopy induced Luminescence (STML) has gathered great interest since its development in the late 1980s as it allows studying optical properties with atomic spatial resolution. With this technique, it has become possible to study quantum light sources like individual molecules exhibiting single photon emission, but obtaining high and reproducible photon yields has proven to remain challenging. With our self-built STML-setup, we achieve count rates about an order of magnitude higher than what has been reported in the past, allowing for measurements on more sensitive systems. Here, we present optical properties of dibenzoterrylene (DBT) molecules which have been reported as single photon sources when encapsulated inside a host lattice of Anthracene and Naphthalene. However, since both materials are not stable, we combine DBT molecules with a host lattice consisting of C_{60} multilayers, which is much more robust and even stable in air at room temperature. We found that light emission of individual DBT on C_{60} multilayers is indeed preserved. The emitted light was analyzed by means of photon maps and photon energy spectra.

O 43.15 Tue 14:00 P2

Influence of Polarons on Tunneling and Optical Spectra of Molecules Adsorbed on Dielectric Layers — •Jan Friese — Institute of Physics, Czech Academy of Sciences, Cukrovarnicka 10, Prague, 16200, Czech Republic

Light-assisted scanning tunneling microscopy has enabled the simultaneous probing of transport and optical properties of individual molecules with atomic-scale precision. This technique relies on electronically decoupling the molecules from the metallic substrate by depositing them on dielectric spacer layers. However, these spacers are often formed by ionic crystals, such as NaCl. The phononic response of these ionic layers can significantly impact the observed experimental features due to polaronic effects. Their understanding requires a bottom-up theoretical description accounting for the dynamics of the dielectric layer triggered by electronic transitions in the molecule.

Here we address this challenge and use the polaron-formalism to model the interaction of phonons in the dielectric layer with changes of the charge density in the molecule due to optical or charge transfer excitations. With that, two-time correlation functions and consequently spectral functions can be derived to account for the dynamics involved in substrate reorganization processes following a change of charge density in an adsorbed molecule. The results can be used to calculate features like the reorganization energy, and positions, widths and shapes of peaks in tunneling and optical spectra.

O 43.16 Tue 14:00 P2

Optics of Edge-Modified Graphene Nanoribbons: A Theoretical Perspective — •Jian Cheng Wong[1], Song Jiang[2], Guillaume Schull[2], and Tomáš Neuman[1] — [1]Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, 16200 Prague, Czech Republic — [2]Université de Strasbourg, CNRS, IPCMS, UMR 7504, F-67000 Strasbourg, France

Atomic-scale engineering of graphene nanoribbons (GNRs) provides a versatile means to tune their electronic and optical properties. We present a theoretical study of edge-modified GNRs that describe the process resulting in excitonic emission under scanning tunneling microscopy-induced luminescence (STML). The modified edge structure forms localized states in GNR similar to the end states studied formerly[1]. From the electroluminescence maps, we explore how interactions between two of these localized states change the optical properties depending on the GNR structure. For this, we construct a many-body model which describes the dynamics of tip-induced charging/discharging and relaxation that eventually leads to light emission.

[1] Song et al., Science, 379(6636), 1049-1054 (2023).

O 43.17 Tue 14:00 P2

Utilizing a Tunable Laser for Tip Enhanced Photoluminescence of Single Molecules — •Maximilian Rödel[1], Rodrigo Cezar De Campos Ferreira[1], Jiři Doležal[1], and Martin Švec[1,2] — [1]Institute of Organic Chemistry and Biochemistry (IOCB), Czech Academy of Sciences, Flemingovo náměstí 542/2. CZ16000, Praha 6, Czech Republic — [2]Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10/112, CZ16200, Praha 6, Czech Republic

The study of organic molecules and their optical properties provides insight into molecular interactions, guiding the design of materials for advanced optoelectronic devices. In this contribution, we present a tip-enhanced photoluminescence (TEPL) scanning tunneling microscope (STM) setup by utilizing a tunable Ti:Sapphire laser not only for resonant excitation of organic molecules like MgPc, but, moreover, for disentangling optical signals.

For this purpose, a parabolic mirror is used for coupling the laser into the nanocavity, ensuring wavelength-independent imaging and minimizing aberrations, enabling a consistent performance across the entire visible wavelength range. By doing so, high-resolution spectra of single-molecule MgPc at temperatures of <7 K on a Ag111/NaCl surface can be detected and by changing the excitation wavelength the vibronic contribution and the Raman signal can be distinguished. With this model system, we are able to complement our optical data set and even hope to establish photoluminescence excitation spectroscopy for future measurements.

O 44: Scanning probe techniques: Method development – Poster

Time: Tuesday 14:00–16:00 Location: P2

O 44.1 Tue 14:00 P2

Determining the electrical transmission to the junction of a scanning tunneling microscope — •Guido Hiller, Gaël Reecht, and Manuel Gruber — University of Duisburg-Essen

Stochastic resonance spectroscopy has recently been implemented in STM to probe dynamics at the atomic scale over a wide range of timescales, down to the picosecond range [1]. A key requirement for this method is a modulation voltage at the STM junction with an amplitude independent of the frequency. This, in turn, demands an accurate characterization and compensation of the frequency-dependent transmission of the cabling.

Several studies have focused on quantifying such transmissions. In particular, Paul et al. [2] quantitatively analyzed the radio-frequency induced broadening

of a sharp feature in dI/dV spectra. Building on this method, we carried out such analysis in the Fourier space and discuss the associated advantages.

[1] Betz et al., arXiv:2412.12647 (2024) / Hänze et al., Sci. Adv. 7, no. 33 (2021) [2] Paul et al., Rev. Sci. Instrum. 87, no. 7 (2016)

O 44.2 Tue 14:00 P2

Upgrading an LT-STM with a qPlus-AFM system — •René Knispel, Patrick Härtl, and Matthias Bode — Physikalisches Institut, Experimentelle Physik 2, Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

The invention of the scanning tunneling microscope (STM) by Binnig and Rohrer in 1981 enabled direct imaging of atomic-scale structures in real space [1]. Shortly thereafter, the recognition of tip–sample interactions enabled the development of the atomic force microscope (AFM) [2]. In 1995, Giessibl achieved true atomic resolution with AFM [3] by measuring the force gradient-induced resonance frequency shifts of a silicon cantilever. Quartz-based cantilevers with enhanced stiffness and sensitivity enabled the development of the so-called qPlus-AFM technique, which surpasses STM in spatial resolution and allows STM measurements to be performed concurrently.

To extend the capabilities of our low-temperature STM, we upgraded it with a qPlus-AFM system. The Pan-type scanner was redesigned to enable cantilever excitation and to integrate both differential oscillation signals and the STM tunneling current. A UHV-LT preamplifier for the oscillation signals was also build and mounted inside the liquid-helium shield of the cryostat. The technical implementation and performance of the upgraded microscope will be demonstrated using suitable test samples.

[1] G. Binnig *et al.*, Phys. Rev. Lett. **49**, 57 (1982).
[2] G. Binnig *et al.*, Phys. Rev. Lett. **56**, 930 (1986).
[3] F. J. Giessibl, Science **267**, 68 (1995).

O 44.3 Tue 14:00 P2

Multifrequency Tunnelling Spectroscopy — •Gleb Neplyakh, Philipp E.J. Maier, Carolina A. Marques, Berk Zengin, Kevin Hauser, Rian Ligthart, Alexander LaFleur, and Fabian D. Natterer — Department of Physics, University of Zurich, Winterthurerstrasse 190, CH-8057, Switzerland

Scanning tunnelling spectroscopy (STS) probes the local density of states by measuring differential conductance as a function of energy. Traditional STS acquires N energy points by sweeping a DC bias with a small modulation superimposed. This requires N sequential measurements, making it impractical for large mapping tasks.

We have developed Parallel Spectroscopy (PS) to overcome this limitation. PS exploits the nonlinearity in the $I(V)$ curve of the materials: a single or multitone AC voltage drive generates a set of higher harmonics that encode the full spectrum. Demodulating N harmonics within one leakage-free integration window enables the energy dependence to be recovered in a single measurement, providing substantial speedups.

We compare conventional STS and single- and multi-frequency PS with respect to signal-to-noise ratio, potential artefacts, and spectral resolution. Using PS in conjunction with compressive sensing could allow us to conduct high-resolution studies of many-body effects in quantum materials.

O 44.4 Tue 14:00 P2

Tip-enhanced Raman Microscopy simulation methods — •Pablo Planelles Prensa, Harshit Sethi, Orlando Silveira Junior, and Adam Foster — Konemiehentie 1, 02150 Espoo / P.O. Box 15600, FI-00076 AALTO

Tip-enhanced Raman Microscopy (TERS) has emerged as a promising technique that overcomes Abbe diffraction limit, which dictates that for green light around 500 nm the spatial resolution is limited to only 250 nm, which is insufficient for studying nanomaterials. In TERS, by using a strongly localized plasmonic field produced at the tip apex, the Raman signal is significantly enhanced, and submolecular resolution can be achieved.

Similar to Scanning Tunneling and Atomic Force Microscopy techniques, TERS relies on a sharp tip. TERS offers the additional advantage of providing not only topographic information about the sample, but also chemical.

Despite the rapidly increasing interest in TERS, progress remains limited by the difficulty of interpreting the resulting experimental images.

In this context, we aim to contribute by presenting ab-initio simulation methods and demonstrating how they can be used to greatly facilitate the interpretation and prediction of TERS images. Moreover, we will study the influence of the substrate on the images, and how different tip geometries and materials affect resolution and induce image asymmetry. We will also compare several simulation methods with different levels of complexity and computational cost.

O 44.5 Tue 14:00 P2

Automatic tip functionalization with CO on Ag(111) using machine learning — •Johanna Schnorrenberg, Jonas Heggemann, Paul Laubrock, and Philipp Rahe — Universität Osnabrück, Institut für Physik, Barbarastraße 7, 49076 Osnabrück, Germany

Functionalization of scanning probe microscopy tips with CO molecules enables high-resolution imaging, sub-molecular contrast and access to charge distributions of adsorbed molecules. [1, 2]

However, the manual functionalization procedure is time-consuming and limits experimental throughput. To address this, tip functionalization can be automated. [3]

Here, we implement a full pipeline for CO tip functionalization on Ag(111). The process includes localizing a CO molecule during scanning the surface, performing the pick-up of this CO molecule and evaluating the resulting tip condition. Tip quality is assessed by imaging CO molecules on the substrate and classifying the achieved resolution as "good" or "bad" for a CO-tip using a convolutional neural network (CNN). The CNN performance is compared to a conventional image analysis algorithm, in this case a template matching algorithm.

We expect this automated approach to significantly improve the efficiency of AFM experiments and thereby enabling faster and more systematic data acquisition on molecular systems.

[1] B. Schulze Lammers et al., Nanoscale, 13, 13617 (2021)
[2] L. Gross et al., Angew. Chemie Int. Ed., 57, 3888 (2018)
[3] B. Alldritt et al., Comp. Phys. Commun., 273, 108258 (2022)

O 44.6 Tue 14:00 P2

Spectral interferometry scanning near-field optical microscopy; investigating resonant tip-sample near-field interactions — •Tom Jehle, Sam S. Nochowitz, Juanmei Duan, and Christoph Lienau — Institute of Physics, University of Oldenburg, 26129 Germany

Localized phonon polaritons and plasmon polaritons resonantly enhance near-field mediated light matter interactions and are key for strong coupling between single quantum emitters and nanocavities (1). Localized polariton resonances with high oscillator strength show tip-sample distance dependent frequency shifts in scanning probe experiments, requiring spectroscopic analysis at explicit tip-sample distances (2). Here, we introduce a broadband interferometric scattering-type SNOM technique (3) to reconstruct spectral amplitude and phase of visible light scattered from a gold taper. Harmonic sampling with a fast line camera allows reconstruction of spectra with high tip-sample distance resolution. Spectral amplitude, phase and the evaluation of the distance dependence of the near-field interaction allows the retrieval of the temporal near-field dynamics with sub-cycle precision. We demonstrate our technique by measuring the tip-sample distance dependent time dynamics of the near-field at the apex of a resonant gold taper coupled to its image. Our results pave the way towards hyperspectral imaging in the visible with nm spatial resolution and fs temporal resolution of the reconstructed time dynamics. (1) S. Hu et al., Nat. Commun. 15, 6835 (2024); (2) H. Wang et al., Nat Commun. 9, 2005 (2018); (3) J. Zhan et al., Nano Lett. 24 (49),15738 (2024)

O 44.7 Tue 14:00 P2

Cryogenic Band Pass Amplifier for measuring Atomic Shot Noise — •Benjamin Frölich, Kevin Hauser, Lebin Yu, Gleb Neplyakh, Ajla Karić, and Fabian D. Natterer — Department of Physics, University of Zurich, Winterthurerstrasse 190, CH-8057, Switzerland

Scanning tunneling microscopy provides access to the texture and correlation of charge carriers in quantum materials by listening to their characteristic shot noise signatures that reveal 1e and 2e charge quantization effects at the atomic scale. Previous studies introduced a band pass amplifier with center frequency of 3 MHz based on their in house made high electron mobility transistor (HEMT) and LC tank circuit to measure such shot noise. Here we build a similar band pass amplifier with a center frequency of 17 MHz based on a comercially available InP HEMT. Another goal is the evaluation of resonating circuits like the LC tank at cryogenic temperatures. We achieve 26 dB single stage amplification at liquid nitrogen temperatures. Simulations suggest a noise figure of < 0.12 dB. Experiments at even lower temperatures present challenges impacting implementation into the cryostat.

O 44.8 Tue 14:00 P2

all-in-one preparation stage of STM/AFM QPlus sensors for ultrahigh vacuum — •reza habibipour, jakob pelster, marco pratzer, michiel reul, and markus morgenstern — II. Institute of Physics B, RWTH Aachen University and JARA-FIT, Germany

QPlus sensors enable the combination of atomic force microscopy (AFM) and scanning tunneling microscopy (STM) with high resolution. We developed a compact preparation stage for positioning, glueing, annealing and tip etching of wires with diameters down to 7.5 um and length down to 200 um. The QPlus sensors are based on a piezoelectric quartz tuning fork with nominal frequency of 32.6 kHz. A tip wire is attached to one prong with the other prong is fixed to a ceramic block on the ultrahigh-vacuum (UHV) sample holder. Two tuning-fork contacts connect to the sample plate for AFM oscillatory function and for STM current. Sensor preparation utilizes a long-working-distance optical microscope (~6 cm) and micrometer manipulators for precise glue and wire positioning. A heater is used to cure the glue. A tungsten-carbide flush cutter trims the wire to within 0.2 mm of the prong edge. Alternatively, an etching ring is employed for tip shaping. Afterwards contacts can be checked in-situ by a Keithley instrument. Q-factors at room temperature and UHV amount to 16.000. The resulting

QPlus sensors will be employed in a 300 mK STM/AFM cryostat mostly for maneuvering towards stacks of 2D materials by AFM prior to STM measurements.

O 44.9 Tue 14:00 P2

Iron Implantation from a Ferrocene Ion Source — •Urs Boison, Ajla Karić, Berk Zengin, Lebin Yu, and Fabian D. Natterer — Department of Physics, University of Zurich, Winterthurerstrasse 190, CH-8057, Switzerland

The scattering of electrons on defects in low dimensional materials provides insight into the electronic structure using quasiparticle interference or tunneling spectroscopy. Since natural defects are mostly spin averaging and obscure magnetic textures, using magnetic impurities would allow a richer inspection of the underlying magnetic properties. At present, magnetic impurities are difficult to produce because chemically active defects are required to chemisorb magnetic atoms, such as hydrogen. We use metal ions in a volatile molecule that can easily and directly be delivered to ion sources commonly used for sample cleaning. Using a conventional sputtering source and heated ferrocene (vapor pressure of 1773 Pa at 400 K), we implant ferrocene molecules between 100 and 3000 eV and use different vapor pressures to investigate the ion implantation efficiency and possible defect generation. We test the optimal dose as a function of these parameters using ion current measurements and mass deposition on a quartz crystal microbalance. To verify successful implantation, we use scanning tunneling microscopy on graphene and superconducting layers. Magnetic defects should exhibit signatures related to Yu-Shiba-Rusinov states, confirming the conservation of their spin upon implantation.

O 44.10 Tue 14:00 P2

Development of a Low-Temperature Scanning Probe Microscope — •Tingwen Miao — Tsung-Dao Lee Institute, Shanghai, China

We independently designed and constructed a low-temperature ultrahigh-vacuum scanning probe microscope (SPM) system which is equipped with a single-axis 9T magnetic field and can be cooled down to 400mK. The system integrates the functionalities of atomic force microscopy (AFM) and scanning tunneling microscopy (STM) into the scanning head, enabling in-situ measurements of both electrical signals and force signals. The cooling curve, current noise, non-contact AFM and STM imaging and I(V) spectroscopy are characterized to verify that the system achieve the fundamental SPM capabilities. Subsequent magnetic field test and low-temperature test will be performed to confirm that the system can achieve all designed performance.

O 44.11 Tue 14:00 P2

Correlative AFM-SEM-EDS microscopy on nanoparticles and -wires — Chris Schwalb[1], •Lukas Stühn[1], Hajo Frerichs[1], Sebastian Seibert[1], Darshit Jangid[1], Marion Wolff[1], Kerim Arat[2], Hamed Alemansur[2], Afshin Alipour[2], Andreas Amann[2], Luis Montes[2], Jost Diederichs[2], Jeff Gardiner[2], Will Neils[2], and Stefano Spagna[2] — [1]Quantum Design Microscopy GmbH, Pfungstadt, Germany — [2]Quantum Design Int., San Diego, USA

Correlative AFM-SEM-EDS microscopy enables multimodal nanoscale analysis but is often hindered by complex sample transfers and the lack of a joined coordinate system. Our approach integrates these techniques to allow simultaneous acquisition of topographical, mechanical, electrical, SEM and EDS data from the same region of interest[1]. We illustrate the advantages of such in-situ correlative measurements through several case studies, including hard-to-access structures such as bone lacunae, individual nanowires on 5 nm TEM grids, and nanoparticles relevant for multimodal characterization workflows[2]. In addition, we present first results on individual ZnO nanowires for energy-harvesting concepts, where SEM enables rapid localization and AFM provides mechanical and electrical characterization[3,4]. Overall, the presented in-situ correlative strategy, the FusionScope, expands the analytical capabilities for nanoscale inspection and process control across a wide range of materials and devices. [1] https://doi.org/10.1093/mictod/qaad083 [2] https://doi.org/10.1093/mam/ozae044.233 [3] https://doi.org/10.3390/mi16080927 [4] https://doi.org/10.1002/adfm.202310110

O 44.12 Tue 14:00 P2

Distance dependent of local work function on Pb/Si(111) islands — •Ajay Kumar[2], Thomas Späth[1], Ben Lottenburger[2], Zeineb Ben Tanfous[3], Daniel Rothhardt[2,4], Paul P. Schmidt[2], Manuel Schulze[2], Ralf Metzler[2], Kurt Busch[3], Gino Wegner[3,5], and Regina Hoffmann-Vogel[2] — [1]Institute of Physics and Astronomy, University of Potsdam, Karl-Liebknecht-Str. 24-25, 14476, Potsdam, Germany — [2]Physikalisches Institute, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [3]Humboldt University of Berlin, 12489 Berlin, Germany — [4]Swiss Federal Laboratories for Materials Science and Technology, CH-8600 Dübendorf, Switzerland — [5]Max-Born-Institute, 12489 Berlin, Germany

A quantitative description of the measured local contact potential difference (LCPD) as a function of tip-sample separation is essential for a deeper understanding of Kelvin probe force microscopy (KPFM), since it permits a more complete characterization of the sample's electronic properties and of the forces acting on the probe. We employ Pb islands on the Si(111)-7*7 reconstruction as a model system of metallic islands on a semiconducting substrate. Using a frequency-modulation scanning force microscope, we have performed frequency-shift bias-approach measurements at 115 K on these Pb islands and have studied the variation of the LCPD with tip-sample distance.

O 44.13 Tue 14:00 P2

Nonlinearity mapping using adaptive control schemes in scanning force microscopy — •Lukas Böttcher[1], Hannes Wallner[2], Niklas Kruse[2], Franziska Dorn[1], Wolfram Just[2], Ingo Barke[1], Jens Starke[2], and Sylvia Speller[1] — [1]Institute of Physics, Universität Rostock, Germany — [2]Institute of Mathematics, Universität Rostock, Germany

When probing surfaces by scanning force microscopy methods using oscillating cantilevers, bistabilities may occur [1,2]. This is a result of nonlinearities arising due to tip-sample interactions. In this work we focus on the attractive regime. Using an adaptive control scheme we track branches of unstable periodic orbits of the oscillating cantilever, arising between the two stable states [3]. Combining this with a topography scan of a polymer blend surface we explore spatial changes of the unstable branch. Parameters, such as the frequency width of the bistable region or the slope at the unstable branch can serve as nonlinearity parameters and respective maps can be acquired. The aim is to connect such nonlinearity maps to material-related properties such as density and elasticity.

[1] Gleyzes, P. et al.: Bistable behavior of a vibrating tip near a solid surface. Appl. Phys. Lett. 58, 2989 (1991) [2] Misra, S. al.: Event-driven feedback tracking and control483 of tapping-mode atomic force microscopy. Royal Society of London Proceedings484 Series A 464, 2113*2133 (2008) [3] Böttcher, L. et al.: Exposing hidden periodic orbits in scanning force microscopy. Commun Phys 8, 57 (2025)

O 44.14 Tue 14:00 P2

Realizing Spin-Polarized Scanning Tunneling Microscopy for an Atomic-Scale Study — •Leon Bojunga, Felix Otto, Jonas Brandhoff, Maximilian Schaal, Christian Haberland, Lorenz Brill, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Spin-polarized scanning tunneling microscopy and spectroscopy (SP-STM/STS) is a powerful tool for investigating spin structures with real-space resolution down to the atomic scale. By combining a spin-sensitive tip with controlled magnetic fields at cryogenic temperatures, SP-STM/STS enables the study of phenomena such as Kondo resonances, spin excitations, organic radicals, and magnetism. Realizing SP-STM/STS requires, beyond standard low-temperature STM stability, a magnetically sensitive tip and a precisely tunable external magnetic field. In this work, we fabricate Ni tips by electrochemical etching and verify their apex geometry via SEM to ensure high quality. This is achieved using a home-built etching setup that enables a reproducible process with consistent results. Testing of the fabricated tips is carried out using an STM at cryogenic temperatures, which, together with a perpendicular magnetic field of up to 3 T, allows controlled magnetization of the tip. To assess the magnetic sensitivity and spatial resolution of the Ni tips, we employ Co bilayer islands on Cu(111), whose well-defined magnetic structure provides an ideal benchmark for validating tip polarization and imaging performance.

O 44.15 Tue 14:00 P2

Low latency, galvanically isolated data transfer architecture for distributed low-level precision measurements — Toni Marković, Shane O'Neill, Aitziber Herrero, David Zurbriggen, Daniel Uehli, and •Alessandro Pioda — SPECS Zurich GmbH, Technoparkstrasse 1, 8005 Zurich

Many recent achievements in the field of quantum devices, spintronics, novel materials and surface science, have been possible thanks to the ability to cool samples to temperatures significantly below 1 Kelvin and to the use of state of the art measurement electronics. Requirements for signal resolution, precision and quality increase significantly at low temperatures, while the growing complexity of experiments and higher measurement throughput require a growing number of signals, larger bandwidths, and push the cost of measurement electronics upwards.

Here we present a data transfer architecture that enables a low-latency, synchronous transfer of raw DAC and ADC data from multiple signal generation and acquisition interfaces to a central processing core. The architecture allows transfer of very high-resolution data with microsecond resolution, high resolution data with nanosecond resolution or a combination thereof. The use of off-the-shelf optical fiber cables for data transfer allows for decentralized measurements, simultaneous experiments on different experimental set-ups, as well as galvanic isolation between the processing core and the signal interfaces. The architecture can handle hundreds of signals, all synchronous and with no multiplexing. We also discuss state of the art signal interfaces and typical applications for this novel architecture.

O 44.16 Tue 14:00 P2

Development of low noise cryogenic circuitry for shot noise measurements in STM — •Anne-Catherine Oeter, Soumyaranjan Jhankar, Christian Ast, and Klaus Kern — Max Planck Institut for Solid State Research

Tunneling currents of electrons are subject to shot noise. Measuring shot noise in a scanning tunneling microscope (STM) can give more insight into the tunneling dynamics and the properties of the tunneling charges. Our goal is to measure shot noise at low tunneling currents simultaneously with the dc tunneling current. To this end, we are developing a low-noise cryogenic pre-amplification circuit. It is made up of a tank oscillator circuit, to filter and amplify the white noise signal at a frequency beyond flicker noise, as well as a HEMT based cryogenic amplification circuit. We will discuss how we want to improve the shot noise circuitry already used in the literature, for example, how to enhance the quality factor of the inductances used to filter the ac signal.

O 44.17 Tue 14:00 P2

Realization of laser-assisted UHV sample surface preparation for STM — •Clara Marie Nieder, Soumyaranjan Jhankar, David Sousa, and Christian Ast — Max Planck Institute for Solid State Research

Scanning tunneling microscopy (STM) enables the study of the electronic properties of superconductors such as vanadium. To achieve reliable STM measurements, the preparation of clean and well-defined metal surfaces under ultra-high vacuum (UHV) conditions is essential. This requirement becomes particularly demanding for reactive transition metals, where surface oxides can form even under high-quality UHV conditions. In this work, we present a laser-assisted UHV sample preparation approach to obtain clean vanadium surfaces. For this method, we utilize a diode laser directed at the front surface of the sample to achieve high temperatures. To prevent mechanical or electrical complications inside the UHV chamber, we place all optical and diagnostic components, including pyrometric temperature monitoring, outside the chamber. This enables a controlled and localized high-temperature annealing for oxide removal. Therefore the method represents a promising way to reproducibly prepare reactive and superconducting surfaces for subsequent STM measurements.

O 45: Organic molecules on inorganic substrates: Adsorption and growth – Poster

Time: Tuesday 14:00–16:00 Location: P2

O 45.1 Tue 14:00 P2

Domain mixing of coronene and nonahelicene with CuO_x species on Cu(110) — •Max Halbauer, Martin Wolf, and Akitoshi Shiotari — Fritz-Haber-Institute, Faradayweg 4-6, 14195 Berlin, Germany

Various surfaces are known to reconstruct as a result of surface energy minimization (e.g. Pt(110)-(2×1), Si(111)-(7×7)). For certain systems, the surface reconstruction is induced by the adsorption of molecules or atoms (e.g. C_{60}/Cu(111) [1]). In this work, we show how the organic molecules, coronene and nonahelicene, interrupt the growth of copper oxide rows of the typical Cu(110)-p(2×1)O reconstruction and mediate the formation of mixed domains instead. The resulting adlayer domains on Cu(110) were imaged by scanning tunneling microscopy (STM) and non-contact atomic force microscopy (NC-AFM) under ultrahigh vacuum and cryogenic conditions. Models for the adsorption structures of the molecules and CuO_x species are discussed and confirmed with simulated images. A mechanism for the mixed domain growth is proposed, whereby surface diffusion and favourable lateral interactions between the molecules and oxide species drive the formation of the observed coordination framework. The finding opens prospects for controlling the lateral chemical and electronic interactions between adsorbed molecules by partial oxidation of the Cu(110) surface.

[1] L. Forcieri, S. P. Jarvis, *et.al.*, *Phys. Rev. B* **2021**, *104*, 205428.

O 45.2 Tue 14:00 P2

Importance of Electrostatic Effects for Interpretation of X-ray Photoemission Spectra of Self-Assembled Monolayers — •Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany

The subject of this contribution is electrostatic effects in X-ray photoemission (XP) from self-assembled monolayers (SAMs), which are application-relevant ultrathin molecular films, coupled to the substrate by a suitable anchoring group. Whereas, in most cases, the standard concept of chemical shift is fully sufficient to describe XP spectra of these systems, consideration of electrostatic effects is frequently necessary for their proper interpretation. Due to the insulating character of the SAM matrix, decoupled electronically from the substrate, the introduction of a dipolar "sheet" at the SAM-substrate interface or within this matrix creates a potential discontinuity, shifting the energy levels above the "sheet" with respect to those below it. This shift is reflected then in the matrix-related spectra, resulting in shifts and splitting of the characteristic photoemission peaks. Representative examples in this context underline the importance of electrostatic effects in photoemission and suggest that they should be considered on equal footing with the chemical shift.

O 45.3 Tue 14:00 P2

Self-assembled quasi-one-dimensional metal-organic framework — Jonas Brandhoff, Jule S. Hölzer, Felix Otto, Torsten Fritz, and •Roman Forker — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

We compare condensed monolayers of 4,5,9,10-pyrenetetrone (Py4O) on Cu(111) in two fundamentally different configurations, namely with and without adatoms. To this end, we employ density-functional theory (DFT) calculations to understand the structural configurations as well as the electronic properties. We uncover the coupling between the organic molecule, surface, and possible adatoms. Furthermore, we demonstrate how a quasi-one-dimensional arrangement including a Cu adatom is thermodynamically stable. This interpretation is substantiated by means of scanning-tunneling microscopy (STM) experiments, along with low-energy electron diffraction (LEED) patterns. Additionally, we use photoelectron spectroscopy to assess the electronic structure. Finally, we elucidate the bond formation between the d-orbitals of the Cu adatom and the p-orbitals of the molecular oxygen.

O 45.4 Tue 14:00 P2

Landing-Energy-Controlled Surface Conformation of Electrosprayed Foldamer Molecules on Au(111) — •Jue Wang[1], Dennis Meier[1,2], Shengming Zhang[1], Patrick Lawes[1], Pengfei Zhao[1], Jinhua Wang[3], Victor Maurizot[3], Andreas Walz[1,4], Annette Huettig[1,4], Hartmut Schlichting[1,4], Anthoula C. Papageorgiou[1,5], Joachim Reichert[1], Ivan Huc[6,7], and Johannes V. Barth[1,7] — [1]TU Munich, DE — [2]Tufts University, US — [3]CNRS, Univ. Bordeaux, FR — [4]pureions GmbH, Gilching, DE — [5]National and Kapodistrian University of Athens, GR — [6]LMU Munich, DE — [7]Cluster of Excellence e-conversion, DE

Preserving the structural integrity of biomimetic foldamers upon surface deposition is essential for their integration into functional molecular architectures. In this study, we investigate the electrospray ion beam deposition of foldamer molecules in ultra-high vacuum and examine how their conformation depends on the mean landing energy during deposition. With a low mean landing energy of about 0.6 eV, intact foldamers are observed on the surface. Higher landing energies predominantly result in unfolded molecules. The unfolded conformation are further accessible by annealing of the adsorbed folded molecules. These results highlight the importance of soft-landing conditions to maintain hydrogen bond-stabilized architectures on surfaces, offering a model platform for studying the structure-function relationship of surface-supported thermolabile biomolecules

O 45.5 Tue 14:00 P2

Adsorption, Dissociation and Chain Formation of 2NHC-azo-iPrI on Au(111) — Ebru Cihan[1], Natasha Khera[1], Franz Plate[1], Ningwei Sun[2], Soyoung Park[2,3], Franziska Lissel[2,3], and •Francesca Moresco[1] — [1]Center for Advancing Electronics Dresden, TU Dresden, Dresden, Germany — [2]Institute of Macromolecular Chemistry Leibniz Institute of Polymer Research, Hohe Strasse 6, Dresden, Germany — [3]Institute for Applied Polymer Physics, TU Hamburg, Hamburg, Germany

In this study, we investigated 2NHC-azo-iPrI molecules on the Au(111) surface. While the central azobenzene core is clearly visible in STM images, in most cases, only two isopropyl groups are present per molecule. Our results indicate the possibility of a reaction between I- counterions and the isopropyl (iPr) side groups, which may lead to the dissociation of iPrI upon heating. Furthermore, experiments using STM lateral manipulation, which facilitate the separation of chain structures on azobenzene bridges, suggest that the chains are likely connected to each other by weak van der Waals or hydrogen bonds. Additionally, to further investigate the azobenzene core of the molecule, voltage pulses were applied to the molecule using the STM tip. This investigation reveals the potential for cis-trans isomerization in the azobenzene core.

O 45.6 Tue 14:00 P2

Tuning molecular self-assembly of BDA on $CsPbBr_3$(100) — •Hannah Loh, Milan Möller, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

$CsPbBr_3$ is a promising alternative to organic-inorganic perovskites in solar cells and light emitting diodes [1]. In these devices, organic layers are often used as

charge transport layers and hence interface properties are of particular interest. Depending on the termination of the $CsPbBr_3$ substrate [2] the adsorption properties can be tuned [3].

In this contribution we invesitgate the self assembly of 4-4-biphenyl dicarboxylic acid (BDA) on epitaxial $CsPbBr_3$ thin films on Au(100). Independent of surface termination the BDA molecules lie flat and form compact islands. On the CsBr-terminated surface, molecules follow a head to tail hydrogen-bridge stabilized arrangement. The interaction with the PbBr terminated surface is stronger causing partially a slight tilt of the molecules to adapt to the substrate unit cell and deprotonation.

[1] Bao C. et al., Organic Electronics, **73**, 299-303 (2019)
[2] Rieger J. et al., Phys. Rev. Mat, **7**, 035403 (2023)
[3] Loh H. et al., ACS Nano, **19**, 10199-10206 (2025)

O 45.7 Tue 14:00 P2

Force mapping of a pyridyl-functionalized platform molecule by noncontact atomic force microscopy — •Hyeji Choi[1], Behzad Mortezapour[2], Martin Wolf[1], Richard Berndt[2], and Akitoshi Shitotari[1] — [1]Fritz-Haber Institute of the Max-Planck Society, Berlin, Germany — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Kiel, Germany

Platform molecules based on trioxatriangulenium (TOTA) form triangular adsorption motifs on metal surfaces with a functional group protruding to the vacuum [1]. However, probing the atomic-scale structure of such steric molecules remains challenging. Here, we study pyridyl-TOTA on Ag(111) and perform single-molecule force mapping, using noncontact atomic force microscopy (NC-AFM) at 6 K. We obtained force and potential maps of the pyridyl group interacting with a metal tip by measuring frequency shift as a function of tip height and location. These maps reveal anisotropy depending on the direction relative to the pyridyl ring plane. Simulations using Lennard-Jones potential reproduce the map appearances, enabling estimation of the preferred ring orientation and directional stiffness. We thus demonstrate the high potential of single-molecule force mapping for the structural characterization of steric adsorbate.

[1] Mortezapour, B., et al., ACS Nano 19, 38773-38780 (2025)

O 45.8 Tue 14:00 P2

Decoupling of Organic Monolayers from Cu(111) Using Blue Phosphorene — •Felix Otto, Wiebke Makowski, Jonas Brandhoff, Maximilian Schaal, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Two-dimensional (2D) materials are promising for future electronics due to their tunable properties. Since graphene's discovery in 2004, materials like MoS_2, h-BN, and Blue Phosphorene (BlueP) have been synthesized, offering high charge mobility and adjustable band gaps. BlueP can be grown on substrates such as Cu(111), making it suitable for decoupling organic layers. This study investigates whether BlueP can effectively decouple PTCDA monolayers from Cu(111). Two BlueP phases – hexagonal and chiral – were prepared and characterized, revealing structures with hexagonal unit cells but significantly stretched lattices compared to free-standing BlueP. Despite structural differences, both phases exhibited similar chemical and electronic properties. PTCDA was deposited on both phases, forming ordered herringbone structures. On the chiral phase, a single structural model sufficed, while two were necessary for the hexagonal phase. Spectroscopic analyses indicated weak interactions and evidence of integer charge transfer, supporting the idea that BlueP acts as an effective decoupling layer. These findings contribute to understanding how 2D-materials can be used to electronically isolate organic monolayers, advancing their application in nanoelectronics.

O 45.9 Tue 14:00 P2

Density functional study of the geometric and electronic properties of a tetracene-adduct molecule on Ag(110) — •Fabian Dixer[1], Eric Fackelman[2], Veronika Schmalz[3], Monja Stettner[2], François C. Bocquet[2], Andrei C. Matetskii[2], Serguei Soubatch[2], Ulrich Koert[3], Frank Stefan Tautz[2], and Peter Puschnig[1] — [1]Institute of Physics, University of Graz, Austria — [2]PGI-3, FZ Jülich and RWTH Aachen University, Germany — [3]Department of Chemistry, Philipps-Universität Marburg, Germany

We present a density-functional theory (DFT) investigation of the adsorption behavior of the tetracene-maleic anhydride Diels-Alder adduct (4A-MAD) on Ag(110). This molecule serves as a model system for studying light induced retro 4+2 cycloadditions on surfaces. Using a repeated-slab approach with a van-der-Waals corrected GGA functional, we explore the adsorption energy landscape by sampling multiple initial configurations and performing local relaxations. The most favorable geometries are examined in terms of work-function changes, charge-density-difference distributions, and projected densities of states. We further simulate photoemission momentum maps of the frontier molecular orbitals within photoemission orbital tomography and compare them with angle-resolved and angle-integrated photoemission data from our experimental collaborators. This combined analysis provides a comprehensive picture of the molecule-substrate interaction and lays the groundwork for future studies of on-surface photochemical cleavage of the Diels-Alder adduct.

O 45.10 Tue 14:00 P2

Theoretical Investigation of Halogenated Polycyclic Aromatic Hydrocarbons on Clean and Coated Metal Surfaces — •Florian Pfeiffer[1], André Schirmeisen[2], Daniel Ebeling[2], and Simone Sanna[1] — [1]Institute for Theoretical Physics, JLU Giessen, Germany — [2]Institute for Applied Physics, JLU Giessen, Germany

Halogenated organic precursors are the building blocks for the on-surface synthesis of complex structures with precisely tuned properties. While chemical synthesis is typically performed on clean metallic surfaces, a NaCl bilayer might be employed to electronically decouple substrate and adsorbates, increasing mobility and thus simplifying manipulation.

To improve our understanding of the fundamental interactions of halogenated precursors on (isolated) surfaces, we examined charge redistribution as well as the adsorption geometry, distance, and energetics for several substrate-adsorbate systems, e.g. Dibromopyrene and Iodotriphenylene on NaCl/Cu and halotetracenes on coinage metals.

The Vienna Ab initio Simulation Package [1] implementation of density functional theory was used to calculate potential energy surfaces and nudged elastic bands for modelling adsorption behaviour and diffusion pathways, respectively. Comparability with experimental results [2] was achieved by simulation of atomic force microscopy using the Probe-Particle Model [3].

[1] G. Kresse and J. Hafner, Phys. Rev. B 47, 558 (1993)
[2] Q. Zhong et al., Nat. Chem. 13, 1133 (2021)
[3] P. Hapala et al., Phys. Rev. B 90, 085421 (2014)

O 45.11 Tue 14:00 P2

Formation and Electronic Interaction of Donor–Acceptor Heterostructures — •Philipp Janzen, Jonas Brandhoff, Felix Otto, Maximilian Schaal, Roman Forker, and Torsten Fritz — Institute of Solid State Physics, Friedrich Schiller University Jena, Helmholtzweg 5, 07743 Jena, Germany

Combining donating and accepting molecules lies at the heart of many electronic devices. These molecular heterostructures allow for a delicate tailoring of charge-transfer interfaces. In this work, we investigate such heterostructures formed by the adsorption and structural organization of 1,4,5,8,9,11-hexaazatriphenylenehexacarbonitrile (HATCN) and 2,3,6,7,10,11-hexahydroxytriphenylene (HHTP) on Au(111). Owing to their shared symmetry, HHTP and HATCN form a well-matched co-assembly on the surface. Employing scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED), we are able to resolve the structural properties of the individual systems, as well as the combined heterostructure. Additionally, X-ray photoelectron spectroscopy (XPS) and photoemission orbital tomography (POT) provide insights into charge-transfer processes and the electronic structure at the interface.

O 46: Organic molecules on inorganic substrates: electronic, optical and other properties – Poster

Time: Tuesday 14:00–16:00 Location: P2

O 46.1 Tue 14:00 P2

Investigation of chiral helicene molecules on the superconducting substrate Pb(111) — •Melvin Grumser[1], Rahel Specht[1], Vincent Herzog[1], Wenhui Niu[2], Narcis Avarvari[3], and Katharina J. Franke[1] — [1]Freie Universität Berlin, Berlin, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany — [3]University of Angers, Angers, France

Chiral molecules have recently garnered a lot of attention for their ability to partially spin polarize currents running through them, which is of interest for the emerging field of spintronics. Chirality induced spin selectivity (CISS) typically manifests itself in experiments in which a current passes through a chiral molecule, as has been done down to the single-molecule scale using scanning tunneling microscopy [1]. However, recent studies suggest that the adsorption of chiral molecules might already lead to magnetization in the surface layer which could locally interact with the Cooper-pairs of a superconducting substrate [2]. Here, we investigate the effect of adsorbed chiral molecules on the elemental superconductor Lead. For this, [7]-Helicene and [6]-Helicene derivatives were evaporated onto a Pb(111) surface and investigated via STM and AFM. The molecules form ordered islands with different orientations of the molecules. In addition, we use scanning tunneling spectroscopy and identified the energy of the HOMO and LUMO. However, we do not observe any signatures of an

alteration of the local superconducting behavior.

[1] Safari, Mohammad Reza, et al. Small 20.22 (2024): 2308233.
[2] Shapira, Tamar, et al. Phys. Rev. B 98.21 (2018): 214513.

O 46.2 Tue 14:00 P2

On-Surface Reaction of Naphthothiadiazole Derivatives on Au(111) — •Mohsen Ajdari[1], Jakob Steidel[1], Larissa Winkelmann[1], Felix Landwehr[1], Jakob Sawatzki[1], Jakob Roth[1], Christian Huck[1], Hendrik Hoffmann[2], Uwe H. F. Bunz[2], and Petra Tegeder[1] — [1]Institute for Physical Chemistry — [2]Institute for Organic Chemistry, Heidelberg University, Germany

Naphthothiadiazole (NTD) and its halogenated derivatives (NTD-Br/Cl) are promising electron acceptor candidates for use in (opto)electronic applications.

In a multi-technique approach, this study utilizes scanning tunneling microscopy, two-photon-photoemission spectroscopy, and temperature-programmed desorption to identify on-surface reactions of adsorbed NTD-Br/Cl on Au(111).

Our findings suggest that the halogenated molecules undergo temperature (NTD-Br) and photo-induced (NTD-Br/Cl) dehalogenation reactions. As a result, we found work function changes, differences in the energy-level alignment as well as changes in the adsorption structure.

O 46.3 Tue 14:00 P2

Second Harmonic Generation in Thin Films of Chiral Organic Molecules — •Martin Richter[1], Gayani Liyanage[1], Marjan Krstic[2], Erik Misselwitz[3], Milan Kivala[3], Carsten Rockstuhl[2], and Petra Tegeder[1] — [1]Institute for Physical Chemistry, Heidelberg University, Germany — [2]Institute of Theoretical Solid-State Physics, Karlsruhe Institute of Technology, Germany — [3]Institute of Organic Chemistry, Heidelberg University, Germany

Nonlinear optical (NLO) techniques enable increased sensitivity to chiroptical features. In contrast to linear circular dichroism (CD), second harmonic generation (SHG) chiroptical features can be explained within the dipole approximation. This includes electric as well as magnetic dipolar contributions. The latter are usually much weaker and specific measurement schemes are required to detect them. Here, we investigated thin films of chiral organic molecules using SHG-CD and SHG-ORD (optical rotatory dispersion) to probe the nonlinear CD and optical rotation. Continuous rotation of a quarter-wave plate generates circular and elliptical light to gain insights into the relative amplitudes of the second-order susceptibilities from electric χ^{eee} and magnetic (χ^{mee} and χ^{eem}) dipolar contributions. Our theoretical modelling allowed us to disentangle electric and magnetic dipole contributions.

O 46.4 Tue 14:00 P2

Electronic structure of spiro-bridged N-heterotriangulenes on Au(111) — •Jakob Roth[1], Jakob Sawatzki[1], Christian Huck[1], Angelina Jocic[2], Milan Kivala[2], and Petra Tegeder[1] — [1]Institute for Physical Chemistry — [2]Institute of Organic Chemistry, Heidelberg University

N-heterotriangulenes are versatile p-type organic semiconductors combining enhanced planarity with sterically defined bridges, enabling highly stable amine-centered radical cations, making them promising candidates for semiconducting and energy storage applications.

Here, we investigated the adsorption and electronic structure of two model systems - dimethylmethylene-bridged N-heterotriangulene (TN) and spirofluorene-bridged N-heterotriangulene (FTN) - deposited on Au(111). The spiro-annulated fluorenyl groups of FTN are expected to elevate the molecular core and hence reduce the electronic coupling strength to the metal substrate. Scanning tunnelling microscopy reveals that both species form well-ordered monolayers. Two-photon photoemission spectroscopy quantitatively resolves occupied and unoccupied electronic (transport levels) as well as excitonic states (optical gaps). These results highlight how molecular design controls surface coupling and electronic level alignment in Triphenylamine-based materials.

O 46.5 Tue 14:00 P2

Deprotonation of quinacridone on Ag(100) - an NIXSW/XPS study of the phase transition — Lucas Hirschfeld[1], Morris E. L. Mühlpointner[1], Anna J. Kny[1], Sergey Subach[2], and •Moritz Sokolowski[1] — [1]Clausius Institute for Physical and Theoretical Chemistry, University of Bonn, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich GmbH, Germany

Quinacridone (QA) forms two different phases on the Ag(100) surface. When QA is deposited at room temperature, the formation of the α-phase with a point-on-line (*pol*) structure is observed. After annealing, the commensurate β-phase is irreversibly formed [1]. The mechanism, involving the loss of intermolecular hydrogen bonds, was not disclosed so far. Thus we have performed a detailed Normal Incidence X-ray Standing Waves (NIXSW)/XPS study.

The N1s XPS spectra exhibit a second peak shifted by 2.2 eV to lower binding energies when going from the α- to the β-phase. This reveals that the irreversible reaction from the α- to the β-phase is explained by a deprotonation of 50 % of the amine groups. The deprotonated N-atoms form stronger bonds to the Ag(100) surface, indicated by a drastic approach of the respective N adsorption height from 4.3 Å in the α-phase to 3.4 Å in the β-phase. These results show that the reaction is driven by the energy gain related to N/Ag interfacial bonds, which overcompensate the loss of intermolecular hydrogen bonds.

Support by Diamond Light Source is acknowledged.

[1] JPCC 124.45 (2020), 24861-24873.

O 46.6 Tue 14:00 P2

Fluorescence Spectroscopy of Quinacridone Molecules on thin Epitaxial KCl(100) films. — •Morris E. L. Mühlpointner and Moritz Sokolowski — Clausius-Institut für Physikalische und Theoretische Chemie der Universität Bonn, Germany

Quinacridone forms one-dimensional chains on metal surfaces and thin epitaxial KCl films grown on Ag(100) [1]. TD-DFT predicts the transition dipole moment in the direction of chain growth. The resulting J-like coupling suggests superradiance which can be enhanced by chemical modifications that increase the inter-chain distance. However, no data on the optical properties of QA on KCl surfaces exist.

We have measured the fluorescence at cryogenic temperatures (7 K) of quinacridone (QA) and its fluorinated derivative (FQA) on ultrathin KCl films grown on Ag(100). Isolated QA molecules on KCl have a 0-0 transition at 20200 ± 200 cm^{-1}. The spectral lines have asymmetric shapes with large line widths (400 to 700 cm^{-1}). We relate the broadening to the weak bonding interactions of the molecule and the substrate.

Upon forming a 2D aggregate on the surface, we observe a significant red shift by 1600 cm^{-1} for QA and FQA. This can be understood by the attractive of the transition dipoles.

[1] JPCC **127** (2023): 23814-23826.

Acknowledgements: We thank the DFG for support via the research training group 2591, Mohammad Al Dubel and Sigurd Höger for kindly providing FQA molecules and Harshita Malik and Thomas Bredow for DFT calculations.

O 46.7 Tue 14:00 P2

On-Surface Coupling of Feringa-Type Molecular Motors — •David Le[1], Grant J. Simpson[1], Matthew J. Timm[1], Dongdong Liu[2], James M. Tour[2], and Leonhard Grill[1] — [1]University of Graz, Austria — [2]Rice University, Houston, USA

Artificial molecular motors are fundamental components of nanoscale machines that convert external energy into uni-directional motion. On metallic surfaces, their operation can be probed with sub-molecular precision, allowing observation of rotational pathways and intermediates. In nanomachines, it could be advantageous to have not only one, but several motor units incorporated. However, the synthesis of such complex molecules is very challenging. Here, we studied whether individual Feringa-type motor units can be coupled covalently directly on a Au(111) surface to form bimotors, thus avoiding the complex synthesis and difficult deposition of molecules that contain more than one motor unit. Using low-temperature scanning tunnelling microscopy (STM) under ultrahigh vacuum conditions, we identified individual bimotor molecules after the coupling and could resolve distinct conformations. Moreover, conformational transitions and lateral translation could be induced by STM tip manipulation. The results for bimotors are compared with the mono-motors, i.e. before the coupling. Our results demonstrate controlled reactions and manipulation of molecular motors on a metallic surface, supporting the development of more complex nanomachines.

O 46.8 Tue 14:00 P2

Optical properties of pi conjugated molecule on insulator films supported by metal surface — •harshita malik — Clausius Institute for Physical and Theoretical Chemistry , University of Bonn,Bonn,Germany

Quinacridone (QA) is a pi-conjugated molecule whose optical properties are strongly influenced by hydrogen bonding and by its local environment. To establish consistent reference data, we determined the gas-phase and solution-phase excitation energies of QA using CCSD, TDDFT, and GW-BSE, and compared the results with available experimental spectra. These calculations provide reliable values for the ionization potential, the lowest singlet excitation, and the main vibronic features.

We then examined several structural variants of QA, including tautomers, substituted derivatives, and solid-state polymorphs. Their different packing motifs lead to measurable shifts in excitation energies, which we quantified using periodic GW-BSE.

To investigate QA on insulating surfaces, we used machine-learning potentials (MACE) combined with Bayesian optimization (BOSS) to identify stable adsorption geometries on KCl(100). The monomer and dimer structures obtained from this approach agree with DFT benchmarks and serve as starting points for further excited-state calculations on KCl films supported on Ag(100). I am currently working on computing excitons and other optical properties for QA adsorbed on these KCl/Ag surfaces to understand how substrate screening and adsorption geometry modify its electronic and optical response.

O 46.9 Tue 14:00 P2

Photoemission intermittency from organic quasi-one-dimensional crystals coupled with silver nanoparticles — •Moha Naeimi[1,2], Waqas Pervez[1,2], Frithjof Harmsen[1,2], Ingo Barke[1,2], and Sylvia Speller[1,2] — [1]Institute of physics, University of Rostock — [2]Department of life, light & matter, University of Rostock

Organic, quasi-one-dimensional crystals are suitable platforms for triplet exciton migration, latter only requiring minimal orbital coupling [1]. In organic molecules, triplet excitons can be generated via singlet fission, where excited singlet states convert into two long-lived triplet states [2]. We recently prepared long quasi-one-dimensional rubrene crystals on silicon substrates with a native thin silicon oxide layer (SiO2) [3]. After depositing Ag nanoparticles, we observe strong photoemission intermittency (blinking) at the interface sites and weak blinking on the rod crystal itself. In this work, we characterize the blinking in terms of its time traces and time-of-flight electron spectra. The blinking is consistent with exciton propagation that becomes trapped at nanoparticle-containing interface sites, where apparent electron binding energies shift to lower values. These molecule-nanoparticle systems offer promising pathways for directed energy transport and guided exciton migration.

[1] S. R. Yost et. al., J. Phys Chem C 116, 17369 2012. [2] T. Zhu et. al., J. Phys. Chem. Lett. 9, 6502 - 6510 2018. [3] Naeimi et. al, Adv. Opt. Mater., 2025 (DOI:10.1002/adom.202502744).

O 46.10 Tue 14:00 P2

Tip-induced hysteretic switching in copper-coordinated bipyridine (BIPY) thin films — •Sunny M P Gautam, Ankita Jaiswal, Thiruvancheril G Gopakumar, and Sandeep Verma — Indian Institute of Technology, Kanpur, India

In this work, we present a rationally designed hypoxanthine-based ligand, 1,9-bis(pyridine-2-ylmethyl) hypoxanthine (BIPY), specifically tailored for constructing functional surface-confined metal-organic networks (SMONs). The ligand integrates a π-conjugated purine core with flexible pyridyl donor arms, creating a nitrogen-rich, tridentate coordination environment ideal for forming robust 2D frameworks. Its conformational adaptability around metal centers enables dynamic metal*ligand interactions, offering a pathway toward SMON-based molecular switching driven by electronic-state transitions rather than geometric changes. Such electronically mediated bistability provides enhanced stability and potentially faster switching compared to conventional conformational molecular switches. Our results highlight BIPY as a promising platform for developing adaptive, switchable SMON architectures with potential applications in sensing, spintronics, data storage, and molecular logic systems.

O 46.11 Tue 14:00 P2

Monolayers of Thiols with Very High Dipole Moments Show Surprisingly Small Work Function Changes — Michael Gärtner[1], Andreas Terfort[1], and •Michael Zharnikov[1,2] — [1]Institut für Anorganische und Analytische Chemie, Johann Wolfgang Goethe Universität Frankfurt, 60438 Frankfurt am Main, Germany — [2]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

The recently introduced concept of distributed dipoles in molecular self-assembly was combined with the standard dipolar tail group decoration in the context of electrostatic engineering of surfaces and interfaces by self-assembled monolayers (SAMs). To this end, thiol-anchored molecules, containing dipolar 2,5-bipyrimidine units within their molecular backbones, were decorated with either nitrile or dimethylamino tail groups and assembled on Au(111). The directions of the distributed and tail group dipoles were aligned either upwards or downwards to the anchor to achieve the maximum effect on the work function (WF) of the substrate. Despite a dense molecular packing and an upright molecular orientation, the decoration of the bipyrimidine thiols with the tail groups not only provided no WF gain but even had a detrimental effect in the dimethylamino case. This behavior is explained by the upside-down orientation of a part of the molecules in the SAMs, driven by the minimization of the energy associated with the strong dipole-dipole interaction between the SAM-forming molecules.

O 47: New methods: Theory

Time: Tuesday 14:30–15:30 Location: HSZ/0201

O 47.1 Tue 14:30 HSZ/0201

Energy-resolved tip-orbital fingerprint in scanning tunneling spectroscopy based on the revised Chen's derivative rule — Ivan Abilio[1,2] and •Krisztián Palotás[1] — [1]HUN-REN Wigner Research Center for Physics, Budapest, Hungary — [2]Budapest University of Technology and Economics, Budapest, Hungary

The revised Chen's derivative rule for electron tunneling [1] is implemented to enable computationally efficient first-principles-based calculations of the differential conductance dI/dV for scanning tunneling spectroscopy simulations [2]. By taking pristine and boron- or nitrogen-doped graphene sheets as sample surfaces, the reliability of our implementation is demonstrated by comparing its results to those obtained by the Tersoff-Hamann and Bardeen's electron tunneling models. It is highlighted that the energy-resolved direct and interference contributions to dI/dV arising from the tip's electron orbitals result in a fingerprint of the particular combined surface-tip system. The significant difference between the electron acceptor boron and donor nitrogen dopants in graphene is reflected in their dI/dV fingerprints. The presented theoretical method allows for an unprecedented physical understanding of the electron tunneling process in terms of tip-orbital-resolved energy-dependent dI/dV maps that is anticipated to be extremely useful for investigating the local electronic properties of novel material surfaces in the future.

[1] Phys. Rev. B 91, 165406 (2015).
[2] Phys. Rev. B 111, 245425 (2025).

O 47.2 Tue 14:45 HSZ/0201

Innovative Approaches to Semiconductor Surface Oxidation Studies Using Active Learning and MLIP — •Ondrej Krejci[1,2], Shola Adyemi[2], Konstantinos Konstantinou[2], and Milica Todorović[2] — [1]Department of Chemistry and Materials Science, Aalto University, Espoo, Finland — [2]Department of Mechanical and Materials Engineering, University of Turku, Turku, Finland

Oxygen passivation of InAs surfaces critically affects material performance in electronic devices, but the nature of the oxide surface reconstruction is not well characterized. To address this, we employ a machine learning (ML) driven workflow. Starting from the $\zeta(4\times2)$ reconstruction of pristine InAs(100) [1], we use Bayesian Optimization [2] to identify oxygen binding sites. This allows us to populate the surface with increasing number of oxygen atoms. The oxide models serve as input for a ML interatomic potential based on the MACE model [3], trained via the active learning method PALIRS [4]. The potential is used for molecular dynamics simulations to identify promising candidates for the oxidized InAs(100) surface reconstruction. Our workflow enables an efficient exploration of configurational space surpassing traditional computational approaches.

[1] Appl. Phys. A 75, 89 (2002)
[2] Npj. Comput. Mat. 5, 35 (2019)
[3] NeurIPS 35, 11423 (2022)
[4] Npj Comput. Mat. 11, 324 (2025)

O 47.3 Tue 15:00 HSZ/0201

Complete basis limit with hybrid functionals using LAPW — •Janis Uzulis and Andris Gulans — University of Latvia, Riga, Latvia

We present a systematic framework for achieving the complete basis limit (CBL) for molecules and solids in hybrid functional calculations with density functional theory using the linearized augmented plane wave (LAPW) method. Standard LAPW calculations with nonlocal exchange employ radial basis functions and core orbitals obtained from a (semi)local functional, leading to inconsistencies that prevent the calculations from converging to CBL. We address this issue and achieve the same level of precision that previously was attainable only with local functionals. By applying this method, we obtain the Hartree-Fock total energy for crystals with a few μHa precision. Aside from high-quality reference data (reaction energies, cohesive energies and equation of state) for computational-chemistry and band-structure codes, our work provides an insight into the range of applicability of the standard approach to hybrids in LAPW.

O 47.4 Tue 15:15 HSZ/0201

AI-Driven Optimization Techniques for Density Functional Theory Calculations — Álvaro Fraile-Carmena[1], Damián Sánchez-Maqueda[1], Cristian Ramírez-Atencia[1], and •María Camarasa-Gómez[2] — [1]Universidad Politécnica de Madrid, C/ Alan Turing, s/n, Madrid 28031, Spain — [2]Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), Paseo de Manuel Lardizábal 5, Donostia-San Sebastián 20018, Spain

Accurately determining optoelectronic properties of molecules and solids is an ongoing challenge in first-principles methods. This objective has gained even more relevance, as research on quantum materials evolves rapidly. So far, density functional theory (DFT) has remained the primary computational tool for this task. However, reaching with DFT accuracy levels comparable to many-body perturbation theory still requires significant computational effort [1]. Here we introduce an approach that integrates AI-driven optimization techniques into DFT workflows [2]. Embedding these optimization methods directly in ab initio software enhances both accuracy and efficiency. We present results obtained with surrogate models and state-of-the-art open source optimization libraries

[3], showing their potential to accelerate and improve electronic structure simulations.
[1] M. Camarasa-Gómez, S. E. Gant, et al., npj Comput. Mater. 10, 288 (2024)
[2] Á. Fraile-Carmona, D. Sánchez-Maqueda, C. Ramírez-Atencia, and M. Camarasa-Gómez (2025) [in preparation]
[3] J. Blank, and K. Deb, IEEE Access 8, 89497 (2020)

O 48: Metal & Semiconductor substrates: Structure, epitaxy and growth

Time: Tuesday 14:30–16:00 Location: HSZ/0204

O 48.1 Tue 14:30 HSZ/0204

Electric-field induced formation of a two-dimensional adatom gas on cryogenic Li(110) — Shyam Katnagallu[1], Samuel Mattoso[1], Huan Zhao[1,2], Se-Ho Kim[1,3], Jing Yang[1], Baptiste Gault[1,4], •Christoph Freysoldt[1], and Jörg Neugebauer[1] — [1]MPI for Sustainable Materials, Düsseldorf Germany — [2]State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an, China — [3]Department of Materials Science and Engineering, Korea University, Seoul, Korea — [4]Department of Materials, Royal School of Mines, Imperial College London, UK

The field evaporation behavior of Li at 60 K in atom probe tomography (APT) shows very inhomogeneous distribution on the detector hit map with hot-spot sites accounting for thousands of evaporations, implying an unusual high surface mobility. We therefore investigated the ad-atom energetics and diffusion behavior on the prototypical Li(110) surface in the presence of the very high fields (10^{10} V/m) by density-functional theory. Two key effects are found to jointly explain the experimentally observed behavior. Firstly, free ad-atoms become energetically favorable over kink sites at fields above 10 V/nm, making sizeable ad-atom densities in thermodynamic equilibrium. Secondly, the ad-atom diffusion barrier vanishes at ~11 V/nm due to a degeneracy of the on-top and bridge sites. We suggest that a highly dynamic ad-atom gas forms, that enables efficient transport to evaporation hotspot sites. Our static calculations are corroborated by molecular dynamics simulations, that show the spontaneous ad-atom emission from a kink-site enabled by the field.

O 48.2 Tue 14:45 HSZ/0204

Structural analysis of the interaction of H_2S with the FeO_2 chain phase on Ir(100) — •Alexander Wegerich, Eric Engel, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

On the Ir(100) surface, a self-organised growth of oxide chains of the form Ir(100)-(3 × 1)-MO_2 (M = Mn, Fe, Co and Ni) can be observed. These transition metal oxide chains are shifted by half an Ir(100) lattice constant with respect to the iridium rows [1]. Furthermore, it is possible to reduce these oxide chains to an Ir(100)-(3 × 1)-MIr_2 (M = Mn, Fe, Co and Ni) surface alloy by annealing under H_2 atmosphere, now with the reduced chains aligned to the Ir rows [2].
Using quantitative LEED-IV analyses, STM and DFT, we examine whether the iron oxide chain phase can be structurally changed and/or tuned by reaction with S, the only other non-metallic chalcogen. In contrast to oxygen, sulphur does not create a Ir(100)-(3 × 1)-FeS_2 chain-like phase, but a c(6 × 2) superstructure. Prepared by annealing the FeO_2 chains under a H_2S atmosphere, the oxide chains are reduced and sulphur adsorbes on them. The so-formed c(6 × 2) can be interpreted as a c(2 × 2)-S adphase on the Ir(100)-(3 × 1)-$FeIr_2$ chains.
[1] P. Ferstl et al., Phys. Rev. Lett. **117**, 046101 (2016)
[2] P. Ferstl et al., Phys. Rev. B **96**, 085407 (2017)

O 48.3 Tue 15:00 HSZ/0204

STM study of surface evolution and phase stability in Sn/Pt(111) systems — •Qing Shi, Fumio Komori, Masaki Mizuguchi, and Toshio Miyamachi — Nagoya University, Nagoya, Japan

The formation of Pt_3Sn surface alloys on Pt(111) is of considerable interest for applications in catalysis and topological electronics. Depositing Sn on Pt(111) followed by annealing offers a route to realize atomically flat, single-crystalline Pt_3Sn(111) surfaces suitable for detailed surface studies. Here, we reveal how the annealing process directly controls the surface morphology and local electronic structure in Sn/Pt(111) systems by scanning tunneling microscopy and spectroscopy (STM/S).

In the lower-temperature regime (< 400 K), where a Sn overlayer is stabilized, Sn atomic layers preferentially attach to step edges. The STS measurements indicate that the Sn overlayer is metallic due to hybridization with the Pt substrate. Upon annealing to higher temperatures, the surface undergoes Pt-Sn alloying, leading to the formation of a Pt3Sn phase across the surface. This transition is accompanied by pronounced island coarsening, morphological rounding, and an increase in local disorder, driven by thermally activated atom processes. Equilibrium shape analysis of the alloy islands reveals nearly isotropic step free energies, indicating minimal energetic differences between alternating A- and B-type step edges. Spectra acquired on the Pt_3Sn terraces show a high density of states near the Fermi level, corresponding to contributions from both bulk and surface electronic states.

O 48.4 Tue 15:15 HSZ/0204

Enhanced thermal switching of an azobenzene derivative via metal doping on graphitic surfaces. — •Nidhi Rawat[1], Hariom Birla[2], and Thiruvancheril G. Gopakumar[3] — [1]Indian Institute of Technology Kanpur, Kanpur, India — [2]Indian Institute of Technology Kanpur, Kanpur, India — [3]Indian Institute of Technology Kanpur, Kanpur, India

The thermal isomerization (switching) of azobenzene derivatives is often limited by high activation barriers, limiting efficient switching between trans and cis configurations induced by heat. In this study, we first examined the thermal induced switching of pristine azobenzene-based thin films and observed no isomerization upon heating. Upon introducing a metal dopant into the films, several morphological changes are observed, across varying molecular coverages, upon heating confirming that thermal switching is readily induced in the doped films. The analysis of the morphology and microscopic structure of the film is analysed using AFM and STM. These results clearly demonstrate that metal doping can effectively modulate the energy barrier and facilitate thermally driven molecular switching. This approach offers a promising pathway to tailor the isomerization dynamics of molecular systems, providing new opportunities for the development of thermally responsive devices.

O 48.5 Tue 15:30 HSZ/0204

Evolution of surface superstructures on altermagnetic MnTe thin films — •Marco Dittmar, Franziska Beisler, Hannes Haberkamm, Lena Hirnet, Maximilian Ünzelmann, and Friedrich Reinert — Exp. Physik VII and Würzburg-Dresden Cluster of Excellence ctd.qmat, Universität Würzburg, Germany

MnTe has recently attracted significant attention as a workhorse altermagnet, where real space spin arrangements give rise to symmetry-driven, momentum-dependent spin splitting without net magnetization. In terms of basic research as well as for enabling high-quality interfaces in potential devices, the investigation of the surface atomic structure of MnTe becomes very important. In this talk, we present an electron diffraction surface analysis of epitaxially grown MnTe thin films, highlighting the factors that govern their surface atomic structure. In particular, we discuss how variations in Te flux and surface evaporation conditions guide the formation and stability of different surface reconstructions, we have found experimentally.

O 48.6 Tue 15:45 HSZ/0204

Atomic structure of MBE-grown Ta-Ge alloy on Ge(001). — •Suhani Singh[1], David Sommers[1], Patrick Strohbeen[2], Yi-Hsun Chen[1], Javad Shabani[2], Arkady Fedorov[1], and Peter Jacobson[1] — [1]School of Mathematics and Physics, University of Queensland, St. Lucia, Queensland 4072, Australia — [2]Center for Quantum Information Physics, Department of Physics, New York University, New York, New York 10003, USA

Tantalum-germanium (Ta-Ge) alloys are a promising option for superconducting devices.[1] Here, we study the atomic-scale structure and thermal evolution of an MBE-grown Ta-Ge alloy film on Ge(001) using scanning tunnelling microscopy (STM) and synchrotron-based soft x-ray photoemission (XPS). A series of annealing steps between 673 K and 873 K smoothed the initially corrugated surface and enabled atomic-resolution STM. Short anneals at 873 K, reveal threefold symmetric surface domains. Longer anneals at 873 K led to the appearance of square lattice consistent with Ta(100), coexisting with more corrugated regions. Further temperature increase made the surface progressively rougher and difficult to image. Synchrotron-based XPS shows higher temperature annealing produces a Ge-rich surface, suggesting Ta migrates into the bulk. These preliminary results map out how thermal processing affects the Ta-Ge surface and will guide strategies to obtain cleaner, sharper superconductor-semiconductor interfaces.

[1] Patrick J Strohbeen et al. *Molecular beam epitaxy growth of superconducting tantalum germanide*. Applied Physics Letters 124, 9 (2024).

O 49: Plasmonics and nanooptics: Light-matter interaction, spectroscopy I

Time: Tuesday 14:30–15:45 Location: HSZ/0403

O 49.1 Tue 14:30 HSZ/0403

Beyond-Dipole Approaches to Generating and Applying Twisted Light — •Esra Ilke Albar[1], Franco Bonafé[1], Valeriia Kosheleva[1], Heiko Appel[1], and Angel Rubio[1,2] — [1]Max-Planck-Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, DE — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute, 162 Fifth Avenue, New York, New York 10010, USA

We perform numerical electrodynamics simulations where a nanoplasmonic Archimedean spiral is targeted with a circularly polarized, 8-cycle plane wave pulse to probe the generation of twisted pulses, i.e., fields with orbital angular momentum(OAM). We identify mismatches between the generated pulse and the ideal OAM beams, which motivates us to discuss the spatiotemporal optical vortices (STOVs). All realistic electromagnetic fields are finite pulses, while the structural properties of plasmonic OAM generators are often adjusted to the central wavelength. As a next step, we employ a two-particle point charge system to map the local OAM density and confirm the space dependence of the generated pulse. This pushes us to expand beyond the known electric dipole approximation(EDA). We introduce our beyond dipole formalism and present high harmonic generation results computed within this approach.

O 49.2 Tue 14:45 HSZ/0403

Electro-Optic Phonon Polaritons — •Michael S. Spencer[1], Olga Minakova[1], Maximilian Frenzel[1], Joanna M. Urban[1], Martin Wolf[1], and Sebastian F. Maehrlein[1,2,3] — [1]FHI Berlin — [2]HZDR — [3]TU Dresden

Ultrafast control of fundamental excitations and order parameters represents a major driving force for the rising field of terahertz (THz) cavity electrodynamics. However, most efforts to date have not taken full advantage of THz sampling capabilities. By using an electro-optic crystal to fill a cavity, we directly measure intra-cavity electric fields, and polarizations arising from dipole-active excitations, all in the time domain. We identify that under cryogenic conditions, and in high-quality cavities, a polaritonic state is formed from the superposition of cavity photons and optical phonons. We explore the relationship between the light-matter coupling strength and temperature, and between the polariton splitting and cavity quality factor. With our novel electro-optic cavity design, we are able to investigate the detuning-dependence of the strong coupling behavior, obtaining the full picture of light-matter interactions. Furthermore, we reveal fluence-dependent polariton dynamics, indicative of significant coupling beyond the harmonic approximation. This identification of strong light-matter interactions in electro-optic cavities opens an important new testing ground for measuring novel, light-matter-entangled states.

O 49.3 Tue 15:00 HSZ/0403

Femtosecond and attosecond correlations in multi-electron pulses — •Rudolf Haindl[1,2], Valerio Di Giulio[1,2], Armin Feist[1,2], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Göttingen, Germany

In femtosecond electron emission from nanoscale field emitters, Coulomb interactions result in structured few-electron states exhibiting strong correlations in energy [1,2], transverse momentum [1], and time [3]. Here, we combine femtosecond-gated, event-based detection with inelastic electron-light scattering to directly map the phase-space distribution of two-electron states [4].

Our experiments reveal a bimodal structure in longitudinal phase space, distinguishing contributions from interparticle interaction and dispersion. Furthermore, we demonstrate that global phase modulation coherently shapes the few-electron distribution to exhibit attosecond temporal correlations. We show how this controlled phasing drives a multi-electron quantum walk, a phenomenon that can be harnessed to produce tailored excitations and superradiance via two-electron energy post-selection.

[1] R. Haindl et al., Nat. Phys. 19, 1410-1417 (2023).
[2] S. Meier et al., Nat. Phys. 19, 1402-1409 (2023).
[3] J. Kuttruff et al., Sci. Adv. 10, eadl6543 (2024).
[4] R. Haindl et al., Phys. Rev. Lett. 135, 165002 (2025).

O 49.4 Tue 15:15 HSZ/0403

Quantum-electrodynamical density-functional theory for periodic solid-state materials — •Benshu Fan[1], I-Te Lu[1], Michael Ruggenthaler[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter — [2]Center for Computational Quantum Physics (CCQ), The Flatiron Institute

Quantum-electrodynamical density-functional theory (QEDFT) has emerged as a powerful first-principles framework for describing properties of materials coupled to quantized electromagnetic fields. While it has been successfully applied to capture cavity-induced modifications of electronic structures mainly for atoms and molecules, a consistent treatment of phonon-related and optical properties for periodic solids remains elusive. In this work, we present a unified QEDFT framework that incorporates collective light-matter coupling in the electronic ground state, density functional perturbation theory for phonons, and real-time time-dependent QEDFT for optical excitations. This approach enables ab initio calculations of cavity-modified electronic and phononic dispersions, Born effective charges, dielectric tensors, and both non-resonant and resonant optical absorption spectra for solids. Using wurtzite gallium nitride (GaN) embedded in an optical cavity as an example, we show how the quantized vacuum field reshapes electronic and phononic properties and gives rise to possible experimentally observable signatures in the dielectric function and absorption spectra. Our results establish QEDFT as a general first-principles framework for exploring and predicting cavity-modified properties of quantum materials.

O 49.5 Tue 15:30 HSZ/0403

Anyonic Chern Insulator in Graphene Induced by Surface Electromagnon Vacuum Fluctuations — •Xinle Cheng[1], Emil Viñas Boström[1], Frank Y. Gao[2], Edoardo Baldini[2], Dante M. Kennes[1,3], and Angel Rubio[1,4] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Department of Physics, The University of Texas at Austin, Austin, Texas, 78712 — [3]Institute for Theory of Statistical Physics, RWTH Aachen University, 52056 Aachen, Germany — [4]Initiative for Computational Catalysis, The Flatiron Institute, Simons Foundation, New York City, NY 10010, USA

Sub-wavelength cavities have emerged as a promising platform to realize strong light-matter coupling in condensed matter systems. Previous studies are limited to dielectric sub-wavelength cavities, which preserve time-reversal symmetry. Here, we lift this constraint by proposing a cavity system based on magnetoelectric materials, which host surface electromagnons with non-orthogonal electric field and magnetic field components. The quantum fluctuations of the surface electromagnons drive a nearby graphene monolayer into an anyonic Chern insulator, characterized by anyonic quasi-particles and a topological gap that decays polynomially with the graphene-substrate distance. Our work opens a path to controllably break time-reversal symmetry and induce exotic quantum states through cavity vacuum fluctuations.

O 50: Electronic structure theory II

Time: Tuesday 14:30–16:15 Location: TRE/PHYS

O 50.1 Tue 14:30 TRE/PHYS

Efficient DFPT for 2D Films in the FLAPW Code FLEUR — •Thomas Bornhake[1,2], Alexander Neukirchen[1], Gregor Michalicek[1], Daniel Wortmann[1], Gustav Bihlmayer[1], and Stefan Blügel[1,2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institute for Theoretical Physics, RWTH Aachen University, 52074 Aachen, Germany

Interest in structural instabilities, magnetism, transport, and superconductivity in 2D films is rapidly increasing, and all of these phenomena involve phonons. However, *ab initio* phonon calculations for films typically require large supercells, which include substantial vacuum. As a result, they become computationally expensive. In this talk, we present an efficient and unique DFPT implementation in the context of the all-electron FLAPW code FLEUR [1,2] that treats films as single slabs in a truly 2D geometry perfectly embedded in semi-infinite vacuum [3]. We outline the key features of the method, benchmark it against the commonly employed supercell approach, and show first results on how a homogeneous external electric field modifies the phonon properties.

This work was supported by the CoE-MaX (EuroHPC Joint Undertaking, Grant 101093374) and DFG through CRC 1238 (Project C01).

[1] D. Wortmann *et al.*, 10.5281/zenodo.7576163; www.flapw.de
[2] C.-R. Gerhorst *et al.*, Electron. Struct. **6**, 017001 (2024).
[3] M. Posternak *et al.*, Phys. Rev. B **21** 5601 (1980).

O 50.2 Tue 14:45 TRE/PHYS

Valence only FLOSIC with pseudo core electrons — •Simon Liebing and Jens Kortus — Institute of Theoretical Physics, TU Bergakademie Freiberg, 09599 Freiberg, Germany

Over the past decade, the FLOSIC method [1, 2] has demonstrated its versatility and applicability to a wide range of systems. However, it has been observed that this method can require significant computational time, particularly when adjusting the core electrons in the case of heavier elements. Previous work has shown that FLOSIC calculations can be effectively carried out using pseudopotentials [3]. In the case of heavier atoms, however it is possible that the valence orbital descriptors may shift too close to the core region due to the limitations of pseudopotentials. In this work, the authors introduce a novel approach to also account for the repulsive interactions between the core and valence electron FLOSIC descriptors in case of pseudopotentials. This method has the potential to significantly reduce the computational cost typically associated with SIC calculations compared to standard DFT methods. References: [1] M. R. Pederson et al., J. Chem. Phys., 140, 121103 (2014) [2] S. Schwalbe, et al., J. Chem. Phys., 153, 8, 2020. [3] S. Liebing et al., DPG Verhandlungen Berlin, O, Session 82, Contribution 8, 2018.

O 50.3 Tue 15:00 TRE/PHYS

Spectroscopy of chemisorped systems from a first-principles local-orbital representation — •Simiam Ghan and Jens Nørskov — Technical University of Denmark DTU

We present a local-orbital representation of density functional theory (DFT) which elucidates the properties of chemisorped systems. A direct calculation of orbital overlap and coupling matrix elements between the adsorbate and surface allows us to construct the hybridization function, familiar from e.g. Anderson-Newns-Grimley models, which encodes rich orbital phase interactions[1]. Beyond a qualitative tool, we demonstrate the quantitative correspondence of this object to observables in ultrafast spectroscopy and scanning-tunneling spectroscopy. The scheme is generally useful to assess the coupling between a local state and its environment from first principles.

[1] S. Ghan *et al*., J. Chem. Phys. 158, 234103 (2023).

O 50.4 Tue 15:15 TRE/PHYS

Quantum-mechanical analysis of the 4H-SiC surface — •Kateřina Dočkalová[1,2], Martin Friák[2], and Jana Pavlů[1] — [1]Dept. Chem., Masaryk Uni., Brno, Czech Rep. — [2]Inst. Phys. Mater., Czech Acad. Sci., Brno, Czech Rep.

Silicon carbide (SiC) is a key wide-bandgap semiconductor employed in high-power and high-voltage electronic devices. Among its polytypes, 4H-SiC is particularly promising for next-generation power electronics. We investigated the atomic and electronic structure of the 4H-SiC (0001) surface with a specific focus on the challenges of modelling polar orientations. To accurately capture the intrinsic surface properties, we evaluate the planar-averaged electrostatic potential and the electron localisation function (ELF) using various models (differing in bottom-surface termination, passivation with pseudohydrogens, and vacuum thickness) and applying electrostatic corrections. These strategies suppress artificial dipole moments and eliminate spurious internal electric fields that often compromise surface calculations. We find that either carbon termination at the bottom surface or pseudohydrogen passivation can individually introduce a spurious internal electric field manifested in the vacuum potential. Interestingly, applying electrostatic corrections does not improve the electrostatic-potential profile for models in which the vacuum region is already sufficiently thick. Financial support from the Czech Academy of Sciences (Praemium Academiae, M.F.) and Masaryk University (MUNI/A/1691/2024) is acknowledged. Computational resources were provided via e-INFRA CZ (ID:90254).

O 50.5 Tue 15:30 TRE/PHYS

Quantifying conductance variations in single molecule junctions using machine learning — •Hector Vazquez — Inst. of Physics, Czech Academy of Sciences

In single molecule circuits, conductance (the inverse of resistance) is strongly dependent on the junction geometry. Break-junction experiments are often carried out at room temperature, where many molecular conformations are sampled during the measurements. In contrast, the computational cost of DFT-NEGF calculations restricts them to only a few geometries.

We recently developed a computationally efficient method to calculate molecular conductance within DFT for thousands of geometries, based on small Au-molecule-Au clusters [1,2]. Their geometry is taken from MD simulations of the junction at room temperature. We can thus compute within DFT the conductance for tens of thousands of thermally-accessible molecular geometries.

We study typical conjugated and alkane molecules and interpret these large conductance datasets with machine learning methods including regression models, feature importance techniques, and SHAP analysis. Our work identifies which of the bond lengths, angles, or dihedral angles in the molecule, all of which are changing continuously and simultaneously, have a larger impact on conductance.

[1] H. Vazquez, J. Phys. Chem. Lett. 13 9326 (2022)

[2] E. Montes, W.Y. Rojas and H. Vázquez, J. Phys. Chem. C 129, 9947 (2025)

O 50.6 Tue 15:45 TRE/PHYS

Towards Accurate Surface Adsorption Through a Numeric-Orbital FDET Framework — •Danjo De Chavez[1] and Reinhard J. Maurer[1,2,3] — [1]Department of Chemistry, University of Warwick, UK — [2]Department of Physics, University of Warwick, UK — [3]Faculty of Physics, University of Vienna, AT

Multiscale embedding methods balance accuracy and computational efficiency in modeling extended materials by combining high-level treatments of active regions with lower-level descriptions of their environments. We implemented Frozen Density Embedding Theory (FDET) with Freeze-and-Thaw (F&T) cycles in the numeric atomic orbital code FHI-aims, enabling consistent cluster and periodic calculations. Initial electron densities are constructed from free-atom superpositions, with one subsystem kept frozen while the other is optimized. The implementation leverages the efficient parallelization of FHI-aims. Embedding potential and subsystem density are decomposed using an auxiliary basis set via an RI framework, facilitating reconstruction in the real space. This method enables accurate predictions with high-level theory for adsorption, bond dissociation, optical excitation, and charge-transfer phenomena relevant to surface catalysis and spectroscopy.

O 50.7 Tue 16:00 TRE/PHYS

Brillouin zone sampling in ONETEP — •Chengcheng Xiao, Peter Haynes, and Arash Mostofi — Department of Material, Imperial College London, London SW7 2AZ, United Kingdom

ONETEP is a parallelised linear-scaling density-functional theory (DFT) simulation software package designed for large-scale calculations of properties of materials. It was engineered under the premise that, for self-consistent calculations of systems with thousands of atoms, the Brillouin zone only needs to be sampled at its centre - the Gamma-point.

Whilst this is a suitable approximation for large systems, it often leads to the unnecessary use of large supercells of structures where periodicity can be exploited. For those systems, a more suitable method is to sample the Brillouin zone along the periodic directions.

In this work, we introduce a new Brillouin zone sampling technique in ONETEP where the localisation constraint imposed on the basis functions is selectively lifted along the periodicity directions, making it possible to perform a "hybrid" calculation where the best scaling can be achieved by incorporating both Brillouin zone sampling and linear-scaling techniques. Furthermore, if the unit cell is small along all directions, all localisation constraints can be lifted, which effectively turns ONETEP into a plane-wave code. This enables us to compare the algorithmic accuracy of ONETEP to other DFT codes on the same footing. These developments enable much more efficient calculations on short and intermediate-scale periodic systems, such as bulk crystals, nanowires, surfaces, and interfaces.

O 51: Focus Session: Structure and Dynamics of Solvent at Electrochemical Interfaces II

Understanding how solvent molecules organize and move at electrochemical interfaces is central to catalysis, energy conversion, and electrochemical materials science. This Focus Session will bring together experimental and theoretical leaders using complementary surface specific spectroscopies as vibrational sum frequency generation, advanced X ray/electron techniques, and multiscale simulations to reveal intermolecular structure, hydrogen bond networks, ion-solvent coupling, and field driven dynamics from single crystal electrodes to complex battery interfaces. By highlighting recent breakthroughs in time-resolved measurements and operando platforms, the session aims to connect fundamental interfacial physics with macroscopic performance in electrocatalysis, corrosion, and electrochemical energy storage.

Organized by Yujin Tong (U Duisburg-Essen) and Angelika Kühnle (U Bielefeld).

Time: Tuesday 14:30–15:45 Location: TRE/MATH

Invited Talk O 51.1 Tue 14:30 TRE/MATH

Ultrafast aqueous electric double-layer dynamics — •Mischa Bonn — Max Planck Institute for Polymer Research

The formation of electric double layers (EDLs) at solid-liquid interfaces is universal, yet their molecular structure and dynamics remain incompletely understood. Building on recent advances in interface-specific spectroscopy and nanofluidic model systems, this talk will address how interfacial polarization, geometric confinement, and charge density collectively shape the structure and dynamics of water at electrochemical interfaces. We will highlight new femtosecond-resolved optical spectroscopy measurements that access the genuine ultrafast response of the aqueous EDL, revealing that field-driven ionic rearrangements and solvent reorganization occur on time scales of only a few tens to hundreds of picoseconds - significantly faster than expected from classical diffusion-limited models. These results demonstrate that collective many-body interactions and short-range correlations dominate the EDL response long before macroscopic diffusion sets in. Taken together, the studies provide a molecularly consistent picture in which interfacial polarization and charge act in concert to control water structure and dynamics across electrochemical interfaces, with direct implications for energy conversion, ion transport, and operando spectroscopies of electrified surfaces.

O 51.2 Tue 15:00 TRE/MATH

Second-order nonlinear vibrational spectroscopy: from depth-resolved studies at charged aqueous interfaces towards determining excitonic-vibrational coupling in hybrid heterostructures — •Debojyoti Roy, Sarabjeet Kaur, Álvaro Díaz Duque, Martin Wolf, Alexander P. Fellows, and Martin Thämer — Fritz-Haber-Institut of the Max Planck Society, 14195 Berlin, Germany

The properties of charged aqueous interfaces are governed by interfacial electric fields that influence ion distributions in the liquid phase, forming an electric double layer. While the evolution of the electric potential is relatively well described by theoretical models, much less is known about the influence of the DC fields on the interfacial molecular structure of water and its evolution with depth. Using our recently developed combined sum- and difference-frequency generation spectroscopy (SFG/DFG), we investigate the depth-dependent water structure at charged interfaces as a function of ionic strength, obtaining deep insight into the anisotropic orientational distribution of water and detailed information on the properties of the hydrogen bond network at different distances from the phase boundary.

Besides depth-resolution, the complementary information from SFG and DFG responses can also be used to isolate coupling terms in doubly-resonant studies. Here we also explore this possibility conceptually and propose such studies on exciton-vibrational coupling in 2D material/organic interfaces, which have various applications in solar cells but still lack understanding of their physicochemical properties.

Invited Talk O 51.3 Tue 15:15 TRE/MATH

Interface-specific nonlinear THz spectroscopy — •Chuanshan Tian — Department of Physics, Fudan Univ. China

Quantum confinement and proximity effects at material interfaces give rise to a range of novel physical and chemical phenomena, substantially advancing our ability to understand and control material properties. The development of in situ and interface-sensitive characterization techniques is therefore critical for uncovering the microscopic mechanisms governing interfacial systems and for improving device performance. This presentation will outline recent advances in interface nonlinear optical spectroscopic techniques, with a particular focus on their extension into the (multi-)terahertz spectral regime. Applications of these methods in probing interfacial microstructures and dynamic processes will be discussed, highlighting their potential for resolving complex interfacial phenomena with high specificity.

O 52: Oxide and insulator surfaces: Structure, epitaxy and growth I

Time: Tuesday 14:30–16:00 Location: WILL/A317

Invited Talk O 52.1 Tue 14:30 WILL/A317

Dynamics of catalytically active, atomically precise clusters on reducible oxide supports under the (fast) scanning tunneling microscope — •Friedrich Esch — TU Munich, Garching, Germany

Reducible oxides are versatile supports for catalytically active particles. Their reducibility offers the possibility to steer fundamental properties such as cluster stability and shape, charge transfer, lattice oxygen reverse spillover, or encapsulation. In this talk, I present our fundamental studies on the dynamics of atomically precise Pt clusters on two complementary supports, $Fe_3O_4(001)$, where reduction leads to interstitial diffusion and hole formation, and $CeO_2(111)$, where it leads instead to the formation of surface-near vacancies. As a local probe, we employ scanning tunneling microscopy (STM) at elevated temperatures and under reactive gas environments, upgraded with sophisticated tools for fast movie acquisition and cluster tracking. We complement this structural characterization with integral pulsed valve molecular beam "sniffer" activity and x-ray photoemission measurements. While on magnetite stabilization of even very small clusters via encapsulation is observed [1,2], on ceria, a dimensionality crossover from 3D to 2D clusters occurs, triggered by the degree of surface reduction [3].

[1] S. Kaiser et al., ACS Catal. 11 (2021) 9519.
[2] S. Kaiser et al., ACS Catal. 13 (2023) 6203.
[3] J. Reich et al., ACS Catal. 15 (2025) 18369.

O 52.2 Tue 15:00 WILL/A317

Segregation effects in 2D mixed oxide nano-islands: edge structure and composition in V(2-x)FexO3 monolayer islands — Ying Wang[1], Piotr Igor Wemhoff[1], Ghada Missaoui[1], Niklas Nilius[1], Jacek Goniakowski[2], and •Claudine Noguera[2] — [1]Carl von Ossietzky Universität Oldenburg, D-26111 Oldenburg, Germany — [2]CNRS-Sorbonne Université, Institut des Nanosciences de Paris, Paris, France

Low-coordinated atoms located at the surface or edges of oxide nanostructures play a crucial role in adsorption and reaction processes in heterogeneous catalysis. Contrary to binary compounds, there is a significant lack of information on their nature and behavior available for ternary materials. In this study, high-resolution scanning tunneling microscopy, DFT calculations and Monte Carlo simulations have been used to decipher the edge structure and composition of mixed V(2-x)FexO3 honeycomb monolayer islands grown on Pt(111).

DFT calculations and MC simulations demonstrate that, in contrast to a clear preference for VO-terminated edges in the pure V2O3 system, Fe segregation to the edges of mixed films tends to produce undercoordinated edge Fe cations, with a ratio of Fe/VO edge species highly sensitive to the oxygen environment. We show that the different oxygen affinity of V and Fe cations, yielding different bonding strengths of terminal vanadyl and ferryl groups are the main cause of the segregation pattern. The sensitivity of edge composition to the oxygen environment thus represents a lever for manipulating the edge configurations and tuning their catalytic response.

O 52.3 Tue 15:15 WILL/A317

Ultra-high THz-confinement in $LaAlO_3$ twin-walls — •Jakob Wetzel[1], Javier Taboada-Gutiérrez[2], Susanne C. Kehr[1], Alexey B. Kuzmenko[1,3], Lukas M. Eng[2], and Samuel D. Seddon[1] — [1]TU Dresden, Institute of Applied Physics, Nöthnitzer Straße 61, 01187 Dresden, Germany — [2]University of Geneva, Department of Quantum Matter Physics (DQMP), Geneva 1211, Switzerland — [3]ct.qmat: Dresden-Würzburg Cluster of Excellence EXC 2147, TU Dresden, 01062 Dresden, Germany

Recent advancements in polaritonics and nano-photonics have focused on the confinement of optical modes in ultra-thin films, 2D materials, and interfaces in order to uncover pathways toward ultra-compact nanophotonic circuits and sub-diffraction imaging technologies. Such approaches to THz-confinement face fundamental challenges such as inherent strain, defects, and lattice mismatches.

Here we present the experiment- and simulation-based investigations of ferroelastic twin-walls in $LaAlO_3$, which provide a *perfect* strain-free interface to explore optical effects emergent from the coincidence of two equal but directionally rotated optical axes. Scanning near-field optical microscopy (s-SNOM) in combination with the HZDR free electron laser FELBE shows an ultra-high confinement (>250) of THz-fields at these twin-wall. Experimental results are reproduced by COMSOL-simulations and understood with an adapted dipole model.

O 52.4 Tue 15:30 WILL/A317

Atomic-scale effects of surface modifications on mixed conducting oxides — •Matthäus Siebenhofer, Claudia Steinbach, and Jürgen Fleig — TU Wien, Institute of Chemical Technologies and Analytics, Vienna, Austria

Mixed ionic and electronic conducting (MIEC) oxide surfaces play a critical role in various technologies due to their high catalytic activity for processes such as oxygen reduction, oxygen evolution, and (photo)electrochemical water splitting. Recent advances have shown that even minute amounts of surface modifications can dramatically alter the work function and the catalytic performance but the detailed mechanisms behind these effects remain poorly understood.

This contribution discusses our efforts to understand the fundamental processes that occur during modification of MIEC oxide surfaces with ultra-thin oxide layers and acidic contaminants. We employ in-situ impedance spectroscopy during pulsed laser deposition (i-PLD) to monitor changes in the oxygen exchange activity of pristine thin film surfaces; X-ray photoelectron spectroscopy (XPS) and density functional theory (DFT) provide insights into atomic-scale processes induced by these modifications.

Our results demonstrate that surface modifications introduce charge redistribution between the modification and the MIEC oxide. These effects are governed by the ionic potential and acidity of both the host material and the modifying species. Based on these observations, we provide design strategies to tailor optimized material combinations for targeted catalytic applications.

O 52.5 Tue 15:45 WILL/A317

Probing electron-transfer between layers of a CrOx/Pt(111) thin film via workfunction and adsorption measurements in the STM — •Ghada Missaoui[1], Claudine Noguera[2], Jacek Goniakowski[2], and Niklas Nilius[1] — [1]Carl von Ossietzky University, Institute of Physics, D-26111 Oldenburg, Germany — [2]CNRS-Sorbonne University, UMR 7588, INSP, F-75005 Paris, France

Low-temperature tunneling spectroscopy has been employed to probe the workfunction of atomically flat Cr-oxide single- and double-stack films grown on Pt(111). The single-stack Cr3O6 trilayer exhibits an exceptionally high workfunction of more than 7.0 eV, decreasing to 5.0 eV for Cr6O11 double-stacks. The charge redistribution behind this workfunction drop was analyzed by density functional theory. The high workfunction of Cr3O6 trilayers originates from a massive electron transfer from the Pt(111) support into empty Cr-states that reduces 2/3 of the oxide cations from their formal 4+ to a 3+ charge state. The negative surface dipole diminishes upon growing a Cr-O honeycomb plane on top of the trilayer, forming a Cr6O11 double-stack. The ad-layer acts as electron donor, allowing the charge transfer from the platinum to decrease substantially. The charge redistribution not only triggers the detected workfunction drop but also leads to a different reactivity of single- versus double-stack CrOx films, as demonstrated with MgPc adsorption experiments performed with the STM.

O 53: Topical Talk Parkinson

Time: Wednesday 9:30–10:15 Location: TRE/PHYS

Topical Talk O 53.1 Wed 9:30 TRE/PHYS

Single-Atom Catalysis: Insights From Model Systems — •Gareth S. Parkinson — Institute of Applied Physics, TU Wien, Vienna, Austria

Single-atom catalysis promises maximal atom efficiency, tunable active sites and improved selectivity, and is now a key concept in the design of sustainable catalysts. Yet many of the central claims about what single-atom catalysts are, how they operate, and whether they remain truly isolated under reaction conditions are still under debate. In this overview talk I will use oxide-supported single atoms as case studies to examine what can really be established about structure, stability and mechanism, and where the evidence remains ambiguous. I will show how atomically well-defined model surfaces, probed by STM, noncontact AFM, XPS and vibrational spectroscopy, in tight integration with theory, can test key assumptions about single-atom catalysis. I will close with a perspective on outstanding challenges, from adsorbate induced restructuring and water to the transfer of insight from model systems to working catalysts.

O 54: Nanostructured surfaces and thin films

Time: Wednesday 10:30–12:30 Location: HSZ/0201

O 54.1 Wed 10:30 HSZ/0201

Advanced Characterization of Black Silicon via AFM and XPS: Geometric and Chemical Insights for better characterization of PV materials — •Jens Neurohr[1], Hendrik Hähl[1], Karin Jacobs[1], Michael Klatt[2], and Frank Müller[1] — [1]Experimental Physics and Center for Biophysics, Saarland University, Campus E2 9, 66123 Saarbrücken, Germany — [2]German Aerospace Center (DLR), Institute for Material Physics in Space, 51170 Köln, Germany

Understanding the link between surface geometry and chemical properties is crucial for photovoltaic (PV) applications, especially in nanostructured materials like black silicon (b-Si). RMS roughness is commonly used to describe nanorough surfaces, but it cannot capture their complexity or predict behaviors such as bacterial adhesion [1] or chemical composition.

On steep, irregular surfaces, chemical analysis techniques such as X-ray photoelectron spectroscopy (XPS) becomes challenging. To overcome this, we use Minkowski functionals and tensors [2,3] to relate XPS data to detailed Atomic Force Microscopy (AFM) topography.

Our results show that nanoscale geometry strongly influences chemical surface analysis and that geometric descriptors provide a powerful framework for studying complex surfaces.

[1] C. Spengler et al., Nanoscale, 11 (2019) 19713.
[2] R. Schneider, W. Weil, Springer (2008).
[3] G. E. Schröder-Turk et al., Advanced Materials, 23 (2011) 2535.

O 54.2 Wed 10:45 HSZ/0201

Systematic Investigation of Colloidal Au Nanoparticles for High-Density III-V Nanowire Growth — •Pavithira Manoharan, Chris Yanic Bohlemann, Peter Kleinschmidt, Thomas Hannappel, and Juliane Koch — Fundamentals of Energy Materials,Technical University of Ilmenau, 98693 Ilmenau, Germany

Over the past two decades, nanoscale structures such as III-V nanowires (NWs) have become versatile components for electronic and photonic applications, including high-performance photovoltaic and photoelectrochemical systems. Many simulation studies show that the density and lateral arrangement of NWs play a decisive role in optimizing light absorption, charge separation, and surface reactions. However, growing ordered NW arrays remains technologically challenging and costly. In this work, we present a simple and cost-effective method for producing high-density, disordered III-V NW using commercially available Au colloid solutions as a source of the catalyst particles. We perform a systematic study on how experimental parameters, such as surface preparation and substrate deposition conditions, affect the resulting nanowire density and diameter. This comprehensive approach provides insight into catalyst behavior prior to the vapor-liquid-solid growth and enables controlled modification of the NW structures. We also evaluate the limitations and potential of this method for NW-based energy conversion architectures.

O 54.3 Wed 11:00 HSZ/0201

Imaging the transition from diffusive to Landauer resistivity dipoles — •Serhii Kovalchuk[1,2], David Kämpfer[1,3,4], Jonathan K. Hofmann[1,3,4], Timofey Balashov[1,3,5], Vasily Cherepanov[1], Bert Voigtländer[1,3,4], Ireneusz Morawski[2], F. Stefan Tautz[1,3,4], and Felix Lüpke[1,6] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institute of Experimental Physics, University of Wrocław, 50-204 Wrocław, Poland — [3]Jülich Aachen Research Alliance (JARA), Fundamental of Future Information Technology, 52425 Jülich, Germany — [4]Lehrstuhl für Experimentalphysik IV A, RWTH Aachen University, 52074 Aachen, Germany — [5]Lehrstuhl für Experimentalphysik II A, RWTH Aachen University, 52074 Aachen, Germany — [6]II. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany

A point-like defect in a current-carrying conductor produces an electrochemical potential dipole that opposes the applied field. When the carriers mean free path is shorter than the defect size, the dipole reflects diffusive transport; when it is longer, ballistic scattering leads to a size-independent residual resistivity dipole as predicted by Rolf Landauer.

We investigate this behaviour around nanoscale holes in thin Bi films on Si(111) using scanning tunneling potentiometry. The measured dipole amplitudes show a clear crossover from linear to constant scaling with decreasing hole size, marking the transition from diffusive to Landauer-type dipoles. This crossover allows us to extract the Fermi wave vector and estimate the carrier mean free path in the Bi films.

O 54.4 Wed 11:15 HSZ/0201

Current-driven Rb^+ intercalation for on-chip tuning of superconductivity in Rb_xC_{60} thin films — •Konstantin Shchukin[1,2], Oliver Gallego Lacey[3], Baptiste Coquinot[4], Jacek Jakowski[5], Jingsong Huang[5], Patrik Staudenmayer[1], Yannic Falke[2], Ram Prakash Pandeya[1], and Alexander Grüneis[1] — [1]Institut für Festkörperelektronik, Technische Universität Wien, Gußhausstraße 25, 1040 Vienna, Austria — [2]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [3]CEA, Université Grenoble Alpes, IRIG-Pheliqs, 38000 Grenoble, France — [4]Institute of Science and Technology Austria (ISTA), Am Campus 1, 3400 Klosterneuburg, Austria — [5]Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, Tennessee, 37831, USA

Superconducting fullerides are usually synthesised by thermal or solution intercalation of alkali ions, which limits control of stoichiometry. We use electro-intercalation to drive Rb^+ into C_{60} thin films. Our on-chip setup combines *in-situ* growth, Raman spectroscopy and four-terminal transport, so that the stoichiometry x of Rb_xC_{60} is obtained from the $A_g(2)$ mode and linked to the superconducting transition temperature Tc. By varying the Rb/C_{60} ratio, we tune the films to superconducting Rb_3C_{60} and change T_c from 7 K to 26 K. Time-dependent Raman and transport data show that the Rb^+ electro-intercalation follows Butler-Volmer-type kinetics. Electro-intercalation enables precise, on-chip control of superconductivity in ultrathin fulleride films and is extendable to other porous and layered materials.

O 54.5 Wed 11:30 HSZ/0201

Mesoporous Cobalt Ferrite Thin Film Oxygen Evolution Electrocatalysts: The Role of Fe-Content on Structure, Activity and Stability — •Ann-Kristin Stief, Barbara Gonzalez-Navarrete, Stefan Lauterbach, Jan Philipp Hofmann, and Marcus Einert — TU Darmstadt, Darmstadt, Germany

Cobalt Ferrite is a promising alkaline Oxygen Evolution Reaction (OER) catalyst to replace state-of-the-art but expensive Ir- and Ru-based acidic OER catalysts in green hydrogen production. Given the limited and contradictory literature on the optimum stoichiometry of $Co_{3-x}Fe_xO_4$, we conducted a systematic stoichiometry study from x = 1.0 - 2.0 in increments of 0.2. To this end, mesoporous thin films were synthesized via dip-coating combined with soft-templating, using the commercially available polymer Pluronic F-127 for the first time. Electrochemical testing revealed that the x = 2.0 composition achieved the lowest iR-corrected overpotential (342 mV at 10 mA/cm^2), the smallest Tafel slope, and the lowest charge transfer resistance. Structural characterization disclosed enhanced crystallinity, reduced grain size and higher degree of inversion upon Fe-enrichment. X-ray Photoelectron Spectroscopy (XPS) further indicated that Fe-rich precatalysts form higher surface concentrations of hydroxide or defective oxide. Together, these findings contribute to the understanding of composition-structure-activity relations of Cobalt Ferrite OER catalysts, thereby laying a foundation for tailoring their catalytic performance. This work was supported by BMFTR within SINATRA (TWOB, Award Nr. 033RC036).

O 54.6 Wed 11:45 HSZ/0201

Probing Electromagnetic Chirality in Nanoresonators Using Scanning Reflection Anisotropy Microscopy — •Fabian Haake — ETH Zurich, Switzerland

We report on the application of a Scanning Reflection Anisotropy Microscope (SRAM) to study metasurfaces consisting of chiral nanoresonators. SRAM is a polarization-modulated optical method previously applied to strain mapping in crystalline materials and, more recently, demonstrated for amorphous systems (Sendra *et al.*, 2023; APL. 124, 171102, 2024). The structures were fabricated on Si_3N_4 TEM membranes using electron-beam lithography and metal deposition. Arrays of left- and right-handed resonators were fabricated and probed, showing a wavelength-dependent RAS contrast between the two enantiomorphic forms. Finite-element simulations under circularly polarized illumination reproduce the observed handedness-dependent responses. The results demonstrate that SRAM sensitively resolves enantiomer-specific optical signals at the microscopic scale, enabling direct characterization of electromagnetic chirality in metasurfaces.

O 54.7 Wed 12:00 HSZ/0201

Self-assembly of linear three-ring aromatic thiols on Au(111) and their conversion into 2D molecular materials — •Verena Müller[1], Anna-Laurine Gaus[2], Daniel Hüger[1], Julian Picker[1], Christof Neumann[1], Max von Delius[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, Lessingstrasse 10, 07743 Jena, Germany — [2]Ulm University, Institute of Organic Chemistry, Albert Einstein Allee 11, 89081 Ulm, Germany

Self-assembled monolayers (SAMs) allow surface modification at the molecular level and moreover have the ability of crosslinking with low-energy electrons to form mechanically stable and transferable 2D materials, so-called carbon nanomembranes (CNMs).

We investigate the self-assembly of linear, three-ring aromatic thiols on Au(111) and their subsequent electron-induced conversion into carbon nanomembranes (CNMs). Our study examines terphenylthiol (TPT) derivatives with distinct terminal groups (-F, $-CF_3$, $-NO_2$) as well as a pyridinebiphenyl compound. Utilizing complementary surface science techniques - X-ray photoelectron spectroscopy (XPS), low-energy electron diffraction (LEED), and scanning tunneling microscopy (STM) - we elucidate the structural properties of the resulting self-assembled monolayers (SAMs) and investigate their transformation into CNMs. The resulting CNMs exhibit tunable gas permeation characteristics, governed by the chemistry of the precursor molecules and the SAM structure.

O 54.8 Wed 12:15 HSZ/0201

Liquid Flame Spray Enables Durable, Transparent, and Super-repellent Silica Coatings — •Suhad Sbeih — German Jordanian University, Amman, Jordan

Developing coatings that are simultaneously transparent, durable, and highly water-repellent remains a long-standing challenge in materials science. In this work, we show that the liquid flame spray (LFS) technique offers a fast and scalable solution. In this process, a silica precursor is combusted to generate nanoparticles that deposit on moving substrates, forming a hierarchical surface texture in a single step. By carefully adjusting the burner-substrate distance, precursor concentration, and coating velocity, we produced coatings that combine optical clarity with extreme water repellency, reaching contact angles above 150° and roll-off angles below 10°.

Beyond these surface properties, the coatings exhibited outstanding durability and retained their performance after rinsing, condensation, tape, and scratch tests. The results highlight LFS as a versatile approach for engineering multifunctional surfaces that bring together transparency, robustness, and superrepellency. Such coatings open new opportunities for large-area applications in optics, energy devices, and biomedical technologies.

O 55: Oxide and insulator surfaces: Structure, epitaxy and growth II

Time: Wednesday 10:30–12:30 Location: HSZ/0204

O 55.1 Wed 10:30 HSZ/0204

Modulated structures in complex 2D oxides — •Muriel Wegner, Loi V. Tran, Oliver Krahn, Stefan Förster, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, Germany

Crystalline materials are typically characterized by a set of lattice vectors that reflect the materials dimensionality. In surface science we are used to two vectors spanning the lattice. However, systematic lattice modifications, which can be displacive in nature or connected to a different periodicity in a given materials property like magnetism, can call for the need of additional modulation vectors for a proper interpretation of the diffraction pattern. Such modulated structures are rarely discussed in surface science. Here we present the structure of a Ba-Ti-O monolayer film grown on Pd(111) and Pt(111). On Pd(111) this structure is commensurate and fully determined by two lattice vectors. In contrast, on Pt(111) four vectors are needed, two describing the average structure and two

additional modulation vectors. This Ba-Ti-O structure is a complex network of Ti-O rings, in which 53% of the rings are decorated with Ba atoms. On Pd(111) it forms a rhombic structure with a periodicity of 23.2 Å and an inner angle of 129.7°. On Pt(111) it grows with the identical lattice parameters. However as a consequence of the modified substrate spacing, the domain size is restricted by systematic inclusions of defects, which cause a modulation period of about 100 Å.

O 55.2 Wed 10:45 HSZ/0204

How coordination preferences dictate the mixing behavior of 2D oxide films: Fe/Cr spinel-type oxides on Pt(111) — Ghada Missaoui[1], Claudine Noguera[2], Jacek Goniakowski[2], and •Niklas Nilius[1] — [1]Carl von Ossietzky University, Institute of Physics, D-26111 Oldenburg, Germany — [2]CNRS-Sorbonne University, UMR 7588, INSP, F-75005 Paris, France

Fe/Cr mixed oxide films, prepared by reactive co-deposition of both elements on Pt(111), are analyzed by STM and DFT calculations. The mixed oxide grows into bi- (h=0.5 nm) and tri-stack films (h=0.7 nm) terminated either by open (2x2) (bi-stacks) or dense (1x1) atomic patterns (bi- and tri-stacks). The former is identified as Cr6O11 phase composed of an interfacial O-Cr-O trilayer and a Cr2O3 honeycomb plane. The latter develops upon substituting Fe into the surface plane, where it forms a hexagonally dense-packed Fe-O bi-layer. Two polymorphs with different mixing enthalpy occur as a function of mixing ratio. At high Fe content, X6O9-type bi-stacks prevail (X = Fe,Cr) with Cr preferentially accumulating in octahedral sites at the interface and Fe filling tetrahedral sites at the surface. At low Fe content, the Cr interface stack reconstructs to stabilize more oxygen, while the surface stack remains Fe-dominated. The resulting film has X6O11 stoichiometry and deviates from the X6O9 structure not only by the oxygen content but also by its workfunction and surface buckling, in agreement with STM data. The observed cationic stacking, with alternating Fe and Cr planes resembles the bulk ilmenite structure (FeCrO3).

Invited Talk O 55.3 Wed 11:00 HSZ/0204

Cationic Mixing in Ultrathin Oxide Films: How substrate and oxygen conditions control nanoalloying. — •Jacek Goniakowski — Institut des NanoSciences de Paris, CNRS & Sorbonne Université, Paris, France

While alloying is a powerful strategy for tuning material properties, the fundamental physics and chemistry of cation mixing in metal-supported ultrathin oxide films, including those relevant to inverse catalysts, remain poorly understood, and only a few doped or mixed phases have been characterized at the atomic scale. Here, density functional theory, combined with recent surface science experiments, is used to elucidate how oxygen conditions and substrate properties govern the formation of mixed two-dimensional oxide phases through a subtle interplay of structural and electronic effects.

The study shows that, although bulk V-Fe-O mixed oxides are rare, reduced V-Fe-O monolayers on Pt(111) are stable across a wide range of cation compositions. However, oxidation of the film strongly narrows the accessible compositional window. Likewise, substrate passivation (e.g., oxidized Ru(0001)) restricts the range of stable compositions. For somewhat thicker films, exemplified by V-Cr-O bistacks, the presence of crystallographically distinct cation sites further promotes mixing, enabling the stabilization of spinel-like V-Cr phases with no direct bulk counterparts. Our results highlight key effects governing compositionally complex supported ultrathin oxide films and suggest pathways to explore novel mixed phases.

O 55.4 Wed 11:30 HSZ/0204

Surface reconstruction of the polar spinel $MgAl_2O_4$(001) surface — David Kugler[1], Andrea Conti[1], Johanna I. Hütner-Reisch[1], Soumyajit Rajak[2], Matthias Meier[1], Nan Jiang[2], Florian Mittendorfer[1], Michael Schmid[1], Ulrike Diebold[1], Gareth S. Parkinson[1], and •Jan Balajka[1] — [1]Institute of Applied Physics, TU Wien, Vienna, Austria — [2]Department of Chemistry, University of Illinois Chicago, USA

The atomic-scale surface structure governs the surface chemistry of materials. Magnesium aluminate ($MgAl_2O_4$) spinel, a wide-gap insulator, poses considerable challenges for experimental surface characterization. Using noncontact atomic force microscopy (nc-AFM), we resolve the atomic structure of the $MgAl_2O_4$(001) surface. The surface adopts a c(2×4) reconstruction accompanied by altered surface stoichiometry. The reconstructed surface is enriched in aluminum and contains ordered pairs of octahedrally coordinated Mg atoms that, in bulk, occupy tetrahedral sites. This cation redistribution stabilizes the otherwise polar $MgAl_2O_4$(001) termination. The resulting structure closely resembles reconstructions observed on other spinel oxides, suggesting a common mechanism for polarity compensation across the spinel group.

O 55.5 Wed 11:45 HSZ/0204

Size Matters: Size-dependent non-equilibrium dynamics of fluxional subnanoclusters — •Patricia Poths[1], King Chun Lai[2], Christoph Scheurer[1], Sebastian Matera[1], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der Max-Planck Gesselschaft, Berlin — [2]Max Planck Computing and Data Facility, Garching

Sub-nanoclusters are known to be fluxional, thermally populating multiple structural isomers, and to have size-dependent catalytic behavior. Due to computational limitations, only quasi-static equilibrium properties could be addressed by first-principles methods so far. Here, we investigate the kinetic evolution underlying isomer fluxionality by coupling machine-learned interatomic potentials (MLIPs) with our recently introduced automatic process explorer (APE) [1]. With this methodology, we construct comprehensive isomerization networks of Pdn (n=3-11) clusters deposited on the MgO(100) surface, and evaluate the corresponding state-to-state dynamics. Using methods from Markov State Modeling, we find that the intrinsic timescales for equilibration can vary by several orders of magnitude based on cluster size. Furthermore, intrinsic timescales for each cluster isomer can vary by multiple orders of magnitude, indicating the existence of metastable sets with quasi-liquid behavior, i.e. rapid conversion between isomers within the set but only slow transition to isomers outside. These simulations reveal that the prevalent quasi-static picture is of limited use for nonequilibrium problems like catalysis, but also that relaxation dynamics should be observable on experimental timescales.

[1] K.C. Lai et al., Phys. Rev. Lett. 134, 096201 (2025).

O 55.6 Wed 12:00 HSZ/0204

Structural and electronic evolution of noble metal-deposited CeO2 catalysts: from model to powder systems — •Zairan Yu, Shuang Chen, Wangtao Li, Alexei Nefedov, Christof Wöll, and Yuemin Wang — Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen, Germany

The interaction between noble metals and oxide supports is crucial in heterogeneous catalysis, governing key reactions such as CO oxidation and the water-gas shift. Pt- and Pd-ceria systems show particularly strong electronic and structural metal-support interactions among these reactions. Despite extensive investigation, the atomic-scale structure and reactivity of these interfaces remain incompletely understood. Here, we combine polarization-resolved IRRAS on single-crystal surfaces and in situ UHV-FTIR transmission studies on ceria nanoparticles, using CO as a probe to elucidate surface structural dynamics and active sites. For Pt/CeO2(111), IRRAS and DFT results reveal that isolated Pt single atoms are not stabilized on the surface, but instead migrate into subsurface interstitial sites at low coverages, giving rise to a characteristic blue-shifted CO band at 2169 cm-1. In the Pd/CeO2/γ-Al2O3 system, highly dispersed Pd cations embedded in the ceria matrix with nearby interfacial oxygen vacancies are identified, correlating with superior catalytic performance in STD reactions. This work was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation)-Project-ID 426888090-SFB 1441.

O 55.7 Wed 12:15 HSZ/0204

Titanium intermixing into cuprous oxide thin films: An STM and XPS study — •Bo-Yi Zhong and Niklas Nilius — Carl-von-Ossietzky University, Institute of Physics, D-26111 Oldenburg, Germany

According to DFT calculations, gap size and p-type conductivity of binary Cu2O can be tuned over wide ranges by doping the material with transition metal ions. To test this assumption, we have prepared Cu/Ti mixtures and exposed them to different oxidation conditions. Mixing is only revealed at low temperature and gives rise to amorphous oxide films without diffraction pattern. Annealing in oxygen triggers a gradual phase separation, with TiOx moving to the surface and CuOx remaining at the interface to the Pt(111) support. The phase separation produces a distinct intensity behavior of the Ti 2p and Cu 2p XPS peaks as a function of temperature. Morphologically, the Ti ions get embedded into the surface reconstruction of Cu2O(111) at low Ti content, as observed in atomically resolved STM images. With rising Ti level, the surface Ti-O forms large crystallites exposing distinct stripe-patterns on their surface, suggesting a TiO2(110)-type morphology. Moreover, STM spectroscopy finds a gap state at 1.5 eV in Ti-poor preparations, compatible with the empty-state resonance of the Ti impurities. At higher Ti content, the gap state broadens and evolves to the TiO2 conduction band. The electronic response of the phase-separated system, with Cu2O at the interface and TiO2 at the surface, resembles the one of a pn-junction.

O 56: Scanning probe techniques: Method development II

Time: Wednesday 10:30–12:15 Location: HSZ/0401

O 56.1 Wed 10:30 HSZ/0401

Simulation of coupled AFM and constant current STM images — •Marvin Krenz[1,2], Miguel Wiche[1,3], Daniel Ebeling[1,3], and Simone Sanna[1,2] — [1]Center for Materials Research, Justus-Liebig University, Giessen, Germany — [2]Institute of Theoretical Physics, Justus-Liebig University, Giessen, Germany — [3]Institute of Applied Physics, Justus-Liebig University, Giessen, Germany

We present a simulation method for AFM images with a constant current STM feedback loop. In contrast to regular AFM constant height images, those images can picture the features of bulky or corrugated molecules, as shown by experiment [1].

The method is based on the electronic density of the molecules, and thus applicable to virtually any DFT code. We apply this method to two test systems, the 6F-Pentacene molecule at Cu(111) and the iodotriphenylene at Ag(111), at different level of approximation.

Both systems compare well to the experimental images; at the highest level of approximation nearly all features of the experiment are reproduced.

[1] Martin-Jimenez, D.; Ahles, S.; Mollenhauer, D.; Wegner, H. A.; Schirmeisen, A.; Ebeling, D. Physical Review Letters 2019, 122, 196101.

O 56.2 Wed 10:45 HSZ/0401

High spatial resolution of Si(111)-7x7 using LFM with a CO-tip — •Shinjae Nam[1,2], Thomas Holzmann[1], Franz Giessibl[1], and Alfred Weymouth[1] — [1]University of Regensburg, Regensburg, Germany — [2]Center for Quantum Nano Science, Seoul, South Korea

The Si(111) 7x7 reconstructed surface has long served as an iconic benchmark for proving the capabilities of scanning probe microscopes. Since STM first resolved the 7x7 pattern in 1983, advances in frequency-modulation AFM have enabled true atomic resolution and quantitative access to short-range chemical and frictional interactions. In this work, we report unprecedented atomic resolution and quantitative mapping of site-dependent lateral forces on the Si(111) 7x7 surface using a qPlus-based lateral force microscope. The tip is terminated with a CO molecule, and oscillating laterally with an amplitude of 50 pm. Unlike reactive Si tips, the CO tip provides a chemically inert and well-defined probe apex, enabling exceptionally sharp contrast and resolving subtle differences between faulted and unfaulted half-cells. The measured lateral force maps agree quantitatively well with theoretical models. These results establish CO-tip LFM as a powerful technique for probing lateral interactions with single-atom precision.

O 56.3 Wed 11:00 HSZ/0401

Spatially Resolved Mode Analysis of Ultra-Long qPlus Probes for STM/AFM — •Aleksander Bogucki[1,3], Yeon-Ji Kim[1,2], Yewon Kim[1,2], Sarah Yi[1,2], German Orlov[1,3], Lei Fang[1,3], Wonjun Jang[1,3], and Andreas Heinrich[1,2] — [1]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS), Seoul 03760, Republic of Korea — [2]Department of Physics, Ewha Womans University, Seoul 03760, Republic of Korea — [3]Ewha Womans University, Seoul 03760, Republic of Korea

Combined scanning tunneling and atomic force microscopy (STM/AFM) based on quartz tuning forks (qPlus) typically relies on short tip lengths (<0.5 mm) for optimal performance. However, restricted sample environments such as liquid cells or setups requiring significant clearance for high-numerical-aperture optical elements demand probe geometries far exceeding standard dimensions. While tips in the 1-3 mm range have been recently explored [1], the dynamics of significantly longer tips are less well characterized.

We present a systematic study of qPlus sensors with ultra-long tips (>8 mm). We correlate electrical response spectra with spatially resolved optical vibrational analysis to map eigenmodes and identify non-vertical components. Supported by FEM simulations, we demonstrate that tip material and geometry can be optimized to tune the spectral response. Finally, we assess the potential of these ultra-long designs for specialized SPM setups.

References: [1] T. Yamada et al., Nanoscale Adv. 5, 840-850 (2023).

O 56.4 Wed 11:15 HSZ/0401

Comparative Analysis of SPM-Based Work Function Measurement Techniques with Application to Work Function Engineering of Superconducting Nb(110) — •Daryoush Nosraty Alamdary, Matthias Bode, and Artem Odobesko — Physikalisches Institut, Lehrstuhl für Experimentelle Physik 2, Julius-Maximilians-Universität Würzburg, Germany

The engineering of the work functions at the interface of complex materials for energy band tuning [1] requires precise and reliable measurement methods, sensitive to atomic monolayer thin films. While there are handful of established methods that allow a precise determination of the work function, scanning probe microscopy-based methods constitute a class of their own since they are based on a local probe. In this work, we present a comparative study of three techniques, i.e., $I(z)$ spectroscopy, field emission resonances, and Kelvin probe force spectroscopy, regarding their complexity and reliability to determine the local work function. For a few well-studied model systems we analyze the respective benefits and challenges. Using the most reliable methods, established by the comparative analysis, we systematically study the coverage-dependent crystal structure and work function of epitaxial Ir films on superconducting Nb(110) [2] and discuss the suitability for work function engineering towards induced superconductivity.

[1] P. Rüßmann *et al.*, Proximity induced superconductivity in a topological insulator, arXiv:2208.14289 (2022)

[2] P. Beck *et al.*, Structural and superconducting properties of ultrathin Ir films on Nb(110), Phys. Rev. Mater. **6**, 024801 (2022)

O 56.5 Wed 11:30 HSZ/0401

Towards Atomically Precise Fabrication through STM with Flat, Crystalline Probes — •Marc Savoie, Eduardo Barrera Ramirez, Bheeshmon Thanabalasingam, and Marco Taucer — CBN Nanotechnologies Inc, Ottawa, Canada

Scanning Tunneling Microscopy (STM) enables the fabrication of atomically precise structures. Traditionally, STM probes manipulate atoms on the sample surface, but this presents challenges for fabricating covalently bonded structures. The high strength of covalent bonds means that detailed knowledge and control over both the probe and sample sides of the tunneling junction is required to form the desired bond and avoid unwanted changes. We introduce inverted-mode STM, an approach that reverses the roles of probe and sample to enable mechanically controlled chemical reactions for atomically precise fabrication. We have developed flat, crystalline Si(100) STM probes that act as the substrate for atomic manipulations. The flat probe is imaged by tailored, 3D molecules deposited on a surface. By determining the orientation of the molecule, the challenge of knowing the atomic configuration on both sides of the junction is effectively resolved. Treating the two sides of the tunnel junction as reagents whose relative positions can be controlled with sub-angstrom precision, we show that hydrogen atoms can be reproducibly abstracted from a locally flat, crystalline region of the probe apex at zero volts using a novel molecule terminated in an alkynyl radical. Multiple surface-bound reagents can sequentially address the same build site on a probe apex. The approach is expected to apply to abstraction and donation of other elements and moieties.

O 56.6 Wed 11:45 HSZ/0401

Atomically Precise Si Abstraction by Inverted-Mode STM — •Rosemary Cranston, Zehra Ahmed, Eduardo Barrera, Brandon Blue, Adam Bottomley, Christian Imperiale, Alex Inayeh, Mathieu Morin, Marco Taucer, and Bheeshmon Thanabalasingam — CBN Nano Technologies Inc., Ottawa, Canada

Direct 3D manipulation of covalently bonded atoms remains a challenge for atomically precise fabrication. Here, we introduce inverted-mode scanning tunneling microscopy (STM) as a new approach for controlled atomic-scale reactions and demonstrate its application to individual Si atom abstraction. A Si probe chip (SPC) with an atomically clean Si(100)-2x1 crystalline terrace at the apex serves as the probe, while a Si wafer bearing isolated, custom-synthesized, surface-bound molecular tools act as the sample. These molecules function both as imaging agents and as tools for chemical manipulation. As the sample is scanned with the SPC, each protruding molecule provides a mirror image of the probe apex and can immediately participate in surface reactions. For subtractive Si patterning, we employ tripodal molecules featuring an ethynyl iodide moiety. After bias-induced cleavage of the iodine, the resulting radical is aligned with a target Si dimer of the SPC. A controlled approach-retraction process transfers a Si atom to the molecule, leaving unique Si vacancies at the target site. Imaging with new iodinated molecules elsewhere on the sample surface confirms changes to the SPC lattice, and allows iterative targeting for the next abstraction, thus enabling a new method for atomically precise fabrication, and the manipulation of Si atoms in 3D.

O 56.7 Wed 12:00 HSZ/0401

Graphene Coated Nanoprobes for Local Conductivity Measurements — •Maria Saavedra-Fredes, Valeria del Campo, and Tomas P. Corrales — Universidad Técnica Federico Santa María, Valparaíso, Chile.

Here we explored the fabrication of AFM cantilevers coated with graphene (Gr) with the aim of detecting local electrical currents. The fabrication process begins with the growth of Gr on copper foils via Chemical Vapor Deposition (CVD). Subsequently, the copper substrate is dissolved using a ferric nitrate solution and then replaced with water, leaving a Gr film floating at the water air interface. This film is transferred onto an AFM cantilever using a three-axis hydraulic micromanipulator. Raman spectroscopy and SEM confirm the presence of graphene on our Gr-coated nanoprobes This technique differs from traditional methods because the Gr is collected directly from the air water interface without the use

of polymer films in the process (10.3390/cryst7090269). Then, to detect currents using conductive mode AFM (10.1002/adma.201200579) and study the conduction between our Gr-coated nanoprobe and a graphene layer deposited on silicon.

O 57: Plasmonics and nanooptics: Light-matter interaction, spectroscopy II

Time: Wednesday 10:30–12:30 Location: HSZ/0403

Invited Talk O 57.1 Wed 10:30 HSZ/0403

From Plasmonic Near-Fields to Electron Dynamics - A Photoemission Perspective — •Pascal Dreher — Faculty of Physics and Center for Nanointegration, Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47048 Duisburg, Germany — Present Address: Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg

Electromagnetic near-fields are ubiquitous in solid-state physics. At surfaces, interfaces, and in nanostructures they control dynamical processes and shape optical and electronic material properties. By concentrating electromagnetic energy to subwavelength volumes, near-fields enable tailored nanoscale light-matter interactions relevant to plasmonics, nanophotonics, and ultrafast carrier dynamics. A detailed understanding of these interactions, however, requires experimental access to the full three-dimensional, time-dependent vectorial structure of near-fields, ideally in conjunction with direct probes of the electronic excitations they launch.

In this talk, I will address these needs using two complementary experimental approaches: polarimetric photoemission microscopy that maps vectorial near-fields at surfaces, and time- and angle-resolved photoemission that probes the resulting charge-carrier dynamics. Using surface plasmon polaritons as a prototypical platform, it will be demonstrated how these methods allow to relate near-field dynamics and light-matter interactions at the native length, momentum, time, and energy scales.

O 57.2 Wed 11:00 HSZ/0403

Steps Towards Excitation of Quantum Emitters with Switchable Nonlinear Near Fields — •Valentin Dichtl, Thorsten Schumacher, and Markus Lippitz — Experimental Physics III, University of Bayreuth

The third-order nonlinear material response of noble metals enables the formation of the third-harmonic near field around a plasmonic nanostructure. The corresponding spatial emission pattern of the third-harmonic hot spots changes drastically when the fundamental wavelength is slightly tuned over a linear resonance of the nano antenna [1]. This effect can be used to spatially tailor the near field for excitation of various emitters – such as molecules or quantum dots – beyond the diffraction limit.

We identified distinct differences in the nonlinear scattering behavior between the complentarry plasmonic structures rod and slit [2]. Building on this insight we compare these geometries in terms of their suitability for single emitter excitation.

We demonstrate non-destructive third-harmonic generation in close proximity to fluorescent dyes. Finally, we discuss spectral and temporal strategies for discriminating photons originating from fluorescence versus those from harmonic generation.

[1] Wolf, D. *et al.* Shaping the nonlinear near field. *Nat. Commun.* 7:10361 (2016). doi: 10.1038/ncomms10361

[2] Dichtl, V. *et al.* The Nonlinear Limit of Babinet's Principle. *Nano Lett.* 2025, 25, 11084-11088. doi: 10.1021/acs.nanolett.5c02210

O 57.3 Wed 11:15 HSZ/0403

Intrinsic plasmon canalization in the natural biaxial van-der-Waals material $MoOCl_2$ — •Farid Aghashirinov[1], Andrea Manchini[2], Lin Nan[2], Giacomo Venturi[2], Nicola Melchioni[2], Florian Mangold[1], Bettina Frank[1], Antonio Ambrosio[2], and Harald Giessen[1] — [1]4-th Physics Institute, University of Stuttgart, Stuttgart, Germany — [2]Vectorial Nano-Imaging, Istituto Italiano di Tecnologia, Milano, Italy

We investigate directional near-infrared plasmon polaritons in exfoliated $MoOCl_2$ flakes on SiO_2 substrates, excited using gold disk nanoantennas and probed with scattering-type scanning near-field optical microscope (s-SNOM). $MoOCl_2$ is a natural van der Waals material that supports low-loss, in-plane hyperbolic plasmons and exhibits strong optical anisotropy: polarization along the short axis yields metallic behaviour, while alignment with the long axis produces a dielectric response [1]. Using a widely tunable broadband laser from Stuttgart Instruments, we map the polariton dispersion across a broad spectral range and identify distinct propagation regimes. In our work, we observe plasmon-polariton canalization for the first time, where wavefronts propagate without divergence. These measurements highlight $MoOCl_2$ as a broadband, highly directional natural polaritonic platform.

[1] G. Venturi et al., Nat Commun 15, 9727 (2024)

O 57.4 Wed 11:30 HSZ/0403

Toward Plasmonic Neuronal Architectures at the Nanometer Scale — •Christopher Weiss[1], Tobias Eul[2], Emily Kruel[1], Mario Pfeiffer[1], Bert Lägel[1], Benjamin Stadtmüller[2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, Germany — [2]Experimentalphysik II, Institute of Physics, University of Augsburg, Germany

Classical von-Neumann computers face severe energy and speed limitations when operating large artificial neural networks, motivating alternative computing concepts beyond the traditional architecture. Plasmonic nanostructures offer a promising route toward ultrafast and highly integrated neuromorphic systems by enabling strong optical confinement at the nanoscale. We present a concept for a plasmonic neuronal cell that combines multiplexed signal reception, static weighting, and nonlinear activation within a single device. Optical inputs encoded in the orbital angular momentum of light are directed into separate dielectric-loaded surface-plasmon-polariton waveguides. Synaptic weighting is implemented through nanoscale gaps, whose attenuation characteristics are analyzed using finite-difference time-domain simulations and experimentally validated by photoemission electron microscopy. Nonlinear activation is provided by plasmon-enhanced two-photon photoemission. These results establish the essential functional components required for ultrafast plasmonic neuromorphic architectures.

O 57.5 Wed 11:45 HSZ/0403

Optical resonance tuning of single polystyrene microspheres using the phase-change material In_3SbTe_2 as a switchable mirror — •Rebecca Rahmel, Hristiyana Kyoseva, Lukas Conrads, Thomas Taubner, and Gero von Plessen — I. Institute of Physics (IA), RWTH Aachen University

The optical resonances of dielectric nanoparticles and microparticles can be modified via their size, shape and configuration [1]. Dielectric particles in particle-on-mirror (PoM) geometries show rich optical responses due to their low losses and electric and magnetic multipolar Mie modes [2]. Cueff et al. introduced the concept of a switchable mirror to tune the resonances of dipole emitters using the phase-transition material VO_2 [3]. Here we tune the infrared multipolar Mie resonances of dielectric polystyrene (PS) microspheres using a switchable mirror made of the phase-change material In_3SbTe_2 (IST). IST exhibits a phase change between an amorphous dielectric and crystalline metallic phase in the infrared [4,5] and can be locally switched under the PS microspheres, creating a PoM geometry. Measuring the scattering spectra of the PS microspheres before and after switching, we achieve huge shifts of the resonance wavelength from 5.2 to 8.9 μm. Our work is a first step towards the controlled tuning of multipolar Mie modes of various particles using reprogrammable IST mirror structures.

[1] Kuznetsov et al. *Science* **354**, aag2472 (2016) [2] Yao et al. *ACS Nano* **18**, 26, 16545-16555, (2024) [3] Cueff et al. *Nat. Com.* **6**, 8636 (2015) [4] Heßler et al. *Nat. Com.* **12**, 924 (2021) [5] Conrads et al. *Opt. Mat. Ex.* **15**, 2664-2687 (2025)

O 57.6 Wed 12:00 HSZ/0403

Spectral tuning of hyperbolic shear polaritons in monoclinic gallium oxide via isotopic substitution — •G. Carini[1], M. Pradhan[2], E. Gelzinyte[1], A. Ardenghi[3], S. Dixit[4], M. Obst[5,6], A. S. Senarath[4], N. S. Mueller[1], G. Alvarez-Perez[1,7], K. Diaz-Granados[4], R. A. Kowalski[4], R. Niemann[1], F. G. Kaps[5], J. Wetzel[5], R. B. Iyer[2], P. Mazzolini[8], M. Schubert[9,10], J. M. Klopf[11], J. T. Margraf[12], O. Bierwagen[3], M. Wolf[1], K. Reuter[1], L. M. Eng[5,6], S. Kehr[5,6], J. D. Caldwell[4], C. Carbogno[1], T. G. Folland[2], M. R. Wagner[3], and A. Paarmann[1] — [1]FHI, Berlin, Germany — [2]University of Iowa, Iowa City, IA, USA — [3]PDI, Berlin, Germany — [4]Vanderbilt University, Nashville, TN, USA — [5]TUD, Dresden, Germany — [6]EXC 2147 (ct.qmat), Dresden, Germany — [7]IIT, Lecce, Italy — [8]University of Parma, Parma, Italy — [9]University of Nebraska, Lincoln, NE, USA — [10]Lund University, Lund, Sweden — [11]HZDR, Dresden, Germany — [12]University of Bayreuth, Bayreuth, Germany

This contribution reports a significant spectral tuning of hyperbolic shear polaritons (HShPs) in monoclinic gallium oxide (bGO) via isotopic substitution. HShPs are imaged in real-space with near-field optical microscopy, allowing for a model-free estimation of the frequency shift. Complementary far-field measurements and *ab initio* calculations - in good agreement with the near-field data - confirm the effectiveness of this estimation. This combined study demonstrates the possibility to support such highly directional polaritons in a hitherto inaccessible range, with great promise for future applications.

O 57.7 Wed 12:15 HSZ/0403

Vibrationally Induced Resonances in Nanolasers based on Plasmonic Cavities — •Kai Müller[1], Kimmo Luoma[2], and Christian Schäfer[3] — [1]Institut für Theoretische Physik, Technische Universität Dresden, D-01062 Dresden, Germany — [2]Department of Physics and Astronomy, University of Turku, 20014 Turku, Finland — [3]Institute of Applied Physics, TU Wien, Wiedner Hauptstrasse 8-10/134, Vienna, 1040, Austria

Optical circuits and light sources, such as lasers, undergo continuous miniaturization. In recent years, this trend has been taken to its extreme with lasers comprising only a few molecules confined in plasmonic nanocavities. Here, we use a novel method that combines the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy with the hierarchical equations of motion (HEOM) to provide theoretical predictions for the quantum dynamics of this few-emitter lasing system. Our approach is informed from first principles and explicitly accounts for the entire vibrational manifold of each molecule in addition to the cavity. We show how the form of the vibrational spectrum influences the lasing process and uncover resonant enhancements in the lasing intensity, which are absent if the coherent drive and vibrational relaxation are combined into the commonly used effective incoherent drive.

O 58: Organic molecules on inorganic substrates: Adsorption and growth III

Time: Wednesday 10:30–12:30 Location: TRE/PHYS

O 58.1 Wed 10:30 TRE/PHYS

Probing weak chemical interactions of metal surface atoms with CO-terminated AFM tips identifies molecular adsorption sites — Jalmar Tschakert[1], Qigang Zhong[1], Alexander Sekels[1], Pascal Henkel[2], Jannis Jung[2], K. Linus H. Pohl[2], Hermann A. Wegner[3], Doreen Mollenhauer[4], André Schirmeisen[1], and •Daniel Ebeling[1] — [1]Inst. of Applied Physics, Justus Liebig University Giessen — [2]Inst. of Physical Chemistry, Justus Liebig University Giessen — [3]Inst. of Organic Chemistry, Justus Liebig University Giessen — [4]Inst. for Technical and Environmental Chemistry, Friedrich Schiller University Jena

Understanding reaction mechanisms of adsorbed organic molecules is key to neat on-surface synthesis of functional nanomaterials. Low temperature atomic force microscopy has become an invaluable tool for studying on-surface reaction mechanisms as it allows to visualize the chemical structure of the reactants and products. However, directly accessing the molecule-surface interactions that are responsible for the pathway of on-surface reactions is difficult. Here, we measure chemical interactions between CO-terminated tips and coinage metal surface atoms in all spatial directions with picometer resolution. Identifying the small covalent bonding contributions in the background of the dispersion-dominated interaction enables revealing insights into the nature of chemical bond formation with metal surface atoms and a reliable determination of molecular adsorption sites. The latter can serve as a starting point and for a comparison with theoretical studies.

[1] Tschakert et al., *Nature Communications* **16**, 7874 (2025)

O 58.2 Wed 10:45 TRE/PHYS

Rare earth modified silicon surfaces: A promising template for ordered organic growth — •Milan Kubicki, Philipp Gruber, Marie-Louise Fraser, Mario Dähne, and Martin Franz — Technische Universität Berlin, Institut für Physik und Astronomie, Berlin, Germany

The formation of self-assembled layers of organic molecules on solid surfaces is an important research field because of their possible application in advanced (opto)electronic devices. While the formation of self-assembled layers is well established on metal surfaces, the growth on silicon surfaces, which are still the material of choice in present semiconductor technology, is much less studied. On pure silicon, however, the formation of ordered organic films is usually hindered by its high dangling bond density, so that an appropriate surface modification is required.

Here we demonstrate the high potential of a rare-earth modification of the Si(111) surface for promoting ordered growth. Using scanning tunneling microscopy, the adsorption of different organic molecules on rare-earth modified silicon surfaces was examined, exemplarily for highly reactive N-heterocyclic carbenes and less reactive transition metal phthalocyanines. Our data demonstrate that single molecules remain mobile on the surface at room temperature. At a coverage of one full monolayer highly ordered films can be formed, demonstrating the great potential of rare-earth modified silicon surfaces as template for organic film growth.

[1] M. Kubicki *et al.*, J. Phys. Chem. C **128**, 13347 (2024).

O 58.3 Wed 11:00 TRE/PHYS

N-Heterocyclic Carbenes on GaAs: From Chain Formation to Ordered Monolayers — •Martin Franz[1], Ankita Das[2], Sandhya Chandola[3], Milan Kubicki[1], Mowpriya Das[2], Andrea Sette[4], Domenico Corona[4], Maurizia Palummo[4,5], Letizia Chiodo[6], René Schöder[1], Preeti Chahar[2], Benjamin Fuhrmann[1], Jonathan Engelhardt[1], Oskar Düren[1], Mario Dähne[1], Conor Hogan[4,7], Norbert Esser[1,3], and Frank Glorius[2] — [1]Technische Universität Berlin, Institut für Physik und Astronomie, 10623 Berlin, Germany — [2]Organisch-Chemisches Institut, Universität Münster, 48149 Münster, Germany — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, 14109 Berlin, Germany — [4]Dipartimento di Fisica, Università di Roma "Tor Vergata", Rome 00133, Italy — [5]CNR Centro S3, CNR-Istituto Nanoscienze, Modena 41125, Italy — [6]Department of Engineering, Università Campus Bio-Medico, Rome 00128, Italy — [7]CNR-Istituto di Struttura della Materia (CNR-ISM), Rome 00133, Italy

N-Heterocyclic carbenes (NHCs) have emerged as well-established ligands for metal surfaces. First studies on silicon exist as well, while III-V compound semiconductors are the materials of choice for opto-electronic devices. Here, the adsorption behavior of NHCs on GaAs is studied in detail [1]. A covalent binding to the surface and a formation of well-ordered monolayers is found, accompanied by exceptionally large work function reductions. The monolayers consist of NHC chains being the result of an attractive interaction between the molecules.

[1] M. Franz et al., Angew. Chem. Int. Ed., 64, e202511094 (2025).

O 58.4 Wed 11:15 TRE/PHYS

Tuning the adsorption of Subphthalocyanine molecules on Au(111) by peripheral and axial functionalization — •Franz Plate[1], Soyoung Park[2,3], Ebru Cihan[1], Natasha Khera[1], Ningwei Sun[2,3], Dmitry A. Ryndyk[1], Franziska Lissel[2,3], and Francesca Moresco[1] — [1]Center for Advancing Electronics Dresden, TU Dresden, 01062 Dresden, Germany — [2]Institute of Macromolecular Chemistry Leibniz Institute of Polymer Research, Hohe Strasse 6, Dresden, Germany — [3]Institute for Applied Polymer Physics, TU Hamburg, 21073 Hamburg, Germany

Subphthalocyanine (SubPc)-based molecules have been shown to be chemically versatile and tunable molecules, which can be functionalized with a variety of different chemical groups. This makes them promising candidates for designing single molecule machines to store and convert energy. Examples include vertical molecular rotors on surface. Although SubPc is nonplanar, SubPc-based molecules have been shown to form well-ordered molecular assemblies on surfaces, enabling them to function as modular rotor bases. Their chemically stable and rigid core, allows for a functionalization with different axial ligands as well as extensions at the peripheral positions of the π-conjugated base, which leads to different orderings on the surface. We have studied different SubPc based molecules with different axial and peripheral functionalizations on Au(111) using low-temperature scanning tunneling microscopy, supported by simulations. Depending on the peripheral functionalization with methoxy and thiophene groups, we found different adsorption behaviors, ordering, and intermolecular interactions.

O 58.5 Wed 11:30 TRE/PHYS

From Inert Nitrogen to Reactive Metal Nitrene: An On-Surface Route to N-Heterocycles — •Marco Thaler[1], Ricardo Ruvalcaba Briones[2], Shadi Fatayer[2], and Laerte Patera[1] — [1]Department of Physical Chemistry, University of Innsbruck, Innsbruck, Austria — [2]Applied Physics Program, Division of Physical Science and Engineering (PSE), King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia

Nitrenes are highly reactive intermediates in organic chemistry and play a key role in the synthesis of nitrogen containing compounds. In solution, nitrenes are typically generated from chemically activated precursors (e.g., azides), whereas direct conversion of primary amines remains challenging due to the inherent strength of N-H bonds. On surfaces, reactive nitrenes have likewise been formed from organic azides [1]; however, azides are thermally and photochemically labile and can decompose violently upon exposure to heat, light, or mechanical shock, posing safety risks. Here, using combined scanning tunneling microscopy (STM), non contact atomic force microscopy (nc AFM), and density functional theory (DFT), we demonstrate the thermally activated formation of a surface stabilized metal-nitrene intermediate from a chemically inert amine, which mediates the on-surface formation of a nitrogen-containing heterocycle. Our findings establish non activated nitrogen functionalities as viable nitrene precursors and reveal new mechanistic pathways for on-surface synthesis of N-heterocyclic compounds.

[1] Hellerstedt et al., Angew. Chem. 131, 2288-2293 (2019).

O 58.6 Wed 11:45 TRE/PHYS

Mirror domains and adsorption induced dipoles in organic semiconductor films revealed by LEEM and μLEED — •Franz Niklas Knoop, Klaus Stallberg, and Winfried Daum — Institute of Energy Research and Physical Technologies, TU Clausthal, Germany

We apply low-energy electron microscopy (LEEM) and microspot low-energy electron diffraction (μLEED) to study the film growth of nonpolar para-sexiphenyl (*p*-6P) molecules on natively oxidized silicon. In their second monolayer, the molecules form μm-sized, 2D-crystals with a bulk-like unit cell. LEEM reveals dark lines that split individual islands along their long axis into two domains of roughly equal size. The corresponding diffraction patterns are laterally shifted relative to each other, allowing for dark-field imaging of each domain. We attribute this apparent shift in k-space to the presence of lateral electric fields pointing in opposite directions on either side of an island. Given *p*-6P's large polarizability, we ascribe these fields to induced electric dipole moments in the tilted molecules. Thus, the observed dark lines represent boundaries between adjacent domains of mirrored tilt. Since the shift in k-space is independent of the LEEM extractor field, the dipoles must be inherent to the adsorbed molecules on the Si substrate. We observe an increased work function for the second-layer islands compared to the substrate. This and temperature-dependent measurements support our conclusion that adsorption-induced charge transfer causes the polarization of the molecules.

O 58.7 Wed 12:00 TRE/PHYS

The Role of Metal Ions in Metal-Phthalocyanine Adsorption on Oxide Surfaces — Matthias Blatnik[1], Fabio Calcinelli[2], Andreas Jeindl[2], Michael Schmid[1], Ulrike Diebold[1], Peter Jacobson[3], Oliver T. Hofmann[2], and •Margareta Wagner[1] — [1]TU Wien, Austria — [2]TU Graz, Austria — [3]University of Queensland, Australia

The interaction of conjugated organic molecules with surfaces is of fundamental interest and also important in many applied areas. Surface science investigations have advanced understanding of organic/metal interfaces, but the second electrode in organic optoelectronic devices – typically the transparent conductive oxide In_2O_3 – remains largely unexplored. Our work aims at closing this gap by examining the model system phthalocyanines on indium oxide surfaces.

Phthalocyanines adsorbed on the In_2O_3(111) surface were studied experimentally with low temperature STM and AFM, combined with DFT calculations. A key aspect is the comparable size of the molecules and the surface unit cell, which allows a (1×1) arrangement despite the differing symmetries. Various metal phthalocyanines (MPc: CuPc, CoPc, etc.) are investigated to reveal the influence of the metal ion in the selection of adsorption sites, 2D condensation, and the formation of the first layer. We identify a common, robust adsorption site for different MPc that forces the molecules to overlap in the (1×1) structure of the first layer, and a less common site, where a (1×1) packing without overlap is realized.

O 58.8 Wed 12:15 TRE/PHYS

***In Situ* Field-Induced Switching of Global Chirality in Halogen-Bonded Kagomé Networks** — •Nico Kubetschek, Jana Dietrich, and René Matzdorf — Institute of Physics, University of Kassel, Kassel, Germany

We used small organic molecules to construct a chiral Kagomé lattice on the Ag(111) and Au(111) surfaces. The chirality arises from triple halogen bonds that form windmill-like structures. Under certain conditions, we observe a switching in the rotational sense of whole terraces while scanning with STM. The total molecular coverage was used to tune the switching probability between the two chiral states. We demonstrate a bias-dependent attraction or repulsion of the molecules relative to the STM tip position, explaining the observed perturbation leading to the switching events.

O 59: 2D Materials: Electronic structure, excitations, etc. II (joint session O/HL/TT)

Time: Wednesday 10:30–12:30 Location: TRE/MATH

O 59.1 Wed 10:30 TRE/MATH

Polarons in epitaxial single-layer $MnBr_2$ — •Affan Safeer, Oktay Güleryüz, Guangyao Miao, Wouter Jolie, Thomas Michely, and Jeison Fischer — II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany

We investigate polaron formation in insulating single-layer $MnBr_2$ grown by molecular beam epitaxy on three different substrates: graphene on Ir(110), graphene on Ir(111), and Au(111). The polaron number densities and species depend strongly on the underlying substrate, underscoring the crucial role of the substrate. Our findings show that modeling of polarons in such single-layer insulators in contact with conducting substrates must explicitly include the substrate. For $MnBr_2$ grown on graphene/Ir(110), we identify four distinct polaron species, three of which closely resemble those reported for $CoCl_2$ on graphite. These polarons can be created, converted, and laterally manipulated by the STM tip when a tunneling current flows at suitable bias voltages. For graphene on Ir(110) as a substrate, mobile polarons in $MnBr_2$ are guided by the periodic potential imposed by the super-moiré pattern arising from the interaction of $MnBr_2$ with graphene and Ir(110).

O 59.2 Wed 10:45 TRE/MATH

Chirality in the Kagome Metal CsV_3Sb_5 — •Tom P. Lammerskötter[1], H.J. Elmers[2], G. Schönhense[2], O. Tkach[2], Y. Lytvynenko[2], H. Agarwal[2], S. Chernov[3], M. Hoesch[3], D. Kutnyakhov[3], M. Scholz[3], K. Rossnagel[4], A. Gloskovskii[3], C. Schlueter[3], A. Winkelmann[5], A. Haghighirad[6], M. Schmitt[7], T. Lee[7], R. Claessen[8], M. Le Tacon[6], J Demsar[2], and O. Fedchenko[1] — [1]Goethe-Universität Frankfurt (Germany) — [2]JGU Mainz (Germany) — [3]DESY Hamburg (Germany) — [4]Universität zu Kiel (Germany) — [5]AGH University of Krakow (Poland) — [6]KIT Karlsruhe (Germany) — [7]DIAMOND (UK) — [8]Universität Würzburg (Germany)

Kagome metals AV_3Sb_5 (A = Cs, K, Rb) exhibit flat bands, Dirac points, and van Hove singularities that drive unconventional charge-density-wave (CDW) order and topological states. We study chirality in CsV_3Sb_5 using angle-resolved photoemission spectroscopy (ARPES) and x-ray photoelectron diffraction (XPD) with circularly polarized photons. XPD reveals a local crystal chirality in the CDW phase. ARPES shows pronounced magnetic circular dichroism (MCD), demonstrating a chiral electronic structure and indicating orbital moments possibly linked to loop-current order. To probe orbital-moment coupling, we study Nb-doped CsV_3Sb_5, where band broadening and enhanced Dirac-like gaps occur. In the CDW phase, the strongly increased MCD indicates time-reversal-symmetry breaking and couples to the three van Hove singularities at the M points.

O 59.3 Wed 11:00 TRE/MATH

Ab initio and group theory ananlysis of monolayer BiTeI — •Josep Mas-Garcia, Jorge Cervantes-Villanueva, Alejandro Molina-Sánchez, and Alberto García-Cristóbal — ICMUV - University of Valencia - Spain

Monolayer BiTeI is a prototypical polar semiconductor whose remarkable Rashba spin splitting, rooted in strong spin-orbit coupling and non-centrosymmetric structure, offers a fertile landscape for advancing two-dimensional spintronics. This work presents and ab initio and group-theoretical analysis of BiTeI. Employing fully relativistic density functional theory and GW calculations, we obtain electronic structures that serve as benchmarks for the group-theory based Hamiltonian model. Leveraging the systematic method of invariants, we construct symmetry-constrained k-p Hamiltonians near the Γ point. Our implementation of the method of invariants enables precise fitting of the Hamiltoninan eigenvalues to ab initio band dispersions for the obtention of the parameters, and yields a highly compact analytic model that reproduces Rashba splitting and symmetry-dependent features. This framework facilitates straightforward evaluation of key physical quantities, such as effective masses or spin textures, and perturbative responses including electric and magnetic fields and strain effects within a unified and transparent formalism. Moreover our methodology establishes a versatile template for the symmetry-guided modeling of nonmagnetic semiconductors with strong spin-orbit coupling.

O 59.4 Wed 11:15 TRE/MATH

Production of Interstitials in 2D Transition-Metal Dichalcogenides (TMDs) by Ion Irradiation: ab-initio Simulations — •Silvan Kretschmer[1], Joel Davidsson[2], and Kristian S. Thygesen[1] — [1]CAMD, Technical University of Denmark — [2]Department of Physics, Linköping University, Sweden

Defects critically shape the properties of two-dimensional (2D) materials and can be purposefully introduced to tune magnetic, electronic, and optical behavior. Low-energy ion irradiation has recently emerged as an effective route for generating specific defect types via direct implantation [1,2].

First-principles simulations are essential for understanding irradiation-induced defect formation [3], but DFT-based molecular dynamics (MD) is computationally costly and limits broad exploration of materials and irradiation conditions. Machine-learning (ML) interatomic potentials provide a high-accuracy, low-cost alternative, enabling efficient screening of large datasets such as the Impurities in 2D Materials Database [4].

Here, we benchmark a ML potential against ab-initio MD, emphasizing accurate treatment of the short interatomic distances occurring during ion impacts. We apply the fine-tuned ML to study interstitial defect formation in TMDs under low-energy ion irradiation, providing defect formation probabilities and identifying suitable ion-beam parameters for targeted defect engineering in 2D materials.

[1] 10.1038/s41699-022-00318-4 [2] 10.1021/acsnano.4c03475
[3] 10.1103/PhysRevMaterials.8.114003 [4] 10.11583/DTU.19692238

O 59.5 Wed 11:30 TRE/MATH

Long-living metastable electronic states in substituted $1T$-TaS_2 — •Gaël Reecht[1], Jesumony Jayabalan[1], Ričards Knipšis[2], Florian Diekmann[3], Friedemann Queisser[2], Ping Zhou[1], Walter Schnelle[4], Kai Rossnagel[3,5], Ralf Schützhold[2], Manuel Gruber[1], and Uwe Bovensiepen[1] — [1]University Duisburg-Essen, Germany — [2]HZ Dresden-Rossendorf, Germany — [3]CAU of Kiel, Germany — [4]MPI for Chemical Physics of Solids, Dresden, Germany — [5]DESY, Hamburg, Germany

$1T$-TaS_2 is a prototypical correlated material whose low-temperature phase exhibits a commensurate charge density wave forming Star-of-David (SOD) clusters. Each SOD hosts a single electron close to E_F and, due to strong on-site Coulomb repulsion, the system enters a Mott insulating state. Adding or removing an electron creates doublon or holon excitations, which typically relax within few femtoseconds [1]. Here, we manipulate the lifetime of the quasiparticle excitations by substituting some Ta with an electron richer element. Using LT-scanning tunnelling microscopy and spectroscopy (STM/STS) and time-resolved photoemission spectroscopy, we observe metastable doublons with lifetimes ranging from fs to hours. STM/STS further shows that these excitations are locally confined. The experimental observations are corroborated by a theoretical description based on a Fermi-Hubbard model. The disorder induced by the random substitution leads to a spatial localization of holon and doublon wavefunctions at the origin of the long lifetimes observed experimentally.

[1] M. Ligges et *al.*, Phys. Rev. Lett., **120**, 166401 (2018)

O 59.6 Wed 11:45 TRE/MATH

Fingerprints of Excitonic Collective Modes in the Two-Dimensional Electron Gas — •Jakob Wolff[1,2,3], Silvana Botti[2,3], Lucia Reining[4,3], and Matteo Gatti[4,3,5] — [1]Institut für Festkörpertheorie- und Optik, Friedrich-Schiller-Universität Jena, Germany — [2]Research Center Future Energy Materials and Systems, University Alliance Ruhr and Interdisciplinary Centre for Advanced Materials Simulation, Faculty of Physics and Astronomy, Ruhr University Bochum, Germany — [3]European Theoretical Spectroscopy Facility (ETSF) — [4]LSI, CNRS, CEA/DRF/IRAMIS, École polytechnique, Institut Polytechnique de Paris, France — [5]Synchrotron SOLEIL, Gif-sur-Yvette, France

We investigate the collective charge excitations of the two-dimensional homogeneous electron gas in the low density regime within the framework of time-dependent density functional theory. We show that beyond the well-known plasmons new collective excitonic modes emerge, which leave characteristic fingerprints in experimentally accessible quantities, such as asymmetric peak structures in the loss function and enhanced Friedel oscillations. Further, at sufficiently low densities the collective modes become imaginary, indicating an instability towards the formation of a charge-density-wave phase with excitonic origin.

O 59.7 Wed 12:00 TRE/MATH

Moir'e modulated quantum spin liquid candidate 1T-TaSe2 — Ziying Wang, Adolfo O. Fumega, Ana Vera Montoto, Mohammad Amini, Büsra Gamze Arslan, Ales Cahlik, Yuxiao Ding, Jose L. Lado, •Robert Drost, and Peter Liljeroth — Aalto University, Department of Applied Physics

Quantum spin liquids continue to fascinate with their highly entangled quantum states and promises of fractional many-body excitations. Yet there are few tools to probe these materials, and none sensitive enough for applications in 2D materials. This seriously hampers the study of monolayer QSL candidates such as α-RuCl3 and 1T-TaSe2. Scanning tunneling microscopy and spectroscopy may overcome this challenge, as they can access the fundamental excitations of 2D samples through inelastic tunneling spectroscopy. These low-energy excitations can be compared against theoretical models and provide fingerprints of QSL states. We employ this approach against the quantum spin liquid candidate 1T-TaSe2. We observe the emergence of a root 3 reconstruction driven by the substrate, equivalent spectroscopy across all spin sites, and the coexistence of zero and finite energy excitations. These observations are consistent with a QSL ground state. Our results demonstrate that IETS provides a powerful route to obtain atomic-scale insight into the magnetic excitations of two-dimensional materials. Spectral fingerprints may help to identify exotic phases of matter that are otherwise difficult to detect.

O 59.8 Wed 12:15 TRE/MATH

Long-Range Interactions in Twisted Bilayer Materials with Machine Learning for the Electronic Density — •Zekun Lou[1], Alan Lewis[2], and Mariana Rossi[1] — [1]MPI for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Department of Chemistry, University of York, York, U.K.

Moiré superlattices in twisted bilayer (TB) 2D materials exhibit extraordinary quantum phenomena, but first-principles understanding remains limited by computational costs. While most machine learning (ML) methods for density functional theory (DFT) acceleration are based on the locality assumption, we demonstrate that accurate moiré electronic structure prediction requires long-range encoding due to charge rearrangement, orbital hybridisation, and moiré potential modulation. Using long-range representations [1] for electronic-density prediction [2,3], we achieve low-energy band-structure predictions with <15 meV errors across twisted bilayer graphene (TBG), hBN, and transition-metal dichalcogenides (TMDCs), while ~100 times faster than DFT. Descriptor requirements are material-dependent: homoatomic systems (e.g., TBG) are well-described by local descriptors, while hBN and TMDCs require long-range encoding. We summarise the physical implications of these findings that marry machine learning and the fundamental physics that governs the electronic density of twisted bilayer materials.

[1] A. Grisafi, M. Ceriotti, JCP 151, 204105 (2019)
[2] A. Lewis, A. Grisafi, M. Ceriotti, M. Rossi, JCTC 17, 7203 (2021)
[3] A. Grisafi, A. Lewis, M. Rossi, M. Ceriotti, JCTC 19, 4451 (2023)

O 60: Focus Session: Unoccupied States by Inverse Photoemission I

The Other Half of the Picture: 50 Years of Direct Access to Unoccupied States by Inverse Photoemission

In 1981, J. Pendry evaluated the experimental access to electron states in solids: "Currently only half of the picture can be seen with photoemission. Inverse photoemission provides the other half." A complete picture of electron states needs both occupied and unoccupied states in order to describe, understand, and finally tailor macroscopic material properties. In 1976, V. Dose had submitted a first paper on Bremsstrahlung Isochromat Spectroscopy in the VUV range: "The physics involved may be most simply described as an inverse photoelectric effect." The first experiments provided surface-sensitive information on the density of unoccupied states. Later, momentum and spin resolution were added to investigate the spin-dependent E(k) dispersion of unoccupied electron states. During five decades, the technique was further developed by several groups worldwide to enhance the intensity and improve the resolution in energy, momentum, and spin. A wealth of information was gained about metals, semiconductors, ultrathin films as well as adsorbate systems. The experimental studies were accompanied by several theoretical approaches, which are able to accurately describe the unoccupied electronic structure and model the inverse photoemission process. In 2012, H. Yoshida extended the energy range to the near-UV range (low-energy inverse photoemission), which is especially suited to study organic samples due to a lower damage risk caused by the exciting electron beam.

Current research fields for inverse photoemission are, e.g., spin textures of exchange- and/or spin-orbit-induced influenced systems and topological insulators, gap structures in transition metal dichalcogenides, LUMO levels in semiconductors for photovoltaic applications, electronic structure of atomic-layer and quantum materials. This focus session will highlight recent advances obtained by inverse photoemission in different fields and material systems. Also, it will bring together researchers from different areas for addressing current trends and future applications of inverse photoemission from experimental as well as theoretical perspective.

Organized by Markus Donath, Fabian Schöttke and Peter Krüger (U Münster).

Time: Wednesday 10:30–12:30 Location: WILL/A317

Invited Talk O 60.1 Wed 10:30 WILL/A317

Disentangling the origins of spin polarization in (inverse) photoemission from solid surfaces — •Jürgen Henk — Martin Luther University Halle-Wittenberg, Halle, Germany

The spin polarization of electronic states in solids can be probed by various photoemission-based techniques. We discuss how optical excitation modifies the spin polarization of the initial electronic states. Illustrative examples include Rashba-type surface states observed in photoemission (PE) from Au(111), the Dirac-like surface state in inverse photoemission (IPE) from W(110), and magnetic contrast in photoemission electron microscopy (PEEM) from Fe(001). Instead of employing a full group-theoretical analysis, we introduce a simplified symmetry-based approach that enables a clear separation of the different contributions to the photoelectron spin polarization—arising from light polarization, spin-orbit coupling, and intrinsic spin textures. This framework facilitates the interpretation of spin-resolved measurements at surfaces without relying on fully relativistic photoemission calculations.

O 60.2 Wed 11:00 WILL/A317

Inverse photoemission - just the inverse of photoemission? — •Markus Donath — University of Münster, Germany

Photoemission (PE) is known as the most powerful experimental technique to investigate the occupied energy levels of electrons in matter. The photoelectric effect, where electrons are detected after excitation with light, was first observed by H. Hertz and W. Hallwachs in 1887/1888. The reverse effect, the emission of Bremsstrahlung after irradiation of electrons was discovered by W.C. Röntgen in 1895. Bremsstrahlung spectroscopy provides access to unoccupied states. The first Bremsstrahlung spectroscopy experiment in the vacuum ultraviolet (VUV) range was performed by V. Dose fifty years ago [1]. In 1980, J.B. Pendry named this technique inverse photoemission (IPE) [2]. By using light in the VUV spectral range, PE and IPE became valuable complementary tools for studying the energy vs momentum dispersion of electron states below and above the Fermi level, even with spin resolution. After some historical remarks, this talk will review strengths and challenges as well as future perspectives of IPE.

[1] V. Dose, Appl. Phys. **14**, 117 (1977).
[2] J.B. Pendry, Phys. Rev. Lett. **45**, 1356 (1980).

O 60.3 Wed 11:15 WILL/A317

A Retrospective on Spin-Resolved IPES in Milan — •Alberto Calloni, Gianlorenzo Bussetti, and Franco Ciccacci — Dipartimento di Fisica, Politecnico di Milano, Piazza Leonardo da Vinci 32, 20133 Milano, Italy

For over thirty years, the Milan group led by Franco Ciccacci has been a key contributor to the development of spin-resolved Inverse Photoemission Spectroscopy (SR-IPES), advancing both the experimental methods and the study of empty electronic states in solids and interfaces. The activity began in the early '90s, when a dedicated system for spin- and angle-resolved measurements was conceived and built in Milan, drawing on the experience gained earlier with one of the first IPES setups using a UV grating. The new apparatus, featuring a spin-polarized GaAs electron source and a solid-state photon detector that ensured efficient detection of the weak IPES signal, enabled the direct investigation of spin-dependent unoccupied states at a time when such studies were still in their infancy. Building on this capability, the group has carried out a broad range of SR-IPES studies on metallic surfaces, magnetic thin films and multilayers, addressing phenomena such as spin-polarized quantum-well states and surface- or interface-induced spin polarization. More recently, together with studies on systems in which spin-orbit effects define the spin texture of the unoccupied states, the IPES setup has also been applied to hybrid organic/inorganic and molecule/ferromagnet interfaces, offering insight into the stability of the unoccupied states and their possible modifications upon interaction with the surrounding environment.

O 60.4 Wed 11:30 WILL/A317

Spin-Orbit Effects in Atomic-Layer Materials: Tl on Ag(111) — •Sven Schemmelmann[1], Peter Krüger[2], Patrick Härtl[3], Matthias Bode[3], Yuichiro Toichi[4], Kazuyuki Sakamoto[4], and Markus Donath[1] — [1]Physikalisches Institut, Universität Münster, Germany — [2]Institut für Festkörpertheorie, Universität Münster, Germany — [3]Experimentelle Physik II, Universität Würzburg, Germany — [4]Department of Applied Physics, The University of Osaka, Japan

Growing Tl on Ag(111) results in several structures of the Tl adlayers. For low coverage a $TlAg_2$ surface alloy is formed [1]. The Tl monolayer and bilayer exhibits moiré superstuctures with a continuous rotation of the Tl adlayer. Interestingly, all these structures exhibit characteristic spin-orbit-induced effects in their unoccupied electronic structure revealed by spin- and angle-resolved inverse photoemission. The surface alloy is predicted to exhibit states with a Rashba-type spin splitting. In experiment, the intensity of these states is too low for a spin analysis [1]. In the Tl monolayer, spin-dependent hybridization of different overlayer states is observed [2]. Surprisingly, also an image-potential state located in front of the surface is found to hybridize with Tl states. The Tl bilayer, in contrast, exhibits a non-Rashba-like spin-polarized Fermi surface whose origin is found in the dispersion of the unoccupied states.

[1] Härtl *et al.*, Phys. Rev. B **107**, 205144 (2023)
[2] Schemmelmann *et al.*, Phys. Rev. B **109**, 165417 (2024)

O 60.5 Wed 11:45 WILL/A317

Surface state on Au(111): Shockley vs topology — •Patrick Geers, Fabian Schöttke, and Markus Donath — University of Münster, Germany

The *L*-gap surface state on Au(111) is the famous prototype for a Rashba-split Shockley surface state (SS). In 2015, Yan *et al.* posed the question whether Shockley-type SSs may be interpreted as variation of SSs in topological insulators, as both states exist in inverted band gaps [1]. The behaviour of the SS

away from $\overline{\Gamma}$ is important to answer this question. It is crucial to know whether the SS potentially closes the inverted band gap between $\overline{\Gamma}$ and $\overline{M}$. An analysis of not only the existence of SSs but also their spin textures is necessary to show a potential topologically nontrivial character of such SSs.
Inverse photoemission (IPE) as a technique to study the unoccupied electronic states is capable to measure these SSs with spin resolution at expected energies of about 4 eV above the Fermi level. In this talk, we present spin-resolved IPE results for Au(111) showing the energy vs momentum range between $\overline{\Gamma}$ and $\overline{M}$, where the SS merges into the bulk bands.

[1] Yan *et al.*, Nat. Commun. **6**, 10167 (2015).

O 60.6 Wed 12:00 WILL/A317

Combining Spin Polarized Inverse Photoemission Spectroscopy with Angle-resolved X-ray Magnetic Circular Dichroism — •Takashi Komesu[1], Arjun Subedi[1], Bharat Giri[1], Ather Mahmood[1], Will Echtenkamp[1], Mike Street[1], Alpha N'Diaye[2], Xiaoshan Xu[1], Christian Binek[1], and Peter Dowben[1] — [1]University of Nebraska-Lincoln, Lincoln, NE, U.S.A — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA, U.S.A

While angle-resolved magnetometry and angle-resolved X-ray Magnetic Circular dichroism (XMCD) might provide hints of spin or moment canting at a surface, even XMCD taken in the total electron yield (TEY) mode cannot convincingly implicate the surface. Spin Polarized Inverse Photoemission Spectroscopy (SPIPES) is hugely surface sensitive, which is an advantage for characterizing boundary polarization of materials. With in-plane SPIPES, we have convincing proof of deviation from the expected perpendicular anisotropy for boron (B) doped $Cr_2O_3(0001)$ and at the surface of $NiCo_2O_4(001)$. For $NiCo_2O_4(001)$, the Ni magnetic moments are canted slightly off the surface normal, as evident in elemental specific angle-resolved XMCD and consistent with the very surface sensitive SPIPES. In this presentation, we will show the great value of combining SPIPES with XMCD and magnetometry. Furthermore, we can provide an example where an exponential decay of spin polarization is not evidence of a finite paramagnetic correlation length, as in the case of thickness dependent Pd over layers on $Cr_2O_3(0001)$, where Pd is no longer paramagnetic.

O 60.7 Wed 12:15 WILL/A317

On the sign of the Rashba parameter in image-potential states — •Fabian Schöttke[1], Kaishu Kawaguchi[2], Kenta Kuroda[3], Peter Krüger[1], Thorsten Deilmann[1], Sven Schemmelmann[1], Ayumi Harasawa[2], Shuntaro Tani[2], Yohei Kobayashi[2], Takeshi Kondo[2], and Markus Donath[1] — [1]Universität Münster, Germany — [2]Institute for Solid State Physics, The University of Tokyo, Japan — [3]Hiroshima University, Hiroshima, Japan

Image-potential surface states are simple model systems, where spin-dependent effects can be studied in view of spintronic applications. The Rashba effect in surface states at high-Z materials is related to both the strong spin-orbit interaction in heavy atoms and the orbital angular momentum arising from the inversion-symmetry breaking at the surface. Our studies with spin- and angle-resolved inverse photo-emission and three-photon photoemission on image-potential states at Re(0001), Bi_2Se_3 and Bi_2Te_3 show a clear correlation between orbital angular momentum and spin directions. A key factor of our analysis is spin resolution, which enhances the effective resolution to separate spectral features considerably, provided they have different spin character.

O 61: Organic molecules on inorganic substrates: electronic, optical and other properties II

Time: Wednesday 15:00–17:45 Location: HSZ/0201

O 61.1 Wed 15:00 HSZ/0201

Circular dichroism in the photoelectron angular distribution of achiral molecules — Christian Simon Kern[1], Xiaosheng Yang[2], Giovanni Zamborlini[1,3], Simone Mearini[3], Matteo Jugovac[3], Vitaliy Feyer[3], Umberto De Giovannini[4], Angel Rubio[4], Serguei Soubatch[2], Michael G. Ramsey[1], •Frank Stefan Tautz[2], and Peter Puschnig[1] — [1]Institute of Physics, University of Graz, Austria — [2]PGI-3, FZ Jülich & RWTH Aachen University, Germany — [3]PGI-6, FZ Jülich & Universität Duisburg-Essen, Germany — [4]MPI for the Structure and Dynamics of Matter, Hamburg, Germany

Circular dichroism in the angular distribution (CDAD) is the effect that the angular intensity distribution of photoemitted electrons depends on the handedness of the incident circularly polarized light. CDAD has been reported also for achiral organic molecules at the interface to metallic substrates. For this latter case, we investigate two prototypical pi-conjugated molecules, namely tetracene and pentacene, whose frontier orbitals have a similar shape but exhibit distinctly different symmetries. By comparing experimental CDAD momentum maps with simulations within time-dependent density functional theory, we show how the final state of the photoelectron must be regarded as the source of the CDAD in such otherwise achiral systems. We gain additional insight into the mechanism by employing a simple scattering model for the final state, which allows us to decompose the CDAD signal into partial wave contributions.

O 61.2 Wed 15:15 HSZ/0201

Many-body electronic structure of acenes on an MoS2 monolayer — •Jan-Phillip Topmöller and Michael Rohlfing — Institute of Solid State Theory, University of Münster, Germany

TMDCs show great potential in terms of their applicability in optical electronics. Due to their large surface, molecules can easily bind to the TMDC and affect its electronic properties. Here we investigate acenes as a prototypical class of molecule.

We use DFT (GGA) and DFT-D3 to determine the most stable adsorption position of acenes like benzene, naphthalene and anthracene on MoS2. Subsequently, we use many body perturbation theory to calculate the electronic structure of the adsorbate system and its individual components (MoS2 and the molecule) in order to investigate the effect of the molecule on the MoS2 electronic and optical spectrum.

O 61.3 Wed 15:30 HSZ/0201

Azimuthal-Scanning SFG Microscopy for Mapping Packing Motifs and In-Plane Disorder in Molecular Films — •Nasim Mirzajani, Ben John, Alex Fellows, and Martin Thaemer — Fritz-Haber-Institut, Berlin, Germany

Phase-resolved vibrational sum-frequency generation (SFG) microscopy is a powerful tool for probing anisotropic and heterogeneous structure of molecular films. As a second order nonlinear technique, SFG is uniquely sensitive to disorder in film morphology but it has not been yet used to quantify order in molecular film assemblies. Here, we introduce an azimuthal-scanning SFG microscopy approach that extracts detailed information on structure as well as in-plane orientational order by analyzing the full set of rotational frequencies arising from azimuthal dependence. Applying the method to a lipid monolayer, we determine the full 3D structure of the lipids, the packing motif as well as the degree of its in-plane disorder. This technique provides a general framework for probing packing structure in thin films and is broadly applicable to diverse molecular and phononic materials.

O 61.4 Wed 15:45 HSZ/0201

Synthesis and Characterization of a Polyradical Hexaazacycloarene — •Zilin Ruan, Olaf A. Kleykamp, Tim Naumann, Faming Kang, Jörg Sundermeyer, and J. Michael Gottfried — Department of Chemistry, Philipps University Marburg, 35037 Marburg, Germany

Cycloarenes have drawn considerable research interest owing to their unique electronic and topological features. The synthesis of large zigzag-edged cycloarenes, which are predicted to exhibit exotic polyradical ground states, has remained elusive. Here, we report the synthesis of a zigzag-edged hexaazacycloarene incorporating six graphitic nitrogen atoms within its macrocyclic backbone, achieved through a combined in-solution cyclization and on-surface cyclodehydrogenation on a Au(111) surface. The structural and electronic properties of the resulting macrocycle were investigated by STM/STS, nc-AFM and KPFM. DFT and multireference CASSCF calculations reveal that the isolated molecule has an open-shell singlet ground state with six unpaired electrons and undergoes a spontaneous symmetry breaking from C6 to C2, driven by strong electron-electron correlations and a pseudo-Jahn-Teller instability. Notably, the expected low-energy spin excitations are absent on Au(111), which is rationalized by the hybridization between the molecular π-system and the substrate, effectively quenching the intrinsic magnetism. These results provide crucial insight into correlation-driven magnetism and represent a significant advance toward the realization of cycloarenes with π-magnetism.

O 61.5 Wed 16:00 HSZ/0201

Vibrational Spectra of Materials and Molecules with Path Integrals and Machine Learning — •Jorge Castro, Krystof Brezina, and Mariana Rossi — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Vibrational spectroscopy provides fundamental insight into molecular structure and dynamics. Nuclear quantum effects (NQEs) can critically modulate vibrational peak positions, shapes, and intensities. Recently, we showed that the partially adiabatic elevated-temperature centroid molecular dynamics (PA-T_e-CMD) [1] accurately reproduces vibrational spectra across molecular and condensed-phase systems, including low-temperature regimes where NQEs are strongest. This approach enables the simulation of quantum infrared and Raman responses in diverse spectroscopic settings. Tip-Enhanced Raman Spectroscopy (TERS) [2] achieves sub-nanometer spatial resolution and is uniquely sensitive to single-molecule vibrational motion and surface defects. Building on

first-principles finite-field formulations of TERS [3], we combine this framework with PA-T_e-CMD to quantify the role of nuclear quantum motion and anharmonicity in near-field Raman observables. As a first application, we investigate hydrogen-bonded chains of 2,5-diamino-1,4-benzoquinonediimine (DABQDI) and discuss how NQEs imprint on vibrational signatures in simulated TERS images.

[1] J. Castro et al., J. Chem. Phys. 163, 204102 (2025). [2] J. Lee et al., Nature 568, 78*82 (2019). [3] K. Brezina et al., arXiv:2509.13075 (2025).

O 61.6 Wed 16:15 HSZ/0201

Quasiparticle level alignment in anthracene-MoS_2 heterostructures — •Hsin-Mei Ho, Michael Lorke, and Peter Kratzer — Faculty of Physics, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Stacking atomically thin materials through van der Waals (vdW) interaction has opened a new paradigm for fundamental and applied sciences. While preserving the advantages of individual components, heterostructures are predicted to exhibit emergent properties at the interfaces. In the presence of external perturbations, since the behavior of a hybrid system is strongly related to the electronic band structure, it is of interest to find a methodology beyond the ground-state formalism of density functional theory (DFT). In this work, we begin with DFT calculations and consider the organic-inorganic heterostructures composed of anthracene molecules on monolayer MoS_2. Motivated by studies on the crystallinity of organic films, interfacial configurations with different coverage and orientation of anthracene are investigated. We find that both the bandgap values and band offsets are sensitive to whether the molecules are closely packed and whether they adopt perpendicular or parallel orientations on MoS_2. Whereas DFT predicts type-II level alignment, inclusion of quasi-particle corrections via the GW approximation yields type-I alignment. These findings highlight the importance of level-alignment predictions for interpreting experiments and for guiding the design of organic-TMDs heterostructures.

O 61.7 Wed 16:30 HSZ/0201

Magnetic interactions between spins in the Metallacrown CuCu4: bulk vs adsorbed molecule on Au(111) — •Ariyan Tavakoli[1], Stefan Lach[1], Frederik Pütz[1], Dominic Stephan[1], Anne Lüpke[2], Dominik Laible[2], Siegfried Kaidisch[3], Andreas Winidischbacher[3], Eva Rentschler[2], Peter Puschnig[3], Christiane Ziegler[1], and Hans Christian Schneider[1] — [1]RPTU University Kaiserslautern-Landau, Germany — [2]Johannes Gutenberg University Mainz, Germany — [3]University of Graz, Austria

Metal-organic complexes featuring multiple metal ions with unsaturated spin structures are intriguing because of their potential to tune molecular magnetic properties. In this study, we compare the magnetic and electronic properties of the CuCu4 metallacrown [1] in bulk, gas-state, and adsorbed on an Au(111) surface. Using the broken-symmetry approach, we benchmark various (range-separated) hybrid functionals against the computationally efficient GGA+U method to evaluate exchange coupling constants in different states [2]. We compare ultraviolet photoemission spectroscopy (UPS) combined with ab-initio calculations to show how the exchange interactions between Cu spins shift significantly, resulting in a transition from a low-spin state (S = 1/2) in the bulk to a higher-spin state (S = 3/2) on Au(111).

[1] Happ, P.; et al. Phys. Rev. B, 93, 174404 (2016).
[2] Pavlyukh, Y. et al., Phys. Rev. B. 99, 144418 (2019).

O 61.8 Wed 16:45 HSZ/0201

Vectorial spin-to-charge conversion by supramolecular chirality — •Sophie Knewitz[1], Guillaume Schweicher[2], Ashish Moharana[1], Yves Geerts[2], and Angela Wittmann[1] — [1]Johannes Gutenberg-Universität, Mainz, Germany — [2]Université Libre, Bruxelles, Belgium

The chiral-induced spin selectivity (CISS) effect describes how electrons get spin-polarized due to the presence of chiral molecules. The high polarization efficiency makes it promising for future sustainable hybrid chiral molecule magnetic applications. While there are many experimental reports of different aspects of the CISS effect, a complete understanding of the fundamental mechanisms remains an open challenge. In this work, we investigate the role of supramolecular chirality and atomic spin-orbit coupling on the CISS effect in hybrid metal thin film / chiral organic crystal heterostructures. Using spin pumping to inject a pure spin current in the metal thin film, we probe the spin-to-charge conversion at the chiral interface. Based on our recent finding that CISS is a vectorial effect [1], we use a molecular chiral crystal to probe the CISS effect in a well-ordered system in order to maximize the polarization efficiency. Our angle-dependent measurements confirm that the spin selectivity of the chiral supramolecular crystal is highly sensitive to its orientation relative to the spin direction in the metal thin film under the applied magnetic field. These results open new ways for the vectorial manipulation of hybrid spintronic devices by chirality.

[1]: Moharana, A. et al., Sci. Adv. 11, eado4285 (2025).

O 61.9 Wed 17:00 HSZ/0201

Chiral recognition of enantiomers on a superconducting surface — •Lorenz Meyer, Nicolas Néel, and Jörg Kröger — Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany

The adsorption of a racemic mixture of heptahelicene on Pb(111) gives rise to enantiopure domains, in which left-handed and right-handed variants are spatially resolved with submolecular structure. For molecules inside the domains the molecular spiral is oriented along the surface normal, while at domain boundaries the spiral axis is tilted. Both enantiomers leave the Bardeen-Cooper-Schrieffer energy gap of the substrate invariant and exhibit an elevated energy difference between the occupied and unoccupied frontier orbitals. Funding by the Deutsche Forschungsgemeinschaft through KR 2912/21-1 and the Bundesministerium für Bildung und Forschung is acknowledged.

O 61.10 Wed 17:15 HSZ/0201

Unveiling the precise configuration of a molecular junction — Joshua Scheidt[1,3], Jonas Lederer[3], Mong-Wen Gu[1,2], Hadi Arefi[1,2], Jose M. Guevara[1,2], Amin Karimi[1,2], Rustem Bolat[1,2], Marvin Knol[1,2], Klaus-Robert Müller[3], F. Stefan Tautz[1,2], and •Christian Wagner[1,2] — [1]PGI-3, Forschungszentrum Jülich, Germany — [2]JARA, Fundamentals of Future Information Technology, Germany — [3]Institut für Softwaretechnik und Theoretische Informatik, Technische Universität Berlin, Germany

Exploring structure-property relationships of molecular junctions is crucial for future single-molecule applications. While, e.g., a strong scattering of conductance values is found in break-junctions, the responsible structural variations cannot be identified. Here, we describe NC-AFM/STM-based two-contact manipulation experiments on PTCDA (3,4,9,10-perylene-tetracarboxylic dianhydride) on Ag(111) and analyze them using a DFT-based machine learning model of the junction. Our approach allows solving the inverse problem of configuration identification from force gradient data[1] and reveals the origin of the 3-4 fold conductance variations observed upon sub-Angstrom changes in the junction geometry.

[1] J. Scheidt et al., J. Phys. Chem. C 127, 13817 (2023)

O 61.11 Wed 17:30 HSZ/0201

Low-temperature scanning tunneling microscopy and spectroscopy of 1,10-phenanthroline molecules on Au(111) surface — •Yuya Kaneko[1], Takaya Shimokawa[1], Hinata Aso[1], Erlina Tik Man[1], Kenji Hayashida[2], Koutarou Takeyasu[3], Junji Nakamura[4], and Yasuo Yoshida[1] — [1]Dept. of Phys. Kanazawa Univ., Kanazawa, Ishikawa 920-1192, Japan. — [2]Graduate School of Pure and Applied Sciences, Univ. of Tsukuba, Ibaraki 305-8577, Japan. — [3]institute for Catalysis, Hokkaido Univ., Hokkaido 001-0021, Japan. — [4]International Institute for Carbon-Neutral Energy Research, Kyushu Univ., Fukuoka 819-0395, Japan.

Fuel cells are considered a key technology for achieving a low-carbon society. However, current fuel cells rely on precious platinum for the oxygen reduction reaction (ORR). Nitrogen-doped carbon catalysts have attracted attention as promising alternatives due to their low cost and high durability, yet the detailed reaction mechanism remains unclear. Here, we report a scanning tunneling microscopy and spectroscopy (STM/S) study of in situ deposited 1,10-phenanthroline molecules, which serve as ideal model catalytic molecules for ORR activity [1]. [1]Takeyasu K., Furukawa M., Shimoyama Y., Singh S. K., Nakamura J., (2020) Role of Pyr-idinic Nitrogen in the Mechanism of the Oxygen Reduction Reaction on Carbon Electro-catalysts. Angew. Chem. Int. Ed.,60,5121-5124..

O 62: Graphene: Electronic structure, excitations, etc. (joint session O/TT)

Time: Wednesday 15:00–17:45 Location: HSZ/0204

O 62.1 Wed 15:00 HSZ/0204

Magneto-photoelectric effect in graphene via tailored potential landscapes — •Friedemann Queisser[1], Joris Josiek[1,2], Stephan Winnerl[1], and Ralf Schützhold[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

We consider the propagation of charge carriers in planar graphene under the combined influence of a constant transversal magnetic field and an in-plane varying electric potential. By suitably designing the potential landscape, we may effectively steer charge carriers generated by photo-excitation, for example, in order to achieve an efficient charge separation. These finding may pave the way for transport schemes or photoelectric/photovoltaic applications. Funding by the DFG through the SFB 1242 is gratefully acknowledged.

O 62.2 Wed 15:15 HSZ/0204

Topological obstruction in twisted bilayer graphene — Florie Mesple[1], Pierre Mallet[2], •Guy Trambly de Laissardière[3], Clement Dutreix[4], Gérard Lapertot[5], Jean-Yves Veuillen[2], and Vincent T. Renard[5] — [1]Dept. Physics, Univ. of Washington, Seattle, USA — [2]CNRS, Univ. Grenoble Alpes, Inst. Néel, Grenoble, France — [3]CY Cergy Paris Univ., CNRS, LPTM, Cergy-Pontoise, France — [4]Univ. Bordeaux, CNRS, LOMA, Talence, France — [5]Univ. Grenoble Alpes, CEA, IRIG, PHELIQS, Grenoble, France

The rich physics of magic angle twisted bilayer graphene (TBG) results from the Coulomb interactions of electrons in nearly flat bands of non-trivial topology [1]. Here [2], we perform STM/STS measurements on a moiré pattern generated in a TBG tilted by 4.3°, focusing on a point-like defect. We observe quasiparticle interferences (QPIs) resulting from intravalley backscattering between Dirac cones of graphene layers 1 and 2. Rationalized by tight binding calculations and T-matrix theory, our work shows that the QPIs are strongly impacted by the relative chirality of the Dirac cones of layer 1 and 2 in each valley. It establishes that, within a given moiré valley, the two Dirac cones have the same electronic chirality, as expected in the usual continuum model [3]. This peculiar topology leads to a topological obstruction.

[1] B. A. Bernevig, D. K. Efetov, Physics Today **77**, 38 (2024)
[2] F. Mesple, et al., arXiv:2506.08913 (2025)
[3] R. Bistritzer, A. H. MacDonald, PNAS **108**, 12233 (2011)

O 62.3 Wed 15:30 HSZ/0204

Quasiparticle Interferences in 30°-twisted graphene quasicrystal — •Jean-Maxime Schlachter[1], Ahmed El Alouani[2], Vincent S Renard[2], Abhishek Karn[1], Ileana Florea[2], Stéphane Vézian[2], Adrien Michon[2], Clemens B Winkelmann[1], and Vincent T Renard[1] — [1]Univ. Grenoble Alpes, CEA, Grenoble INP, IRIG, PHELIQS, 38000 Grenoble, France — [2]CNRS-CRHEA, Université Côte d'Azur, rue B. Grégory, 06560 Valbonne, France

Quasicrystals are materials that have clean diffraction pattern but no translational symmetry. The advent of van der Waals stacking has opened the possibility to engineer quasicrystals. For example, the moiré pattern in 30°-twisted graphene bilayers has 12-fold rotational symmetry which is not compatible with translation symmetry in 2D, hence it is a quasicrystal (1). Studying this system gives insight into the behavior of Dirac fermions in 2D quasicrystals. ARPES experiments (2) demonstrated the existence of multiple Dirac cone replicas, originating from the incommensurate interlayer coupling. The goal of this study is to determine to what extend these Dirac cone replicas influence the electronic properties of the Dirac fermions. Our low temperature scanning tunneling microscope (STM) experiments evidence the replicated Dirac cones by specific patterns in the local density of states patterns associated with scattering between them, contrary to previous STM experiments (3).

(1) P. Moon et al., Phys. Rev. B, **99**, 16, :165430 (2019) ; (2) S. J. Ahn et al., Science, **361**, 6404, :782-786 (2018) ; (3) C. Yan et al., 2D Mater., **6**, 4, :045041 (2019)

O 62.4 Wed 15:45 HSZ/0204

Machine Learning for Bandstructure-Structure Relationships in Doped Graphene — •Benedict Saunders[1], Lukas Hörmann[1,2], Valdas Vitartas[1], Chen Qian[1], and Reinhard J Maurer[1,2] — [1]University of Warwick, Coventry, United Kingdom — [2]University of Vienna, Vienna, Austria

The introduction of topological defects or dopants to graphene's honeycomb lattice is a common approach to tuning the electronic and transport properties of the material to suit a specific application. Nitrogen is a widely investigated dopant, which can be introduced into the lattice in various configurations, each with a distinct effect on the material's bandstructure. However, due to the combinatorial explosion of possible dopant configurations, conventional first-principles screening of the electronic bandstructure for all possible configurations is not feasible. Here, we address this limitation by employing the recently developed MACE-H machine learning model to predict the electronic Hamiltonian of nitrogen-doped graphene configurations directly for a series of previously generated defect configurations. This allows us to rapidly generate accurate bandstructures and densities-of-states for large numbers of configurations, enabling the identification of structure-property relationships as a function of temperature and composition.

O 62.5 Wed 16:00 HSZ/0204

Electronic structure of intercalated epitaxial graphene: A first principles study — •Andres Unigarro[1], Florian Günther[2], and Sibylle Gemming[1] — [1]Institute of physics, TU Chemnitz, Chemnitz, Germany — [2]UNESP, Rio Claro, Brazil

Two-dimensional materials such as graphene are particularly intriguing due to their exceptional mechanical and electronic properties. A natural next step involves combining different 2D materials to form heterostructures with enhanced functionalities. In epitaxial graphene on silicon carbide (SiC), intercalation provides an effective means to tune the electronic, optical, and transport properties of graphene while preserving its honeycomb lattice. Moreover, intercalation enables the synthesis of otherwise unstable 2D layers. In particular, the intercalation of heavy elements such as Pb [1] and Bi [2] is especially promising, as these can introduce strong spin-orbit coupling (SOC) effects [3] (e.g. Rashba effect, gap opening) in graphene. In this work, we use first-principles calculations to investigate the electronic properties of heterostructures formed by Pb and Bi intercalation.

[1] Schölzel, Franziska, et al. ‚Small Structures (2024), 2400338
[2] Tilgner, N., et al. Nat Commun 16, (2025), 6171.
[3] Unigarro A., et al. J. Phys. Chem. C (2025), 129, 11, 5617-5624

O 62.6 Wed 16:15 HSZ/0204

Domain-resolved electronic structure of AgTe-intercalated graphene on SiC(0001): From semiconducting Te-rich interlayer bands to metallic AgTe alloy states — •Vibha Reddy[1], Sawani Datta[1], Bharti Matta[1], Philipp Rosenzweig[2], Ulrich Starke[1], and Kathrin Küster[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, — [2]Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart

Intercalation at the graphene/SiC(0001) interface provides a powerful route towards engineering the electronic properties of both the graphene and the intercalant. Here, we present the first realization of a transition-metal chalcogen alloy intercalated into the graphene/SiC(0001) interface via AgTe intercalation. The nominally AgTe-intercalated system segregates into multiple microscale intercalation phases, namely, Te-rich, Ag-rich and AgTe alloyed domains. Spatially-resolved and angle-resolved photemission spectroscopy (ARPES) reveals that each domain exhibits distinct graphene doping levels and interlayer band dispersions, highlighting the strong interplay between local intercalation chemistry investigated by X-ray photoelectron spectroscopy (XPS) and electronic band structure. Given the intrinsic spin-orbit coupling and topologically non-trivial states associated with Te- and Ag-based 2D materials, the AgTe alloy-intercalated graphene represents a promising platform for realizing domain-specific emergent quantum phenomena, underscoring the chemical versatility and tunability of alloy-based heterostructures in interface engineering.

O 62.7 Wed 16:30 HSZ/0204

Proximity-induced electronic states in epitaxial graphene/SiC (0001) via Sn intercalation — •Huu Thoai Ngo[1], Zamin Mamiyev[1], Niklas Witt[2,3], Tim Wehling[2], and Christoph Tegenkamp[1] — [1]Solid Surface Analysis, Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]Institute of Theoretical Physics & Centre for Ultrafast Imaging, University of Hamburg, Hamburg, Germany — [3]Institute for Theoretical Physics and Astrophysics, University of Würzburg, Würzburg, Germany

Intercalation of heavy elements at the buffer layer/SiC interface is an effective route to decouple it from the substrate while tailoring its electronic properties, for example, energy gap opening [1] and Mott insulating states [2]. In this work, we investigate the Sn-intercalated buffer layer using low-temperature STM/STS, supplemented by SPA-LEED, and DFT calculations. By precisely controlling the intercalation process, we obtain two distinct Sn phases beneath graphene: Sn(1x1) that induces Kekulé-O distortion, and honeycomb-Sn structure that gives rise to Moiré patterns. Remarkably, our STS results reveal a gap opening in Kekulé-O graphene due to Sn-induced sublattice symmetry breaking. In contrast, the honeycomb-Sn phase exhibits Mott insulating states. These findings demonstrate how Sn intercalants modify the structural and electronic properties of graphene at both nano- and microscale. [1] Ghosal, Tegenkamp, C. et al. Phys. Rev. Lett. 129, 116802 (2022). [2] Ghosal, Tegenkamp, C. et al. Phys. Rev. B 111, 235426 (2025).

O 62.8 Wed 16:45 HSZ/0204

Doping monolayer graphene to the Van Hove singularity — •Guangyao Miao[1], Daniel Jansen[1], Bilal Hawashin[2], Julian Kleeschulte[2], Katharina Offermann[1], Christian Krämer[1], Affan Safeer[1], Abdallah Karaka[1], Jeison Fischer[1], Thomas Michely[1], Michael M. Scherer[2], and Wouter Jolie[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Cologne, Germany — [2]Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany

Tuning correlated states in graphene is an intriguing topic, particularly since the experimental realization of superconductivity, correlated insulator states, and magnetic states in twisted-angle bilayer graphene near the magic angle, along with Van Hove singularities (VHSs) tuned to the Fermi level. Such correlated phenomena have also been predicted in monolayer graphene doped to its van Hove singularity. Motivated by this, we study the effect of Cs doping on a graphene monolayer on Ir(111) using MBE. A $\sqrt{3}\times\sqrt{3}$ superstructure is observed due to the Cs intercalations between graphene and Ir(111). Further deposition of Cs on top of graphene leads to the formation of several surface structures with varying Cs concentrations, including adatoms, stripes, and compact islands. Their morphology and electronic structures are revealed by scanning tunneling microscopy and spectroscopy at low temperature. By optimizing the dosage, we successfully tune the VHS to the vicinity of the Fermi level and observe a $2\sqrt{3}\times2\sqrt{3}$ superstructure with respect to the graphene lattice. Possible origins of the superstructure related to many-body interactions will be discussed.

O 62.9 Wed 17:00 HSZ/0204

Optimizing quantum transport in multi-barrier graphene systems using differential evolution — •Leon Browne and Stephen R. Power — School of Physical Sciences, Dublin City University, Ireland

Potential and mass barriers in graphene introduce electron scattering, modulating transmission probabilities. Complex multi-barrier setups allow electron transmission to be controlled with high precision, but have a huge design space of possible barrier geometries. This work presents a framework to optimize electronic transport in such systems using differential evolution algorithms. First, transfer matrix methods are employed to efficiently compute quantum transport through multi-barrier structures, before optimization is applied to find barrier configurations whose transmission profiles closely match a predefined target profile. To address the trade-off between the accuracy and complexity of resulting barrier configurations, regularization techniques are incorporated into the optimization process. Our approach demonstrates the potential for highly tunable electronic transport in graphene-based systems by exploiting evolution-inspired optimization techniques.

O 62.10 Wed 17:15 HSZ/0204

Comparative study of plasmons in half-filled graphene via Quantum Monte Carlo and kinetic theory — Maksim Ulybyshev[1], •Adrien Reingruber[1], and Kitinan Pongsangangan[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg — [2]Department of Physics, Faculty of Science, Mahidol University, Bangkok

A quantitative description of hydrodynamic electronic transport in strongly correlated materials requires accurate knowledge of collective excitations such as plasmons, which can notably influence viscosity. In free-standing graphene, where long-range interactions are important, standard Dirac-cone perturbation theory misses important finite Brillouin-zone and strong-coupling effects. We investigate plasmons in half-filled free-standing graphene using unbiased Quantum Monte Carlo simulations. Our results reveal well-defined plasmon peaks near the Gamma-point, map their dispersion, and extract the momentum dependence of their quasiparticle residue. Comparing to perturbative predictions, we find substantial deviations arising from the interaction and lattice effects captured only beyond the Dirac approximation. These results underscore the need to incorporate such corrections in analytical theories of electronic transport in graphene.

O 62.11 Wed 17:30 HSZ/0204

NanoARPES Facility in Shanghai Synchrotron Radiation Facility and Investigation of the Moiré bands in Graphene Devices — •Zhongkai Liu — Shanghaitech University

Spatially resolved angle-resolved photoemission spectroscopy (NanoARPES) is an indispensable tool for probing the electronic structure of exfoliated sample flakes, fabricated devices, and more. In this presentation, we describe the construction, specifications, capabilities, and operation of BL07U-the NanoARPES endstation at the Shanghai Synchrotron Radiation Facility (SSRF) [1]. We will showcase our research on the electronic structure of emerging graphene devices, with a focus on moiré and flat bands. For example, our ARPES studies on magic-angle twisted trilayer graphene clearly reveal the coexistence of moiré flat bands and Dirac bands [2]. In aligned bilayer graphene/hBN heterostructures, we demonstrate that in-situ back gating enables precise tuning of the moiré electronic structure [3]. We directly observe the characteristic topological electronic structures of rhombohedral multilayer graphene, from a 3D generalization of the 1D Su-Schrieffer-Heeger (SSH) chain in thin layers to a topological Dirac nodal spiral semimetal in bulk rhombohedral graphite [4]. Finally, we present our work on the moiré band in bulk alternating twist graphene, which becomes flat at "magic momenta".

Reference: [1] H. Gao et al., Synchrotron Radiation News 37, 12-17 (2024) [2] Y. W. Li et al., Advanced Materials 202205996 (2022) [3] H. B. Xiao et al., Advanced Science 202412609 (2025) [4] H. B. Xiao et al., Science Bulletin 70, 1030-1033 (2025)

O 63: Topology and symmetry protected materials & Topological insulators (joint session O/HL/TT)

Time: Wednesday 15:00–17:45 Location: HSZ/0401

O 63.1 Wed 15:00 HSZ/0401

Majorana or Not? An Insight from Atomic-Scale Shot-Noise — •Abhishek Maiti[1], Genda Gu[2], and Freek Massee[1] — [1]Université Paris-Saclay, CNRS, Laboratoire de Physique des Solides, 91405, Orsay, France — [2]Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, NY, USA

The search for non-abelian states of matter has become a central theme of modern quantum material research. Notably, Majorana zero modes are of special interest, as they can serve as the foundation for topological qubits. A robust zero-bias conductance peak, observed in scanning tunneling spectra, is often regarded as the primary signature of a Majorana zero mode. Yet similar features can also arise from trivial bound states, raising a long-standing challenge of how to distinguish a genuine Majorana from imposters. In my talk, I will address this problem with a new approach, atomic-scale shot-noise spectroscopy, that goes beyond conductance measurements. Through a detailed investigation on multiple defect- and vortex-bound zero-bias states in the widely studied (putative) topological superconductor Fe(Se,Te), I will show that while differential conductance measurements might sometimes fail to detect an imposter Majorana state locally, noise measurements consistently provide a conclusive diagnostic, offering a powerful complementary probe. Looking ahead, this technique can be applied to other reported platforms to verify whether their Majorana-like signature in tunneling conductance can pass the shot-noise test.

O 63.2 Wed 15:15 HSZ/0401

Intrinsic topological superconductivity revealed by surface-extended Andreev bound states in $PtBi_2$ — •Xiaochun Huang[1], Lingxiao Zhao[2], Sebastian Schimmel[3,4], Julia Besproswanny[3,4], Patrick Härtl[1], Christian Hess[3,4], Bernd Büchner[4,5], and Matthias Bode[1] — [1]Experimentelle Physik 2, Physikalisches Institut, Universität Würzburg, Germany — [2]Quantum Science Center of Guangdong, Shenzhen, China — [3]Fakultät für Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, Germany — [4]Leibniz-Institute for Solid State and Materials Research, Dresden, Germany — [5]Technische Universität Dresden, Germany

Intrinsic topological superconductivity remains a central question in condensed-matter physics. The three-dimensional Weyl semimetal $PtBi_2$ was recently shown by angle-resolved photoemission spectroscopy to host a superconducting gap that opens exclusively on its Fermi-arc surface states with a nodal structure, establishing it as a prime candidate for intrinsic topological superconductivity [1]. Using scanning tunneling microscopy and spectroscopy, we directly visualize surface-extended Andreev bound states (ABSs) across atomically pristine terraces within a sizable superconducting gap ($\Delta > 10$ meV) in $PtBi_2$. Quantitative analysis of the tunneling spectra within an anisotropic chiral pairing framework identifies these ABSs as signatures of an emergent Majorana-cone dispersion. Our findings provide a definitive real-space spectroscopic fingerprint of intrinsic topological superconductivity in $PtBi_2$.

[1] A. Kuibarov *et al.*, Nature **626**, 294 (2024)

O 63.3 Wed 15:30 HSZ/0401

Probing chiral symmetry with a topological domain wall sensor — •Artem Odobesko[1], Glenn Wagner[2], Titus Neupert[2], Ronny Thomale[1], and Matthias Bode[1] — [1]Physikalisches Institut, Universität Würzburg, Würzburg, Germany — [2]Department of Physics, University of Zurich, Zürich, Switzerland

Chiral symmetry is a fundamental property with profound implications for the properties of elementary particles, that implies a spectral symmetry (i.e. E -> -E) in their dispersion relation. In condensed matter physics, chiral symmetry is frequently associated with superconductors or materials hosting Dirac fermions such as graphene or topological insulators. There, chiral symmetry is an emergent low-energy property, accompanied by an emergent spectral symmetry. While the chiral symmetry can be broken by crystal distortion or external perturbations, the spectral symmetry frequently survives. As the presence of spectral symmetry does not necessarily imply chiral symmetry, the question arises how these two properties can be experimentally differentiated. Here, we demonstrate how a system with preserved spectral symmetry can reveal underlying broken chiral symmetry using topological defects. Our study shows that these defects induce a spectral imbalance in the Landau level spectrum, providing direct evidence of symmetry alteration at topological domain walls. Using high-resolution STM/STS we demonstrate the intricate interplay between chiral and translational symmetry which is broken at step edges in topological crystalline insulator $Pb_{1-x}Sn_xSe$.

[1] G. Wagner et al., Newton **1**, 100009 (2025)

O 63.4 Wed 15:45 HSZ/0401

Quantifying quasiparticle chirality in a chiral topological semimetal — •Jiaju Wang[1], Amit Kumar[1], Markel Pardo-Almanza[1], Jaime Sanchez-Barriga[2], Jorge Cardenas-Gamboa[3], Maia Vergniory[3], Vladimir Strokov[4], Moritz Hoesch[5], Chandra Shekhar[6], Claudia Felser[6], Stuart Parkin[1], and Niels Schröter[1] — [1]Max Planck Institute of Microstructure Physics, Halle (Saale), Germany — [2]Helmholtz-Zentrum Berlin, Berlin, Germany — [3]Donostia International Physics Center, San Sebastián, Spain — [4]Paul Scherrer Institute, Villigen, Switzerland — [5]Deutsches Elektronen-Synchrotron, Hamburg, Germany — [6]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Recently, electron chirality has been proposed as an order parameter to quantify chirality. In chiral topological semimetals with the B20 structure, electron chirality is linked to parallel spin-momentum locking (SML) and spin deviations from SML, which affects numerous physical properties. However, experimental quantification of spin deviation still remains a big challenge. To achieve this, we have used spin and angle-resolved photoemission spectroscopy to directly probe the spin texture of Weyl cones in RhSi, a chiral topological semimetal with strong spin-orbit coupling (SOC). The spin-resolved spectra at different azimuthal angles are intricately fitted to extract numerical values of spin deviation for Weyl cones, allowing us to calculate the normalized electron chirality density (NECD). It was found that deviations can decrease the NECD from 1 down to 0.8. This observation may help interpret physical phenomena in chiral topological semimetals.

O 63.5 Wed 16:00 HSZ/0401

Topology and Real-Space Obstruction: The Phase Diagram of the Triangular p-Orbital Lattice — •Jonas Erhardt[1,2], Sven Schemmelmann[3], Fabian Schöttke[3], Jörg Schäfer[1,2], Giorgio Sangiovanni[2,4], Markus Donath[3], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Universität Würzburg — [2]Würzburg-Dresden Cluster of Excellence ctd.qmat — [3]Physikalisches Institut, Universität Münster — [4]Institut für Theoretische Physik und Astrophysik, Universität Würzburg

Triangular *p*-orbital monolayers (MLs) host a rich topological phase diagram governed by the competition between spin-orbit coupling (SOC) and substrate-induced inversion-symmetry breaking (ISB). The SOC-dominated quantum spin Hall insulator (QSHI) phase arises from a band inversion in the $p_\pm$ manifold and was first realized in indenene, a triangular ML of In atoms on SiC [1]. Real-space interference shifts the associated Wannier centers away from the atoms to interstitial sites A/B, which for the QSHI phase produces an alternating ABAB energy sequence in the charge localization, as demonstrated by scanning tunneling microscopy (STM) [1]. Using the same STM approach, we identify the complementary ISB-dominated regime in a Tl ML on Si(111), where strong adsorption-induced ISB exceeds Tl's SOC. The charge likewise shifts off the atoms but evidences a non-alternating AABB sequence, characterizing Tl/Si(111) as a trivial obstructed atomic insulator. These results complete the experimental validation of the topological phase diagram for triangular *p*-orbital MLs.

[1] Nat. Commun. **12**, 5396 (2021).

O 63.6 Wed 16:15 HSZ/0401

Majorana-metal transition in a disordered superconductor: percolation in a landscape of topological domain walls — Vladimir A Zakharov[1], Ion Cosma Fulga[2,3], •Gal Lemut[4], Jakub Tworzydło[5], and Carlo W. J. Beenakker[1] — [1]Instituut-Lorentz, Universiteit Leiden, PO Box 9506, 2300 RA Leiden, The Netherlands — [2]Institute for Theoretical Solid State Physics, IFW Dresden, Germany — [3]Würzburg-Dresden Cluster of Excellence ct.qmat, Dresden, Germany — [4]Dahlem Center for Complex Quantum Systems and Physics Department, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [5]Faculty of Physics, University of Warsaw, ul. Pasteura 5, 02-093 Warszawa, Poland

Most superconductors are thermal insulators. A disordered chiral p-wave superconductor, however, can make a transition to a thermal metal phase. Because heat is then transported by Majorana fermions, this phase is referred to as a Majorana metal. Here we present numerical evidence that the mechanism for the phase transition with increasing electrostatic disorder is the percolation of boundaries separating domains of different Chern number. We construct the network of domain walls using the spectral localizer as a "topological landscape function", and obtain the thermal metal-insulator phase diagram from the percolation transition.

O 63.7 Wed 16:30 HSZ/0401

fabrication and characterization of the Moiré surface state on a topological insulator — •yi zhang — Shanghai Jiao Tong University, Shanghai, China

A Moire* superlattice on the topological insulator surface is predicted to exhibit many novel properties but has not been experimentally realized. Here, we developed a two-step growth method to successfully fabricate a topological insulator Sb2Te3 thin film with a Moire* superlattice, which is generated by a twist of the topmost layer via molecular beam epitaxy. The established Moire* topological surface state is characterized by scanning tunneling microscopy and spectroscopy. By application of a magnetic field, new features in Landau levels arise on the Moire* region compared to the pristine surface of Sb2Te3, which makes the system a promising platform for pursuing next-generation electronics. Notably, the growth method, which circumvents contamination and the induced interface defects in the manual fabrication method, can be widely applied to other van der Waals materials for fabricating Moire* superlattices.

O 63.8 Wed 16:45 HSZ/0401

Backscattering in topological edge states despite time-reversal symmetry — Jonas Erhardt[1,2], •Mattia Iannetti[3,4], Fernando Dominguez[2,5], Ewelina M. Hankiewicz[2,5], Björn Trauzettel[2,5], Gianni Profeta[3,4], Domenico Di Sante[6], Giorgio Sangiovanni[2,5], Simon Moser[1,2], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Universität Würzburg — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg — [3]Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell'Aquila — [4]CNR-SPIN C/o Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell'Aquila — [5]Institut für Theoretische Physik und Astrophysik, Universität Würzburg — [6]Department of Physics and Astronomy, University of Bologna

Quantum Spin Hall Insulators (QSHI) are promising materials for many applications based on Dirac fermions and topologically-protected edge states. Indium adatoms on a silicon carbide surface, the so-called Indenene, was the first material in which a topological classification solely based on an inspection of the bulk wave functions has been demonstrated. In this work, we present a combined experimental and theoretical study of finite-sized Indenene systems, using STM/STS measurements and a quantitative tight-binding model revealing the rich physics of edge states. We find that a strongly non-linear edge dispersion leads to inter-Kramers pair backscattering, thereby extending the conventional understanding of backscattering protection in topological edge states.

O 63.9 Wed 17:00 HSZ/0401

Quantized Subband Tunneling from Topological Insulator Nanowire Scanning Probe Tips — •Abhisek Kole[1,2], Felix Münning[3,4], Xiaosheng Yang[1,5], Jia G. Lu[6], Oliver Breunig[4], F. Stefan Tautz[1,2], Yoichi Ando[4], and Felix Lüpke[1,4] — [1]Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institute for Experimental Physics IV A, RWTH Aachen University, Otto-Blumenthal-Straße, 52074 Aachen, Germany — [3]Institute of Physics I, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [4]Institute of Physics II, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [5]School of Optical and Electronic Information, Huazhong University of Science and Technology, Wuhan 430074, China — [6]Department of Physics/Electrophysics, University of Southern California, Los Angeles, CA 90089, USA

In topological insulator nanowires, the interplay between size quantization and the surface states wrapping the nanowire circumference gives rise to a magnetic-flux-tunable band structure. We demonstrate the controlled fabrication of (Bi_(1-x) Sb_x)_2 Te_3 (BST) topological insulator nanowires into scanning tunneling microscopy tips. Tunneling spectroscopy reveals a series of distinct peak-like features that exhibit a characteristic 1D DOS, indicating tunneling into the quantized 1D subbands of the BST nanowire tips. Furthermore, a magnetic-field-induced gap-closing and reopening transition is observed, consistent with the Dirac-like gap-closing transition expected for such wires. Moreover, we find indications of spin-selective helical tunneling between the nanowire tip and the Rashba surface states of Au(111).

O 63.10 Wed 17:15 HSZ/0401

Simultaneous Characterization of Dispersion and Orbital Character of the Topological Surface State on the Topological Insulator Bi_2Te_3 — •Christoph Stephen Setescak, Adrian Weindl, and Franz Josef Giessibl — Universität Regensburg, D-93053 Regensburg

Scanning probe microscopy (STM and AFM) allows one to locally probe properties of topological insulators (TIs). On the compound Bi_2Te_3, atomic-scale electronic standing waves can be observed at crystalline step edges, which are associated with the hexagonal warping of the Dirac cone. These real-space oscillations provide a direct means to study the dispersion relation of the topological boundary mode. The interpretation relies on comparing the experimental data to calculations including not only the properties of the TI but also of the tip. In this framework, the tunneling current and differential conductance is modelled using Chen's derivative rule. Bending of the CO molecule at the tip apex due to lateral tip-sample forces is also included in the model. The relevant Bloch functions of the sample are obtained from Wannier-interpolated tight-binding Hamiltonians using maximally localized Wannier functions derived from first-principles DFT + *GW* computations. In combination with the high spatial resolution obtained with CO-terminated tips, not only the dispersion, but also the orbital character of the band structure can be probed.

O 63.11 Wed 17:30 HSZ/0401

Defect-induced displacement of topological surface state in magnetic topological insulator $MnBi_2Te_4$ — •Felix Lüpke[1,2], Marek Kolmer[3,4], Hengxin Tan[5], Adam Kaminski[3,4], and Binghai Yan[5,6] — [1]Peter Grünberg Institute (PGI-3) and JARA-FIT, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [3]Ames National Laboratory, Ames, Iowa 50011, USA — [4]Iowa State University, Ames, Iowa 50011, USA — [5]Weizmann Institute of Science, Rehovot 7610001, Israel — [6]The Pennsylvania State University, University Park, Pennsylvania 16802, USA

The gapped topological surface states of $MnBi_2Te_4$ (MBT) are an attractive platform for the realization of quantum anomalous Hall and Axion insulator states. However, experimentally observed surface state gaps fail to meet theoretical predictions, with the exact mechanism behind the gap suppression still being debated. We report on the effect of intrinsic anti-site defects on the MBT surface states, which we study using scanning tunneling microscopy (STM), angle-

resolved photoemission (ARPES), and density functional theory (DFT). Our results show that high defect concentrations lead to a displacement of the surface states into the interior of the MBT crystal, consistent with theoretical predicitons [PRL 130, 126702 (2023)].

O 64: Surface Magnetism

Time: Wednesday 15:00–17:45 Location: HSZ/0403

Invited Talk O 64.1 Wed 15:00 HSZ/0403

Cantilever based Scanning Force Microscopy: Ultimate Sensitivity and Quantitative Imaging of Nanoscale Spin Textures — •Hans J. Hug — Empa, Ueberlandstrasse 129, 8600 Dübendorf, Switzerland — Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel

Cantilever-based scanning force microscopy operated under vacuum or ultra-high-vacuum (UHV) conditions is a powerful and versatile technique for surface characterization with atomic resolution. Beyond topographic imaging, multimodal and multifrequency approaches enable the simultaneous mapping of Kelvin potential differences and magnetic stray fields with exceptional sensitivity. These advanced methodologies have been applied to quantitatively determine skyrmion diameters in both ferromagnetic and synthetic antiferromagnetic multilayers, revealing skyrmions with diameters down to 25 nm. Furthermore, local tip sample distance control allows MFM imaging on curved substrates, uncovering curvature-induced modifications of the Dzyaloshinskii*Moriya interaction. Finally, we demonstrate the capabilities of UHV multimodal scanning force microscopy by resolving the atomic-scale structure, local Kelvin potential, and magnetic stray fields of NiBr* monolayers grown on Au substrates, highlighting the potential of these techniques for exploring emergent magnetic phenomena in low-dimensional materials.

O 64.2 Wed 15:30 HSZ/0403

Intra-atomic s-f correlation in a single Sm atom probed by ESR-STM — Masahiro Haze[1], Saba Taherpour[2,3], Christoph Wolf[2,3], Jaehyun Lee[2,3], Yaowu Liu[2,3], Andreas Heinrich[2,3], Fabio Donati[2,3], •Yasuo Yoshida[4], and Soo-hyon Phark[2,3] — [1]ISSP Univ. Tokyo, Kashiwa, Japan — [2]Center for Quantum Nanoscience, Seoul, Korea — [3]Ewha Womans University, Seoul, Korea — [4]Kanazawa Univ, Kanazawa, Japan

Correlations between s- and f-electrons are a fundamental topic in condensed matter physics, as they can give rise to exotic phases such as heavy-fermion or non-Fermi-liquid states. Recent work has shown that isolated Sm atoms adsorbed on MgO adopt a monovalent configuration with an S=1/2 spin originating from the 6s orbital, making a single Sm atom an ideal platform for studying s-f correlations at the atomic level. Here, we performed ESR-STM measurements on individual Sm atoms adsorbed on MgO films grown on an Ag(100) substrate. We find that the excitation energy varies strongly with the orientation of the external magnetic field, even though STM probes an S=1/2 spin, which is in principle free from single-ion magnetic anisotropy. The extracted g-values from the ESR measurements range from 1.3 to 6.4. This pronounced anisotropy indicates strong coupling between the s- and f-electrons within a single Sm atom, suggesting that surface-adsorbed Sm atoms may serve as promising building blocks for artificial Kondo lattices.

O 64.3 Wed 15:45 HSZ/0403

Elliptical skyrmions in a hydrogenated Fe double-layer on Ir(110) — Timo Knispel[1], Vasily Tseplyaev[2,3], •Gustav Bihlmayer[2], Stefan Blügel[2,3], Thomas Michely[1], and Jeison Fischer[1] — [1]II. Physikalisches Institut, Universität zu Köln, D-50937 Köln — [2]Peter Grünberg Institute (PGI-1), Forschungszentrum Jülich, D-52425 Jülich — [3]Institut für Theoretische Physik, RWTH Aachen University, D-52074 Aachen

Spin-polarized scanning tunneling microscopy (SP-STM) experiments demonstrate that the magnetic ground state of two pseudomorphic Fe layers on Ir(110) is a Néel-type spin spiral with a unique sense of rotation. Employing density functional theory (DFT) calculations, we show that this spin-spiral is stabilized by frustrated exchange interactions, but the rotation direction is fixed by the Dzyaloshinskii-Moriya interaction [1]. Hydrogen adsorption on the 2Fe/Ir(110) surface significantly modifies the spin-spiral minimum, shifting it to a longer wavelength and causing it to flatten energetically out with increasing H coverage. Using DFT calculations, we can trace back this behavior to electron doping of the surface and atomistic spin-dynamics simulations show that it is possible to induce elliptic skyrmions with an external magnetic field. These spin-textures can also be observed using SP-STM with a perpendicular B-field [2].

We acknowledge funding from the CRC 1238 of the Deutsche Forschungsgemeinschaft.

[1] T. Knispel et al., Phys. Rev. B **111**, L020405 (2025)
[2] T. Knispel et al., Nano Lett. **25**, 14565 (2025)

O 64.4 Wed 16:00 HSZ/0403

Light-driven modulation of proximity-enhanced functionalities in hybrid nano-scale systems — •Mattia Benini[1,2], Umut Parlak[3], Jaka Strohsack[4], Andrea Droghetti[5], Tomaz Mertelj[4], Valentin Alek Dediu[2], and Mirko Cinchetti[1] — [1]Department of Physics, TU-Dortmund, Dortmund, Germany — [2]ISMN-CNR, Bologna, Italy — [3]Department of Physics, Univesity of Konstanz, Konstanz, Germany — [4]Jozef Stefan Institute, Ljubljana, Slovenia — [5]Universitá Ca' Foscari, Venezia, Italy

Recent research on Co thin films surface-hybridized with π-conjugated organic molecules demonstrated that interfacial *p-d* hybridization[1] leads to the establishment of an exotic magnetic configuration, called *Correlated Ferromagnetic Glass* (CFG). It features a glassy-like arrangement of the magnetization and vortex topological defects[2], a strongly enhanced coercivity, and an unexpected complex magnetization dynamics[3]. In this work, we demonstrate that the interface-driven magnetic properties can be actively controlled by optical means, using Co/C_{60} heterostructures as a prototypical system. By generating excitons in the molecular layer with resonant ultrashort light pulses, we achieve up to a 60% reduction of the magnetization precession frequency, ultimately due to a quenching of the interface-induced magnetic anisotropy[4]. References [1] Cinchetti, M. et al., Nat. Mater. 2017, 16 (5), 507*515. [2] Benini, M. et al., Nat Commun 2025, 16 (1), 5807. [3] Strohsack, J. et al., Science Advances 2025, 11 (31), eadw2243. [4] Benini, M. et al., Nat Commun 2025, 16 (1), 7297.

O 64.5 Wed 16:15 HSZ/0403

Layer-dependent magnetic and electronic properties of 2D vdW magnet $FeCl_2$ on Bi(111) — •Shigemi Terakawa[1], Jianqiang Liu[1], Hikaru Ishikawa[1], Ryota Inoue[1], Isamu Yamamoto[2], Amilcar Bedoya-Pinto[3], Niels B. M. Schröter[4], and Kazuyuki Sakamoto[1] — [1]Department of Applied Physics, The University of Osaka, Osaka, Japan — [2]Synchrotron Light Application Center, Saga University, Saga, Japan — [3]Institute of Molecular Science, University of Valencia, Paterna, Spain — [4]Max Planck Institute of Microstructure Physics, Halle, Germany

Two-dimensional (2D) van der Waals (vdW) magnets are promising for future spintronic applications. Recently, transition metal dihalides (TMDHs) have received increasing attention as a new class of 2D vdW magnets. In this study, we report the layer dependence of the magnetic and electronic properties of ultrathin $FeCl_2$, a layered antiferromagnetic insulator, films on Bi(111) from monolayer to four layers. X-ray magnetic circular dichroism (XMCD) measurements revealed that the monolayer film exhibits an in-plane easy axis, while the thicker films have an out-of-plane easy axis with a spin-flip transition, which is consistent with the antiferromagnetic order of bulk $FeCl_2$. The transition field increases with increasing thickness. Angle-resolved photoelectron spectroscopy (ARPES) revealed insulating electronic structure irrespective of the thickness. Layer-dependent change is found as the increase in the width of the bands with large Cl 3p contributions. These results show that both the magnetic and electronic coupling through the vdW interfaces become stronger as the thickness increases.

Invited Talk O 64.6 Wed 16:30 HSZ/0403

Single-spin sensing: A molecule-on-tip approach — •Laurent Limot — Université de Strasbourg, CNRS, IPCMS, UMR 7504, F-67000 Strasbourg, France

Magnetometry plays a pivotal role in advancing ultra-dense data-storage technologies and addressing the challenges that arise as spin qubits are downscaled. A promising route toward atomic-scale single-spin sensing is the use of a magnetic molecule as a spin sensor, although practical implementations of this concept remain at an early stage. To demonstrate its feasibility and potential, we combine a nickelocene molecule with scanning tunneling microscopy to achieve versatile, spin-sensitive imaging of magnetic surfaces.

We investigate model Co islands of varying thickness on Cu(111), which exhibit distinct magnetic properties. Our approach proves robust and reproducible, offering atomic-scale sensitivity to both spin polarization and magnetization orientation through the direct exchange coupling between the nickelocene-terminated tip and the Co surface. This capability enables the acquisition of magnetic exchange maps, whose characteristic magnetic corrugation patterns show excellent agreement with computed spin-density distributions. Building on this foundation, we will apply the method to probe the influence of hydrogen on magnetization, a topic of significant relevance in spintronics. Collectively, these advances substantially enhance our ability to probe and visualize magnetism at the atomic scale.

O 64.7 Wed 17:00 HSZ/0403

Tailoring Robust 1D Atomic and Electronic Textures in Mn Ultrathin Films on Fe(110) via Antiferromagnet-Ferromagnet Interfaces — •Toyo Kazu Yamada[1,2], Eiichi Inami[3], and Peter Krueger[1,2] — [1]Dept. Materials Science, Chiba Univ., Chiba, Japan — [2]Molecular Chirality Res. Centre, Chiba Univ., Chiba, Japan — [3]School of Systems Engineering, Kochi Univ. Tech., Kochi, Japan

Controlling the dimensionality of electronic states on two-dimensional (2D) surfaces has remained a significant challenge over decades. In particular, achieving one-dimensional (1D) electronic ordering on 2D surface could enable anisotropic quantum transport and support quantum-confined functional units for nanoscale device integration. In this study, we demonstrate that even conventional 3d transition metals, ferromagnetic (FM) Fe and antiferromagnetic (AFM) Mn, can give rise to 1D atomic stripe patterns in the local density of states (LDOS) on a 2D surface. This study investigates the emergence of one-dimensional (1D) atomic and electronic ordering in ultrathin manganese (Mn) films grown on atomically flat Fe(110) substrates. By combining scanning tunneling microscopy/spectroscopy (STM/STS) and density functional theory (DFT), we demonstrate that the interplay between antiferromagnetic and ferromagnetic interactions at the interface leads to robust 1D stripe electronic textures that remain stable even at room temperature, persisting in the presence of atomic-scale defects.

O 64.8 Wed 17:15 HSZ/0403

Influence of the light polarization on magnetic dichroism in threshold photoemission — •Frank O. Schumann[1] and Jürgen Henk[2] — [1]Max-Planck Institut für Mikrostrukturphysik, Halle, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Germany

Incoming normal incidence light which is neither purely s- or p-polarized will become in general elliptically polarized inside a metallic surface. We ask how the magnetic dichroism is affected if the incoming light is changed from circularly to linearly polarized, with equally large s- and p-components. This is further compared if the incoming elliptically polarized light is tuned such that it becomes circularly polarized inside the surface. Initial theoretical work on normal emission demonstrated for in-plane magnetized samples a sizeable difference in the dichroism spectra for different light polarizations.[1]

We performed an one-step photoemission calculation for threshold photoemission from a Fe(100) and capture the emission into the full half sphere. The photon energy was 5.2 eV and the angle of incidence was set to 65° as realized in PEEM instruments. We are interested in domain imaging and we determine the relevant asymmetry for magnetic domains.[2] The spectra for a given magnetization direction and polarization state are very different whereas the magnetic dichroism signal displays a weak dependence.

[1] J. Henk and R. Feder, Phys. Rev. B **55**, 11476 (1997) [2] M. Paleschke et al., Phys. Rev. B **112**, 054411 (2025).

O 64.9 Wed 17:30 HSZ/0403

Triple-Q state in magnetic breathing kagome lattice — Hangyu Zhou[1,2], Manuel dos Santos Dias[3], Weisheng Zhao[1], and •Samir Lounis[4,2] — [1]Fert Beijing Institute, Beihang University, Beijing, China — [2]Peter Grünberg Institut, Forschungszentrum Jülich & JARA, Jülich, Germany — [3]Scienti c Computing Department, STFC Daresbury Laboratory, Warrington, United Kingdom — [4]Institute of Physics, Martin-Luther-University Halle-Wittenberg, Halle, Germany

Magnetic frustration in two-dimensional triangular spin lattices produces a variety of exotic states, from multi-Q configurations to disordered spin glasses. The antiferromagnetic kagome lattice, built from corner-sharing triangles, is a paradigmatic frustrated system with macroscopic degeneracy. Building on the kagomerization mechanism we recently introduced [1], we examine the magnetic breathing kagome lattice formed by an Mn monolayer on a heavy-metal substrate capped with h-BN [2]. The Mn kagome geometry induces strong frustration, reflected in the nearly flat bands obtained from spin-spiral energy calculations. Including further-neighbor interactions yields a spin-spiral energy minimum along Γ-K and a triple-Q state with nonzero topological charge, potentially causing highly nonlinear Hall responses. The flat-band character can also stabilize more complex spin textures featuring multiple Q-pockets in the spin structure factor. These findings provide a fertile platform for studying multi-Q states and emergent topological phenomena.

[1] Zhou et al., Nature Communications 15, 4854 (2025)
[2] Zhou et al., npj Spintronics 3, 31 (2025)

O 65: Solid-liquid interfaces: Reactions and electrochemistry II

Time: Wednesday 15:00–18:00 Location: TRE/PHYS

O 65.1 Wed 15:00 TRE/PHYS

Effect of Organic Additives in Aqueous Dye-Sensitized Solar Cells with $TEMPO^{+/0}$ Radicals as Redox Mediator Studied by Perturbation Techniques — •Daniel Holzhacker and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

Understanding the complex interactions among the electrolyte, dye, and semiconductor (TiO_2) in dye-sensitized solar cells (DSSCs) is crucial to uncover and optimize the individual roles of each component. Organic electrolyte additives, such as 1-methylbenzimidazole (1MBI), are commonly used to enhance cell performance. In aqueous $TEMPO^+$ solutions, a distinctive color change was observed upon addition of 1MBI. Cyclic voltammetry revealed that the redox potential of the electrolyte shifted systematically to higher potentials with increasing 1MBI concentration. Photoelectrochemical analysis of DSSCs demonstrated a clear effect of 1MBI on the conduction band edge, which shifted in parallel to the redox potential of the electrolyte. It was shown that reduced recombination losses, i.e., a shift of the electron Fermi level in the TiO_2 closer to the conduction band edge, were responsible for an increased open-circuit voltage. Additionally, the shifts of both the conduction band edge and the redox level of the electrolyte may facilitate electron injection from the dye into TiO_2 and/or the regeneration of the oxidized dye by the redox mediator, thereby explaining the higher photocurrents, also observed at increased 1MBI concentrations.

O 65.2 Wed 15:15 TRE/PHYS

Laser-treated activated carbon derived from date stone for energy storage and environmental remediation applications — •Ahmad Jabr[1], Iyad Sadeddin[1], Amer El Hamouz[1], Hyun Jungb[2], and JeongWon Parkb[2] — [1]An-Najah National university, Nablus, Palestine — [2]Dongguk University, Seoul-Campus, Korea

In this study, Activated Carbon (AC) was synthesized via traditional ZnCl* and KOH routes followed by surface modification process using pulsed Nd:YAG laser (1064 nm) under aqueous conditions to produce laser-modified activated carbon (LAC).

Structural and surface analyses revealed that laser introduced new surface functionalities, increased surface roughness, promoted additional micropores and mesopores formation, resulting in 17% enhancement in SSA. Nitrogen adsorption isotherms indicated higher monolayer adsorption and more developed pore volume distribution in LAC compared with AC. Also, LAC exhibited improved surface chemistry with newly developed OCFGs, attributed to laser bombardment effects.

Electrochemical characterizations showed that AC and LAC exhibit typical EDLC behavior, with LAC achieving 70% higher specific capacitance, enhanced energy and power densities, reduced ESR, and better stability after 10000 cycles compared to AC. Furthermore, adsorption studies showed that LAC overcame AC with 400% enhancement in maximum adsorption capacity and initial rate adsorption, signifying improved surface heterogeneity and multilayer adsorption features.

O 65.3 Wed 15:30 TRE/PHYS

rationalizing capacitance differences across metal/water interfaces within a unified quantum electric double layer model — •Lang Li, Nicolas Hörmann, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin

Electrochemical routes to hydrogen and synthetic fuels promise sustainable energy storage, yet their advancement is limited by an incomplete microscopic picture of the electric double layer (EDL) that governs electrode behavior. Using extensive density-functional theory-based *ab initio* molecular dynamics simulations, we examine a series of noble-metal surfaces and capture the experimental capacitance trend Pt(111) > Cu(111) > Ag(111) ≈ Au(111). Subsequent data analysis rationalizes this trend within a unified EDL picture that rests upon a universal four-state interfacial water structure and material-dependent electron spillover [1]. We probe the generality of this understanding by performing alloy- or strain-mimicking "cross-geometry" simulations at interchanged lattice constants, and obtain capacitance variations in full accordance with the model predictions. This suggests applicability of the model for the rational design of next-generation electrode materials.

[1] L. Li, T. Eggert, K. Reuter, N. Hörmann, *J. Am. Chem. Soc.*, **147**, 22778 (2025).

O 65.4 Wed 15:45 TRE/PHYS

Formic Acid Oxidation on Gold Electrodes — •Johannes M. Hermann[1], Areeg Abdelrahman[1], Heiko Müller[1], Ludwig A. Kibler[1], and Timo Jacob[1,2,3] — [1]Institute of Electrochemistry, Ulm University, Ulm, Germany — [2]Helmholtz-Institute-Ulm (HIU), Ulm, Germany — [3]Karlsruhe Institute of Technology, Karlsruhe, Germany

Adsorption processes are an integral part of electrocatalysis. The use of extensively studied and structurally well-defined Au(111) single crystal electrodes allows for a better understanding of such processes. Formally, the formic acid oxidation (FAOR) is a relatively simple reaction as only one proton and two electrons have to be released to obtain CO_2. However, the reaction exhibits a self-inhibition on Au(111) electrodes due to the blocking of active sites by strongly adsorbed formate indicated by a bell-shaped current density-potential curve [1]. Similarly, the addition of specifically adsorbing anions typically lowers the catalytic activity [2]. In contrast, certain adsorbates enhance the reaction by orders of magnitude. An intersting example is irreversibly adsorbed 4-mercaptopyridine forming a self-assembled monolayer (SAM) on Au(111) with the enhancement being related to the highly ordered SAM structure [3]. Several aspects of FAOR on gold single crystals will be discussed.

[1] L.A. Kibler, M. Al-Shakran, J. Phys. Chem. C 120 (2016) 16238*16245. [2] J.M. Hermann, A. Abdelrahman, T. Jacob, L.A. Kibler, Electrochim. Acta 385 (2021) 138279. [3] J.M. Hermann, H. Müller, L. Daccache, C. Adler, S. Keller, M. Metzler, T. Jacob, L.A. Kibler, Electrochim. Acta 388 (2021) 138547.

O 65.5 Wed 16:00 TRE/PHYS

Improving Carbon Dioxide Reduction Reactivity and Stability of Ultra-High Vacuum Prepared Cu(111) Surfaces by Crystalline Ultrathin Oxide Films — •Patrick Giesbrecht[1], Mauricio Prieto[1], Mikhail Belozertsev[1], Sergio Tosoni[2], Markus Heyde[1], Thomas Schmidt[1], Beatriz Roldan Cuenya[1], and Juan Navarro[1] — [1]Department of Interface Science, Fritz-Haber Institute of the Max-Planck Society, Berlin, Germany — [2]Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, Milano, Italy

Electrocatalytic carbon dioxide reduction reactions (CO2RR) to hydrocarbons at copper cathodes is one promising but complex route towards carbon capture and reutilization, where ultra-high vacuum (UHV) prepared single crystal electrodes can provide precise pre-catalyst structures to inform reactivity trends.[1,2] This work develops ultrathin crystalline Cu oxide phases and silica on Cu(111) electrodes under UHV conditions that activate Cu(111) toward hydrocarbon production and alter corrosion pathways under CO2RR conditions.[3] Ex situ and quasi-in situ UHV surface characterization as well as DFT computational analyses are presented that relate this altered reactivity and surface reconstruction to the pre-catalyst oxide structure, highlighting how atomic scale modifications of the surface can lead to macroscopic changes in electrocatalyst reactivity.

[1] Nguyen, K.C., et al. ACS Energy Lett. 9, 644-652 (2024). [2] Cheng, D., et al. Nat. Commun. 16, 4064 (2025). [3] Navarro, J.J., et al. J. Phys. Chem. C 124, 20942-20949 (2020).

O 65.6 Wed 16:15 TRE/PHYS

Mechanistic insights into liquid phase photocatalysis by studying the photoconversion of tertiary alcohols on titania — •Lucia Mengel, Elena Dietz, Martin Tschurl, and Ueli Heiz — Chair of Physical Chemistry, Technical University of Munich, Lichtenbergstr. 4, 85748 Garching, Germany

Titania loaded with a metal co-catalyst represents a well-studied model photocatalyst, e.g. for investigating hydrogen evolution. For the reaction of most alcohols, the use of a co-catalyst is vital to enable hydrogen evolution and thus a fully catalytic reaction. Tertiary alcohols, however, can be employed as probe for the intrinsic photoactivity of bare titania, as they are catalytically converted in a surface photoreaction discovered by us on single crystals in UHV. In this work, we focus on the applicability of these findings to a liquid phase environment by performing photoconversion of 2-methyl-2-butanol on titania nanopowder. We investigate the catalytic activity under water- and oxygen-free conditions and discuss the reaction behavior under consideration of the catalyst's properties.

O 65.7 Wed 16:30 TRE/PHYS

Simulation of catalytic and corrosive processes via Thermopotentiostat Molecular Dynamics — •Andreas Kretschmer[1], Samuel H. Mattoso[2], Jing Yang[2], Ahmed Abdelkawy[2], Mira Todorova[2], Jörg Neugebauer[2], and Markus Valtiner[1] — [1]Institute of Applied Physics, TU Wien, 1040 Wien, Austria — [2]Max-Planck-Insitute of Sustainable Materials GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

Ab Initio Molecular Dynamics (MD) provides valuable insights in dynamic processes at solid liquid interfaces on the electronic level. However, electrified interfaces have been inaccessible due to the interaction of charged systems with the periodic images. The recently developed thermopotentiostat enables the use of electric fields across a solid/liquid interface by a computational electrode. This electrode consists of a fixed layer of Ne atoms, which confines the water, and provides a compensating charge to keep the cell charge-neutral. The thermopotentiostat updates the charge of the Ne atoms after every MD step to drive the potential difference towards a desired value on average. The electronic minimization then distributes the charge, leading to a corresponding counter charge on the electrode surface, allowing the study of dynamic processes under the influence of electric fields. We apply this method to 2 model systems, one is a single Pt atom supported on two layers of graphene to study catalytic processes with water, the second is a Zn surface to study corrosion processes under H evolution at the interface in anodic and cathodic conditions.

O 65.8 Wed 16:45 TRE/PHYS

First Steps Matter Most: Free Energy Barriers of the Volmer Step in Hydrogen Evolution at Pt(111) — •Barbara Sumić, Karsten Reuter, and Nicolas G. Hörmann — Fritz-Haber-Institut der MPG, Berlin

The Hydrogen Evolution Reaction (HER) plays a central role in hydrogen-based energy conversion. The initial Volmer step, involving proton adsorption at the electrode interface, is key to understanding reaction kinetics and the influence of pH. Conventional approaches to estimating barrier heights based on density-functional theory are limited by the need for reduced system sizes and short simulation times, which restrict statistical sampling and hinder fully converged free-energy calculations, particularly when solvent reorganisation is involved.

Here, we explore machine-learned interatomic potentials (MLIPs) combined with enhanced sampling techniques to gain more comprehensive insight into the reaction mechanism and barrier for the Volmer step at Pt(111) in dynamically described interfacial water. Using data-driven collective variables, we aim to capture dynamic environmental and solvent effects that are difficult to access with standard sampling. We also investigate the applicability of the RAZOR (Response Analysis in z-ORientation) framework [1] for barrier calculations at applied bias to probe potential-dependent behavior.

Together, these approaches provide a pathway toward more consistent and physically grounded modelling of HER across different pH conditions.

[1] N. Bergmann *et al.*, Phys. Rev. Lett. **135, 146201 (2025).**

O 65.9 Wed 17:00 TRE/PHYS

Modeling chemical trends of Hydrogen adsorption and reactivity on Pt (111) surface alloyed with transition metals — •Bingxin Li, Jing Yang, Mira Todorova, and Jörg Neugebauer — MPI for Sustainable Materials, Düsseldorf, Germany

Platinum's near-optimal hydrogen binding energy, as dictated by the Sabatier principle, makes it the benchmark electrocatalyst for the hydrogen evolution reaction (HER). Alloying Pt with transition metals (TMs) is known to enhance catalytic activity, though the underlying mechanisms vary substantially across alloying elements. Here, we employ ab initio molecular dynamics to investigate hydrogen adsorption on Pt (111) surfaces whose top layer is alloyed with different TMs at varying concentrations. By generating lateral free-energy maps of chemisorbed hydrogen and combining them with nudged-elastic-band calculations, we determine the Tafel-step barriers of HER. We find that Tafel-step kinetics improves as on-top-site hydrogen binding is weakened on alloyed Pt surfaces. Electronic-structure analyses, coupled with a machine-learning model, reveal that on-top-site hydrogen binding energy (key HER activity descriptor) can be quantitatively predicted from d-band centre characteristics. These results link compositional tuning of Pt-based alloys to predictable changes in HER-activity, offering a rational design route for next-generation hydrogen evolution catalysts.

O 65.10 Wed 17:15 TRE/PHYS

Atomic-scale insights into enhanced oxygen reduction on Au(100) in alkaline solutions from ab initio molecular dynamics simulations — •Alexander von Rueden[1,2], Mal-Soon Lee[1], Vassiliki-Alexandra Glezakou[3], Roger Rousseau[3], and Manos Mavrikakis[2] — [1]Pacific Northwest National Laboratory, Richland, WA, USA — [2]University of Wisconsin-Madison, Madison, WI, USA — [3]Oak Ridge National Laboratory, Oak Ridge, TN, USA

The unusually high $4e^-$ oxygen reduction reaction (ORR) activity of the Au(100) surface in alkaline environments has motivated numerous experimental and theoretical studies. Even so, atomic-scale insights into the origin of its high activity remain elusive, with static density functional theory (DFT) calculations under vacuum typically proving insufficient. Here, we instead developed atomistic models of Au(100)-water interfaces featuring fully explicit neutral or alkaline solvent environments. Using these models, we performed DFT-based ab initio molecular dynamics (AIMD) simulations to probe the dynamic atomic structures of ORR intermediates adsorbed on Au(100) in different solvent environments. Additionally combining the Blue moon ensemble enhanced sampling technique with AIMD, we demonstrated a low free energy barrier for O_2 dissociation and hydrogenation by water molecules to yield OH* on Au(100), which is consistent with its high experimental activity. Further, our alkaline simulations revealed these OH* products can form complexes with near-surface Na^+ cations, possibly leading to a more downhill reaction free energy.

O 65.11 Wed 17:30 TRE/PHYS

When Charged Intermediates Escape the Surface: Mass Transport Effects on the Electrocatalytic Selectivity of NO_3 Reduction — •Hemanth S. Pillai, Karsten Reuter, and Vanessa J. Bukas — Fritz-Haber-Institut der MPG, Berlin

Electrocatalytic selectivity is often discussed at the atomic level on the basis of the active site, while ignoring effects of mesoscopic mass transport. And yet, transport can critically shape selectivity through the exchange of surface-bound intermediates between the electrode and bulk electrolyte. We recently explored this mechanism, originally coined "desorption–re-adsorption–reaction" [1], by developing a simple model that couples the surface reaction kinetics with diffusion [2]. Here, we advance and extend our approach to describe charged inter-

mediates such as nitrite (NO_2^-) during the electrochemical NO_3 reduction reaction. Ion transport augments a mean-field microkinetic model and is treated at varying levels of sophistication to capture different double layer characteristics. Our simulations show that both the applied potential and catalyst morphology uniquely shape NO_2^- selectivity within the desorption–re-adsorption–reaction mechanism. The emerging trends are in qualitative agreement with experiments, while distinctly different from those obtained for analogous charge-neutral intermediates during e.g. CO_2 reduction. This comparison shows how the double layer affects selectivity due to transport and allows to gauge the level of detail that is required in corresponding reaction models.

[1] H. Wang *et al.*, J. Phys. Chem. B **108**, 19413 (2004).
[2] H.H. Heenen *et al.*, Nature Catal. **7**, 847 (2024).

O 65.12 Wed 17:45 TRE/PHYS

Electroreduction of Acetone on PtRu Model Catalysts — •Robert Hübsch[1], Daniel Schauermann[1], Pankaj Kumar Samal[2], Jan Škvára[2], Frederike Jäschke[1], Lesia Piliai[2], Tomáš Skála[2], Nataliya Tsud[2], Josef Mysliveček[2], Olaf Brummel[1], Yaroslava Lykhach[1], and Jörg Libuda[1] — [1]Interface Research and Catalysis, ECRC, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen, Germany — [2]Charles University, Faculty of Mathematics and Physics, Department of Surface and Plasma Science, V Holešovičkách 2, Prague, 18000, Czech Republic

The isopropanol/acetone system functions as an electrochemically active liquid organic hydrogen carrier (EC-LOHC). In this context, direct electrochemical charging is particularly attractive but requires highly active and selective catalysts. In this study, we investigated acetone reduction on well-defined PtRu model surface alloys. Our approach combined cyclic voltammetry (CV), ex-situ emersion synchrotron radiation photoelectron spectroscopy (SRPES), electrochemical infrared reflection absorption spectroscopy (EC-IRRAS), and differential electrochemical mass spectrometry (DEMS). The PtRu/Ru(0001) surface exhibits low intrinsic catalytic activity; but can be activated through a dealloying procedure. This treatment produces small Pt aggregates on a rough Ru support. In contrast, the PtRu/Ru(10 10) surface, characterized by a lower coordination number, does not require dealloying. Unlike Pt(110), which predominantly produces propane, the PtRu model catalysts selectively yield the target product isopropanol.

O 66: Ultrafast electron dynamics at surface and interfaces III

Time: Wednesday 15:00–17:45 Location: TRE/MATH

Invited Talk O 66.1 Wed 15:00 TRE/MATH

Ultrafast exciton dynamics in 2D semiconductors and electric field gated devices — •Jan Philipp Bange — Georg-August-Universität Göttingen, I. Physikalisches Institut, Germany

Two-dimensional (2D) semiconductors and moiré materials, formed by stacking and twisting atomically thin layers, provide an exciting platform to discover and engineer new quantum states. Precise and reversible control of carrier density and many-body effects is readily achieved through in-situ electric field gating. In combination with angle-resolved photoemission spectroscopy this has been a powerful probe of the static electronic band structure. However, capturing the ultrafast dynamics of excited states in gated 2D materials, including hybrid excitons [1], interlayer excitons [2], and trions [3], remains a fundamental challenge due to the limited real-space resolution of ultrafast time- and momentum-resolved spectroscopy techniques. In this talk, I will present how time-resolved momentum microscopy provides direct access to both the energy landscape and femtosecond dynamics of bright and dark excitons at nanometer length scales. This methodology enables the disentanglement of electron and hole transfer pathways across twisted transition metal dichalcogenide interfaces and reveals the ultrafast formation of quasiparticles as a function of gate voltage.

[1] Bange *et al.*, Science Advances **10**, eadi1323 (2024).
[2] Schmitt *et al.*, Nature Photonics **19**, 187 (2025).
[3] Meneghini *et al.*, arXiv.2511.11448 (2025).

O 66.2 Wed 15:30 TRE/MATH

Ultrafast signatures of Dirac - flat-band hybrid states from time-resolved ARPES — •Maria-Elisabeth Federl[1], Johannes Gradl[1], Franziska Bergmeier[1], Zamin Mamiyev[2], Niclas Tilgner[2], Thomas Seyller[2], Christoph Tegenkamp[2], and Isabella Gierz[1] — [1]University of Regensburg — [2]Chemnitz University of Technology

Hybridization of highly itinerant Dirac electrons with localized flat-band states is predicted to yield emergent phenomena such as exotic heavy-fermion behaviour. Epitaxial graphene resting on a flat-band system at the graphene-SiC(0001) interface offers a promising platform, yet direct spectroscopic signatures - such as avoided crossings in equilibrium ARPES - have remained unresolved. We solved this problem using time-resolved ARPES where evidence of hybridization manifested in three key observations: (1) accelerated Dirac-carrier relaxation due to an increased scattering phase space, (2) transient charging of the Dirac cone enabled by direct optical excitation from the flat bands, and (3) ultrafast charge transfer back into the flat bands on timescales set by the interlayer coupling strength. Our results thus provide a clear dynamical fingerprint of hybridization in a system where equilibrium probes have proven inconclusive.

O 66.3 Wed 15:45 TRE/MATH

Probing topological Floquet states in graphene with ultrafast STM — •Nils Jacobsen[1,2], Melanie Müller[3], Michael Schüler[4,5], Martin Wolf[3], and Angel Rubio[2,6] — [1]University of Bremen — [2]MPSD Hamburg — [3]FHI Berlin — [4]PSI Villingen Switzerland — [5]University of Fribourg Switzerland — [6]CCQ The Flatiron Institute New York USA

The light-induced anomalous Hall effect in graphene driven by circularly polarized light is a hallmark example of Floquet band engineering [1]. It has been observed in ultrafast transport experiments [2] and Floquet Bloch bands in graphene have recently been resolved by time- and angle-resolved photoemission spectroscopy [3]. Here, we propose ultrafast scanning tunnelling microscopy (USTM) as a complementary probe of topological Floquet states in graphene [4]. In our simulations, dynamical band gaps and topological edge states are directly reflected in the local density of states and the ultrafast tunnelling currents. The chirality of the edge states is revealed by the suppression of backscattering at impurities, which could be probed by ultrafast STM. These results establish ultrafast STM as a promising tool to access light-induced topological states in quantum materials. [1] Oka PRB 79, 081406(R) (2009) [2] McIver Nat. Phys. 16, 38-41 (2020) [3] Merboldt, Schüler et al. Nat. Phys. 21 1093-1099 (2025), Choi, Mogi et al. Nat. Phys. 21 1100-1105 (2025) [4] Müller Prog. Surf Sci. 99, 100727 (2024)

O 66.4 Wed 16:00 TRE/MATH

Ultrafast Band-Gap Renormalization in Bilayer Graphene — •Eduard Moos[1], ZhiYuan Deng[1], Hauke Beyer[1], Arpit Jain[4], Chengye Dong[4], Joshua A. Robinson[4], Kai Rossnagel[1,2,3], and Michael Bauer[1,2] — [1]Kiel University, Germany — [2]Kiel Nano, Surface and Interface Science KiNSIS, Germany — [3]Electron Synchrotron DESY, Germany — [4]Pennsylvania State University, United States

We demonstrate, by femtosecond time- and angle-resolved photoemission spectroscopy, that photoinduced interlayer charge transfer in a heterostructure consisting of Bernal-stacked bilayer graphen and a single atomic layer of silver on 6H-SiC(0001) transiently modulates the intrinsic potential landscape across the silver-graphene interface. Acting as an ultrafast electronic gate, this drives momentum-dependent band renormalizations, resulting in a transient band-gap opening on femtosecond timescales. Simultaneously, the photogenerated hot-carrier population enhances electronic screening, leading to a subsequent closing of the band-gap beyond the thermal equilibrium value. These findings reveal two different mechanisms for a photoinduced, reversible control of the electronic band structure in bilayer graphen — interlayer charge transfer and hot-carrier enhanced screening — providing a general framework for the ultrafast control of electronic properties in graphene-based heterostructures. They further open novel pathways for the realization of ultrafast optoelectronic devices and the exploration of correlated quantum phases in bilayer graphene under nonequilibrium conditions.

O 66.5 Wed 16:15 TRE/MATH

Attosecond spin-orbit delays in solid-state photoemission — •Andreas Gebauer[1], Walter Enns[1], Sergej Neb[2], Tillmann Schabbehard[1], Luis Maschmann[1], J. Hugo Dil[3], Ulrich Heinzmann[1], Stephan Fritzsche[4,5,6], Nikolay M. Kabachnik[7,8], Eugene E. Krasovskii[8,9,10], and Walter Pfeiffer[1] — [1]Bielefeld University — [2]ETH Zurich — [3]EPFL, Lausanne — [4]Helmholtz Institute Jena — [5]GSI Helmholtzzentrum für Schwerionenforschung GmbH — [6]Friedrich-Schiller-University Jena — [7]European XFEL GmbH, Schenefeld — [8]DIPC, San Sebastián — [9]Universidad del País Vasco, San Sebastián — [10]IKERBASQUE, Bilbao

Attosecond time-resolved photoelectron spectroscopy allows observation of photoemission dynamics in solids on its natural time scale. Photoelectrons typically need tens to hundreds of attoseconds to be released into the vacuum while various competing effects determine the emission dynamics. We report the first observation of unexpectedly large spin-orbit delays, i.e. relative photoemission delays between spin-orbit split core levels in Bi_2Te_3 and Bi_2Se_3. The observed delays can neither be attributed to intra-atomic delays nor to ballistic photoelectron transport. Instead, calculations based on one-step photoemission theory reveal that strong variations of the final state wave function on the energy scale of the spin-orbit splitting are responsible for the experimental observation. These vari-

ations reflect the complex interplay of propagating and evanescent waves in the photoelectron emission, exhibiting qualitatively different emission dynamics.

O 66.6 Wed 16:30 TRE/MATH

Electron Correlations in Ultrafast Transmission Electron Microscopy — •Nico Stumpp[1], Andreas Wendeln[1], Alexander Schröder[1], and Sascha Schäfer[1,2] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Regensburg Center for Ultrafast Nanoscopy (RUN), Regensburg, Germany

Ultrafast transmission electron microscopy (UTEM) strives to combine an atomic spatial resolution with a femtosecond temporal resolution, yet its performance is inherently limited by Coulomb repulsion within electron pulses. Research in free-electron quantum optics suggests that, rather than avoiding these dynamic interactions, exploiting their induced inter-electron correlations offers a pathway toward quantum-limited imaging performance [1,2].

Utilizing an event-based electron detector with nanosecond temporal resolution, we observe pronounced energy anti-correlations in few-electron states emitted from a high-coherence, laser-driven cold field-emission electron source [3]. Crucially, we demonstrate the ability to actively modify the magnitude and visibility of the induced energy separation depending on angular post-selection. We complement our experimental results with numerical multi-particle simulations of electron pulse dynamics within the electrostatic gun environment, focussing on the interplay between strongly interacting correlated electron pairs and the surrounding electron ensemble of the emitted photoelectron bunch.

[1] R. Haindl et al., Nat. Phys. 19, 1410 (2023).
[2] S. Meier et. al., Nat. Phys. 19, 1402 (2023).
[3] A. Schröder et al., Ultramicroscopy 275, 114158 (2025).

O 66.7 Wed 16:45 TRE/MATH

Ultrafast Investigation of Competing CDW Orders in $LaTe_3$ — •Francesco Sammartino[1], Wibke Bronsch[2], Fulvio Parmigiani[1,2], and Federico Cilento[2] — [1]Università degli Studi di Trieste — [2]Elettra - Sinctrotrone Trieste

The RTe_3 family hosts a rich landscape of charge-density-wave (CDW) phases. All members display a unidirectional CDW aligned along the *c*-axis, while only the heavier rare-earth compounds develop an additional equilibrium CDW along the *a*-axis at lower temperature. Intriguingly, recent ultrafast experiments have shown that $LaTe_3$, whose equilibrium state features only the *c*-axis CDW, can transiently exhibit a rotated CDW component oriented along the *a*-axis.

Building on time-resolved optical studies that first revealed the emergence of this orthogonal order, we investigated $LaTe_3$ through time-resolved ARPES (TR-ARPES) to track, with momentum resolution, the ultrafast evolution of its electronic structure.

We monitored the melting of the equilibrium *c*-axis CDW gap and searched for transient modifications of the electronic dispersions along the *a*-axis that could be linked to the emergence of the rotated order. This study provides direct insight into the nonequilibrium CDW dynamics of $LaTe_3$ and may help clarify the microscopic pathways that enable the formation of the rotated CDW state.

O 66.8 Wed 17:00 TRE/MATH

Electron and exciton dynamics in large-angle twisted bilayer graphene — •Gianmarco Gatti[1], Anders Mortensen[1], Gesa Siemann[1], Zhihao Jiang[1], Alfred Jones[1], Chakradhar Sahoo[1], Thomas Nielsen[1], Naina Kushwaha[2], Jennifer Ridgen[2], Søren Ulstrup[1], Bruce Weaver[2], Yu Zhang[2], Charlotte Sanders[2], Emma Springate[2], Vibha Reddy[3], Ulrich Starke[3], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Aarhus University, 8000 Aarhus C, Denmark — [2]Central Laser Facility, STFC Rutherford Appleton Laboratory, Didcot, Oxfordshire OX11 0QX, UK — [3]Max Planck Institute for Solid State Research, Heisenbergstr. 1, 70569, Stuttgart, Germany

Tunable moiré superlattices naturally form in artificially stacked monolayers through control of their rotational misalignment (twist angle). In large-angle twisted bilayer graphene (TBG), orbital hybridization between the monolayer-derived π/π^* bands leads to avoided crossings and the emergence of pairs of occupied and unoccupied van Hove singularities at fixed wave vectors k*. We investigate the out-of-equilibrium electron dynamics near these points in 10°-TBG using IR-pump XUV-probe time-resolved ARPES experiments. Our measurements resolve the hot electron dynamics in TBG and reveal an additional, unexpected spectral weight within the local electronic band gap at k*. This observation is consistent with the signature of a strongly bound exciton in TBG, whose formation has been attributed by recent theoretical models to a unique destructive coherence between two energy-degenerate subband resonant transitions.

O 66.9 Wed 17:15 TRE/MATH

Hybrid Frenkel-Wannier excitons facilitate ultrafast energy transfer at a 2D-organic interface — •Wiebke Bennecke[1], Ignacio Gonzalez Oliva[2], Jan Philipp Bange[1], Paul Werner[1], David Schmitt[1], Marco Merboldt[1], Anna M. Seiler[1], Daniel Steil[1], R. Thomas Weitz[1], Peter Puschnig[3], Claudia Draxl[2], G. S. Matthijs Jansen[1], Marcel Reutzel[1], and Stefan Mathias[1] — [1]I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Physics Department and CSMB, Humboldt-Universität zu Berlin, 12489 Berlin, Germany — [3]Institute of Physics, NAWI Graz, University of Graz, 8010 Graz, Austria

The combination of two-dimensional transition metal dichalcogenides (TMDs) and organic semiconductors (OSCs) is a highly promising material platform for the realization of future optoelectronic devices. While the excitonic properties of their individual components have been intensively studied, much less is known about excitons at the hybrid interface. Here, we use ultrafast momentum microscopy and many-body perturbation theory to investigate the exciton landscape at the PTCDA/WSe_2 interface [1]. In particular, we find an exciton state formed via Förster resonant energy transfer, which is of hybrid nature: Concomitant intra- and interlayer electron-hole transitions within the OSC layer and across the TMD/OSC interface, respectively, give rise to an exciton wavefunction with mixed Frenkel-Wannier character.

[1] Bennecke *et al.*, Nat. Phys. (2025)

O 66.10 Wed 17:30 TRE/MATH

Electronic friction simulations of laser-driven hydrogen evolution from copper. Does surface coverage matter? — •Alexander Spears[1], Wojciech G Stark[2], and Reinhard J. Maurer[1,3] — [1]University of Vienna, AT — [2]Imperial College London, UK — [3]University of Warwick, UK

Plasmonic catalysts such as metal nanoparticles harness the energy transfer between light, electrons and phonons at interfaces to drive chemical reactivity at interfaces. However, even on clean metal surfaces with a regular structure, it is unclear whether these dynamics are the result of mode-selective energy transfer or photothermal heating effects. Molecular dynamics simulations with electronic friction (MDEF) offer a quantum-classical description of electron-phonon coupling and have previously been used to model ultrafast dynamics on metal surfaces. Using machine learning surrogate models to accelerate MDEF simulations, we show that mode-selective energy transfer has a negligible influence on light-driven hydrogen evolution from copper surfaces. By comparing energy partitioning in desorbed molecules, we conclude the choice of electronic friction approximation only determines the rate of energy transfer, while the energy distributions of desorbing molecules are governed by the potential energy surface. This suggests that thermal and laser-driven desorption may yield similar outcomes at low coverage. However, we expect mode-selective energy transfer to play a stronger role at higher coverage, and show preliminary results for surface coverage dependence in laser-driven desorption.

O 67: Focus Session: Unoccupied States by Inverse Photoemission II

The Other Half of the Picture: 50 Years of Direct Access to Unoccupied States by Inverse Photoemission

In 1981, J. Pendry evaluated the experimental access to electron states in solids: "Currently only half of the picture can be seen with photoemission. Inverse photoemission provides the other half." A complete picture of electron states needs both occupied and unoccupied states in order to describe, understand, and finally tailor macroscopic material properties. In 1976, V. Dose had submitted a first paper on Bremsstrahlung Isochromat Spectroscopy in the VUV range: "The physics involved may be most simply described as an inverse photoelectric effect." The first experiments provided surface-sensitive information on the density of unoccupied states. Later, momentum and spin resolution were added to investigate the spin-dependent E(k) dispersion of unoccupied electron states. During five decades, the technique was further developed by several groups worldwide to enhance the intensity and improve the resolution in energy, momentum, and spin. A wealth of information was gained about metals, semiconductors, ultrathin films as well as adsorbate systems. The experimental studies were accompanied by several theoretical approaches, which are able to accurately describe the unoccupied electronic structure and model the inverse photoemission process. In 2012, H. Yoshida extended the energy range to the near-UV range (low-energy inverse photoemission), which is especially suited to study organic samples due to a lower damage risk caused by the exciting electron beam.

Current research fields for inverse photoemission are, e.g., spin textures of exchange- and/or spin-orbit-induced influenced systems and topological insulators, gap structures in transition metal dichalcogenides, LUMO levels in semiconductors for photovoltaic applications, electronic structure of atomic-layer and quantum materials. This focus session will highlight recent advances obtained by inverse photoemission in different fields and material systems. Also, it will bring together researchers from different areas for addressing current trends and future applications of inverse photoemission from experimental as well as theoretical perspective.

Organized by Markus Donath, Fabian Schöttke and Peter Krüger (U Münster).

Time: Wednesday 15:00–18:00 Location: WILL/A317

Invited Talk O 67.1 Wed 15:00 WILL/A317

New frontiers of one step model of photoemission for quantum materials — •Jan Minar — New Technologies Research Center, University of West Bohemia in Pilsen, Pilsen, Czechia

Quantum materials feature intertwined electronic correlations, topology, and magnetism, requiring realistic treatments of spin-orbit coupling, interactions, and spin fluctuations. Spin- and time-resolved ARPES (STARPES) is a key probe of their electronic and spin structures, but its quantitative interpretation demands advanced theory. I will present a fully relativistic multiple-scattering Green function (KKR) [1] framework for spin-dependent photoemission that incorporates correlations via DMFT, spin fluctuations via the alloy-analogy model, and light-induced electronic excitations [2,3]. Applications include a one-step photoemission description of altermagnets such as RuO* and MnTe, where spin-ARPES reveals lifted Kramers degeneracy relevant for spintronics, and kagome magnets such as FeSn thin films, where persistent flat-band splitting and selective band renormalization expose strong correlation and topological effects. This framework provides a unified route to unravel spin dynamics in complex quantum materials [4,5,6].

[1] H. Ebert et al., Rep. Prog. Phys. 74, 096501 (2011)
[2] J. Minár et al., Phys. Rev. B 102, 035107 (2020).
[3] J. Braun et al., Physics Reports 749, 1 (2018).
[4] J. Krempaský et al., Nature 626, 517 (2024).
[5] A.D. Din et al., arXiv:2511.01690 (2025)
[6] Z. Ren et al., Nature Communications 15, 9376 (2024).

O 67.2 Wed 15:30 WILL/A317

Surface-orientation-dependent unoccupied electronic states of Fe_3O_4 — •Jan Bieling and Markus Donath — Universität Münster, Germany

Experimental studies of the occupied electronic states of magnetite (Fe_3O_4) have revealed that the observed properties, such as band dispersions, are strongly surface-orientation-dependent [1,2]. However, comparable systematic studies of the unoccupied electronic states of different Fe_3O_4 surfaces are still lacking.

We report on the unoccupied electronic states of a well-characterized $Fe_3O_4(111)$ surface using angle-resolved inverse photoemission and compare the results with our previous study of $Fe_3O_4(100)$ [3]. This direct comparison allows for (re)interpreting the spectral features observed for both surfaces.

Finally, we discuss our findings in the context of recent theoretical studies [4,5]. We report a very good agreement between our inverse photoemission spectra of $Fe_3O_4(100)$ and the theoretical results obtained from DFT+U+V for this surface.

[1] Y. Dedkov *et al.*, Phys. Rev. B **70**, 073405 (2004)
[2] W. Wang *et al.*, Phys. Rev. B **87**, 085118 (2013)
[3] J. Bieling and M. Donath, Phys. Rev. B **111**, 075117 (2025)
[4] N. Naveas *et al.*, J. Chem. Theory Comput. **19**, 8610-8623 (2023)
[5] N. Naveas *et al.*, Results Phys. **70**, 108158 (2025)

O 67.3 Wed 15:45 WILL/A317

Beyond the surface: Probing electronic structure with IPES in Valparaíso-Chile — Patricia Martínez[1], Rolando. Esparza[1], Jonathan Correa-Puerta[1], Valeria del Campo[1], Ricardo Henríquez[1], •Patricio Häberle[1], Sanber Viscaya[1], Eric Suárez-Morell[1], Patricio Vargas[1], Jean F. Veyan[2], Marcos Flores[3], and Samuel Hevia[4] — [1]Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso, Chile — [2]Department of Materials Science and Engineering, The University of Texas at Dallas, Richardson, Texas 75080, USA — [3]Physics Department, Facultad de Ciencias Físicas y Matemáticas, Universidad de Chile, Santiago, Chile — [4]Instituto de Física and CIEN-UC, Pontificia Universidad Católica de Chile, Av. Vicuña Mackenna 1860, Macul, Chile

Over the past few years, we have employed angle-resolved inverse photoemission spectroscopy (IPES) at the Valparaíso facility, utilizing both the isochromat mode and photon energy-resolving capabilities. This technique has enabled us to investigate systems exhibiting electronic structures modified by various forms of quantum confinement. We have characterized metallic thin films, carbon nanotubes, self-assembled monolayers (SAMs), and two-dimensional semiconductors. Whenever feasible, we have mapped unoccupied energy bands; however, in many instances, we have relied on simulations and inventive averaging to extract meaningful information from these low-symmetry nanoscale systems. A comprehensive overview of our experimental findings and future directions will be presented.

O 67.4 Wed 16:00 WILL/A317

Inverse photoemission studies of unoccupied electronic states of various Si(111)-based surfaces and interfaces — Younal Ksari, Hela Mrezguia, and •Jean-Marc Themlin — CNRS, Aix-Marseille Univ. University of Toulon, Marseille, France

We operate in Marseille an angle-resolved inverse photoemission (ARIPES) setup working in the isochromat mode. To illustrate the potential of this highly surface-sensitive technique, we give a comparative overview of the unoccupied part of the electronic structure of several Si(111)-based interfaces as revealed by ARIPES, from the hydrogenated H:Si(111) to 2D silicene monolayers grown on passivated Si(111) substrates.

The H-saturated (1x1) termination of Si(111) solely reveals bulk conduction band states. Upon segregation (B) or adsorption (H, As, Au) of foreign atoms on Si(111), specific surface states appear, leading to insulating (H, As, B) or metallic (Au) interfaces.

According to LEED, the adsorption of 1 ML of Si on the $\sqrt{3}\times\sqrt{3})R30^\circ$ reconstructed Au- and B- substrates leads to the formation of a non-covalently bound Si bilayer, alias silicene, which adopts the symmetry of the passivated substrates. Specific unoccupied electronic states appear on each substrate, with dispersions profiles which do not exhibit a $\sqrt{3}\times\sqrt{3})R30^\circ$ symmetry, small overall bandwidths and large bandgaps (resp. > 2 eV and > 1 eV), suggesting important correlation effects.

O 67.5 Wed 16:15 WILL/A317

Layer-Dependent Electronic Signatures of Tl on Ag(111) Revealed by Inverse Photoemission — •Sarah Laufer[1], Sven Schemmelmann[1], Yuichiro Toichi[2], Kazuyuki Sakamoto[2], and Markus Donath[1] — [1]Physikalisches Institut, Universität Münster — [2]Department of Applied Physics, The University of Osaka

The Tl/Ag(111) system is characterised by pronounced changes in its spatial and electronic structure when transitioning from sub-monolayer coverage to the monolayer [1,2] and further to the bilayer [3], making an accurate determination of the layer thickness essential. While low-energy electron diffraction and Auger electron spectroscopy provide valuable information on domain orientations and Tl coverage trends, neither technique allows an unambiguous identification of the bilayer. In contrast, inverse photoemission (IPE) gives direct access to unoccupied electronic states, which are highly sensitive to the Tl film thickness. We show that Tl/Ag(111) exhibits distinct layer-dependent unoccupied states whose characteristic intensity evolution with increasing Tl coverage enables a clear identification of the bilayer. These results highlight the particular strength of IPE as a layer-specific probe for ultrathin metallic films.

[1] P. Härtl *et al.*, Phys. Rev. B **107**, 205144 (2023)
[2] S. Schemmelmann *et al.*, Phys. Rev. B **109**, 165417 (2024)
[3] T. Kobayashi *et al.*, Nano Lett. **23**, 7675-7682 (2023)

O 67.6 Wed 16:30 WILL/A317

Modeling a transient Dirac-like surface state in Floquet-driven SnTe — •Aki Pulkkinen[1], Frédéric Chassot[2], Hugo Dil[3], Claude Monney[2], and Ján Minár[1] — [1]New Technologies-Research Centre, University of West Bohemia in Pilsen, Czechia — [2]Department of Physics and Fribourg Center for Nanomaterials, Université de Fribourg, Switzerland — [3]Institute of Physics, Ecole Polytechnique Fédérale de Lausanne, Switzerland

We present a theoretical analysis of the ultrafast transient cone-like dispersion observed in pump-probe photoemission experiments on SnTe[1]. A semi-infinite (111) surface Hamiltonian is constructed from a Wannier tight-binding model, and the surface Green's function is obtained using the recursive López-Sancho method[2] in extended Hilbert space. The effect of the pump pulse is introduced through a time-periodic Peierls substitution and a Jacobi-Anger expansion of the driven Hamiltonian into Floquet sectors. The Floquet-Green's-function calculations show that photoexcitation induces a transient hybridization between the Floquet replica of the valence band and the conduction band, producing a momentary band inversion at the surface. The inversion generates a short-lived Dirac-cone-like surface state, reproducing the main experimental feature. The results indicate that the transient cone originates from Floquet-induced reconstruction rather than structural or thermal effects, and demonstrate the role of strong periodic driving in reshaping surface electronic structure in SnTe. [1] F Chassot et al. 2025 arXiv:2502.11967 [2] M. P. Lopez Sancho et al. 1985 J. Phys. F: Met. Phys. 15 851

O 67.7 Wed 16:45 WILL/A317

Peak separation analysis for inverse photoelectron spectra: Comparing second derivative, curve fitting, and deconvolution — •ryotaro nakazawa[1,2], haruki sato[2], and hiroyuki yoshida[2] — [1]Institute for Molecular Science, Aichi, Japan — [2]Chiba University, Chiba, Japan

Inverse photoelectron spectroscopy (IPES) is a powerful technique for probing the unoccupied electronic states of materials. Recently developed low-energy inverse photoelectron spectroscopy (LEIPS) can significantly advance the study of unoccupied states, owing to minimal sample damage and suppressed dark counts compared to conventional IPES. However, the instrumental resolution remains at around 0.2 eV, which is one order of magnitude lower than that of photoelectron spectroscopy. Spectral broadening caused by the low instrumental resolution often results in overlapping peaks. Peak separation is therefore crucial in the analysis of LEIPS spectra. In this study, we compared three peak separation methods: second derivative, curve fitting, and deconvolution. These methods were applied to modeled and experimental LEIPS spectra of the lowest unoccupied molecular orbital-derived band of pentacene, which consists of two splitting peaks due to the two inequivalent molecules in the unit cell. We systematically and quantitatively evaluated the performance of each method in terms of analysis parameters and discussed its robustness to noise as well as its peak separation and detection capabilities. This work offers a practical framework for peak separation in LEIPS, with extensions to PES and a wide range of spectroscopies.

O 67.8 Wed 17:00 WILL/A317

The role of light polarization in inverse photoemission — •Marcel Holtmann, Pascal J. Grenz, and Markus Donath — Physikalisches Institut, Münster University, Germany

In inverse photoemission (IPE), electrons are directed onto a surface and the light emitted during radiative transitions into unoccupied states is detected. By detecting the emitted photons as a function of the kinetic energy of the electrons impinging at a defined angle of incidence, the dispersion of conduction-band states can be traced. We focus on the role of light polarization in IPE and how the simultaneous detection of photons with multiple detectors provides additional symmetry information.

In the spirit of "50 years of IPE", this talk aims to give an overview of this aspect of IPE analysis. Building on early work from the 1980s [1,2], we will present measurements of the AgTe/Ag(111) surface alloy. The polarization contrast allows us to identify the orbital character of spin-dependent unoccupied states. We will also discuss the recent improvement of our setup, in which a polarizing mirror was added to the photon detector [3], enabling us to select the detected light polarization.

[1] M. Donath *et al.,* Solid State Commun. **60**, 237 (1986)
[2] T. Fauster *et al.,* Phys. Rev. B **40**, 7981 (1989)
[3] P. J. Grenz *et al.,* Rev. Sci. Instrum. **96**, 033905 (2025)

O 67.9 Wed 17:15 WILL/A317

Sub-100 meV low-energy inverse photoelectron spectroscopy using an electrostatic monochromator — •Tomoko Onishi[1], Taichi Suruga[1], Daichi Honma[1], Masaya Kai[1], Issei Ishimori[1], François C. Bocquet[2], F. Stefan Tautz[2], Harald Ibach[2], and Hiroyuki Yoshida[1] — [1]Chiba University, Chiba, Japan — [2]Forschungszentrum Jülich, Jülich, Germany

Inverse photoelectron spectroscopy (IPES) is the optimal experimental method for probing unoccupied electronic states but its applicability has been limited by modest energy resolution. This resolution is determined by the convolution of the electron energy spread and photon-detector bandwidth. The best reported resolution to date is 165 meV, limited by the photon detector [1]. Low-energy IPES (LEIPS) [2], using an optical bandpass filter, achieves a photon-detection resolution of 38 meV. However, the total resolution remains limited to 250 meV due to electron-beam thermal broadening [3]. In this work, we report a LEIPS system with an electron source consisting of a LaB6 cathode, electrostatic monochromator, and deceleration lens system. This design is based on high resolution electron energy loss spectroscopy (HREELS). We modified it to deliver several hundred nA with a capability of energy scan for LEIPS [4]. An electron energy spread of 90 meV is obtained, resulting in a total LEIPS energy resolution of 98 meV. [1] M. Budke et al., Rev. Sci. Instrum. 78, 083903 (2007). [2] H. Yoshida, Chem. Phys. Lett. 539*540, 180 (2012). [3] H. Yoshida, J. Electron Spectrosc. Relat. Phenom. 204, 116 (2015). [4] H. Ibach et al., Rev. Sci. Instrum. 94, 043908 (2023).

O 67.10 Wed 17:30 WILL/A317

Towards high resolution IPES in the VUV range — Giacomo Merzoni[1], Samuele Comizzoli[1], Giacomo Panzera[1], Lucio Braicovich[1,2], and •Giacomo Ghiringhelli[1,3] — [1]Politecnico di Milano, Italy — [2]ESRF, Grenoble, France — [3]CNR/SPIN, Politecnico di Milano, Italy

Since its concept was introduced and its feasibility was demonstrated, the conceptual interest of angle-resolved inverse photoemission (ARIPES) has not declined. Unfortunately, for decades technical challenges have kept ARIPES in a niche. At the same time direct photoemission, ARPES, has become a popular and unmissable technique for the determination of the electronic structure of solids. ARPES spectra are commonly measured with energy resolution better than 30 meV, a figure still unachieved in ARIPES. Which explains the different popularity of the two complementary techniques.

Is it possible to design today an ARIPES instrument that better exploits the technological progress undergone over the years by detectors and optical elements for VUV radiation, and by monocromatized electron-beam sources?

We present some ideas guiding the realization of an ARIPES apparatus working in the 20-100 eV energy range. Aiming at a combined instrumental bandwidth smaller than 50 meV, it is based on a high-luminosity grating spectrometer and a 2D position sensitive semiconductor detector.

O 67.11 Wed 17:45 WILL/A317

2D IPES intensity maps of MoS_2 — •Patricia Martínez-Rojas, Sanber Vizcaya, Rolando Esparza, and Patricio Häberle — Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso, Chile

Inverse photoemission spectroscopy (IPES) offers direct access to the unoccupied electronic structure of solids and is particularly well suited for investigating layered transition-metal dichalcogenides such as MoS_2. We present momentum-resolved IPES measurements on a bulk 2H-MoS_2 single crystal, performed with a normal-incidence grating spectrometer operated at a fixed electron kinetic energy of 25.6 eV. The sample was prepared by ex-situ exfoliation and subsequently annealed, in UHV, up to 400°C to remove surface contaminants. By recording the photon intensity as a function of emission energy and incidence angle, we constructed two-dimensional maps of the unoccupied states along the ΓK and ΓM directions of the Brillouin zone. The data reveal several dispersive features whose energy-momentum dependence closely matches density-functional theory (DFT) band-structure calculations. In particular, the conduction-band minimum is experimentally found away from high-symmetry points, consistent with theoretical predictions. These results highlight the capability of momentum-resolved IPES to characterize the unoccupied band structure of MoS_2 and provide a benchmark for future studies of two-dimensional materials.

O 68: Nanostructured surfaces and thin films – Poster

Time: Wednesday 18:00–20:00 Location: P2

O 68.1 Wed 18:00 P2

Electrospray Ion-Beam Deposition of Organic Molecules — •Grigori Pasko, Florian Münster, Lukas Heuplick, Jan Herritsch, and J. Michael Gottfried — Fachbereich Chemie, Philipps-Universität Marburg, Germany

The preparation of molecular adsorbates on surfaces is often constrained by limitations of conventional deposition methods. While small molecules can typically be thermally evaporated from a Knudsen cell, this approach becomes unsuitable for larger or non-volatile species. Electrospray ion-beam deposition (ESIBD) provides a powerful alternative, enabling the transfer of intact, non-volatile molecules from solution into ultrahigh vacuum. Although its use is increasing, ESIBD remains an emerging technique, and the chemical state of the molecules after deposition is often insufficiently understood. Determining the oxidation state and overall chemical composition of the deposited species therefore represents a central challenge. In this study, meso-tetraphenylporphyrin (TPP) serves as a model system for evaluating the chemical integrity of ESIBD-prepared films. By combining X-ray photoelectron spectroscopy (XPS), scanning tunneling microscopy (STM), and density functional theory (DFT) calculations, we demonstrate that the porphyrins preserve the protonation state acquired during the electrospray process and remain intact upon deposition.

O 68.2 Wed 18:00 P2

Nitrogen plasma induced surface modification of nickel electrodes for enhanced electrochemical performance — •Karla Siecker[1], Christina Meinert[1], Christian Marcks[2], Timo Wagner[1], Nicolas Wöhrl[1], and Axel Lorke[1] — [1]Faculty of Physics, University Duisburg-Essen — [2]Electrochemical Reaction Engineering, RWTH Aachen University

Nickel sheets are widely used as electrode materials for electrolyzers due to their low cost and ease of handling. Here, we report on the use of a microwave-induced remote nitrogen plasma to modify the sample surface, adjusting both the electrochemical and mechanical properties of the nickel electrode. The plasma treatment leads to the formation of coral-like nanostructures on the nickel surface and promotes measurable surface nitridation. As a result, the surface roughness and wettability increase, directly affecting the electrochemical activity. For this purpose, contact angle measurements, 3D optical profilometry and electrochemical measurements were conducted to evaluate the catalytic activity of the modified electrodes.

O 68.3 Wed 18:00 P2

Nanostructured TiO_2 surfaces by low-energy ion erosion — •Berk Yildirim and Jens Bauer — Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, D-04318 Leipzig, Germany

Ripple nanostructures on titanium surfaces are explored as a means to enhance protein adsorption and potentially introduce directionality for implant applications. We aim to produce large areas of consistent nanostructuring on titanium surfaces. Firstly, titanium/titanium oxide thin films are deposited using argon ion beam sputtering (IBS), followed by low-energy oxygen ion etching at an angle to create the ripple structures. Four main parameters are used for control. 1) thin-film composition, adjusted by supplying a background oxygen during deposition to produce fully TiO_2 films, or by depositing without oxygen to obtain titanium films, 2) etching time, 3) etching ion beam energy, where we applied 1.4 kV and 800 V, and 4) etching ion beam incidence angle. The morphology was analysed using AFM, SEM, Thin-film Reflectometry and the composition using XPS, ToF-SIMS. At 80°, the shadowing effect dominates and produces ripples or nanoneedles aligned in the same direction as the beam, which we consistently observe across a 5 cm radius sample. Roughnesses of the unetched films were $Sq = 1$ nm (Ti) and $Sq = 4.8$ nm (TiOx). We obtain much rougher and larger structures on the titanium oxide thin films with $Sq \approx 15$ nm, and smoother ripple structures on the titanium thin films with $Sq \approx 3$ nm. Controlling etching time and beam voltage allows fine-tuning of roughness and topography.

O 68.4 Wed 18:00 P2

Anomalous morphologies in ion-beam induced surface nanopatterning — •Denise J. Erb and Stefan Facsko — Ion Beam Center, Helmholtz-Zentrum Dresden-Rossendorf, Germany

Irradiating solid surfaces with broad beams of low-energy ions often results in nanaoscale patterning, emerging from a combination of erosive, ballistic and diffusive processes between ions and surface atoms. Typical pattern morphologies comprise ripples, dots, or pits and mounds. The patterning outcome was typically explained as being dominated by either adjustable properties of the ion beam such as incident angle or ion energy, or by inherent properties of the solid material such as elemental composition or crystal symmetry. However, under appropriate experimental conditions, unexpected pattern morphologies can be formed and their understanding requires considering a more complex interplay between ion beam and solid surface. We present such anomalous surface patternings as well as the current state of understanding and modeling these morphologies.

[1] D.J. Erb et al., Intermediate morphology in the patterning of the crystalline Ge(001) surface induced by ion irradiation, PRB 109 (2024) 045439

[2] D.J. Erb and S. Facsko, Tuning the Morphology of Self-Assembled Nanopatterns on MgO(001) Surfaces by Sequential Broad-Beam Ion Irradiation, Phys. Status Solidi RRL (2025) 2500117

O 68.5 Wed 18:00 P2

Fabrication of Self-Assembled Carbon Nanodot Patterns on Quartz Glass Surfaces by Means of Ion Beam Processing — •Jamal Ghaith and Jens Bauer — Leibniz-Institut für Oberflächenmodifizierung, Permoserstraße 15, D-04318 Leipzig, Germany

Graphite Nanodot patterns can be used as a negative mask for subsequent etching of quartz glass surface to bring about anti-reflective properties required in high-power laser applications. This requires uniformity in size and distribution of the nanodots over large areas. Silicon wafers with a $\sim 200\,nm$ thick thermal oxide layer are used as silica test sample material. A carbon layer is initially deposited using Ion Beam Sputtering (IBS), followed by 800 eV Argon ion etching at an angle, with sample rotation. The parameters used to control the nanodot formation are incidence angle of the ion beam, etch time, and carbon layer thickness. We found that an incidence angle of 70 degrees produces the most uniform nanodot distribution. Interestingly, increasing etch time does not necessarily lead to larger (or higher amplitude) dots. Instead of an increased size coalescence of the dots is observed, at least as long as the carbon layer thickness is high enough. The morphology was analysed using AFM and SEM, and the composition using ToF-SIMS.

O 68.6 Wed 18:00 P2

Reversible and persistent changes in nanofilms of the ionic liquid BMP DCA after application of an electric current — •Mirco Wendt[1,2], Anton Schün[2], Regina Lange[2], Jens Berdermann[1], Ingo Barke[2], and Sylvia Speller[2] — [1]Deutsches Zentrum für Luft-und Raumfahrt, Institut für Solar-terrestrische Physik, Neustrlitz — [2]Universität Rostock, Institut für Physik

1-Butyl-1-methylpyrrolidinium dicyanamide (BMP DCA) layers with a thickness of 10 to 20 nm were shown to be effective as charge mitigation layer in the context of spacecraft charging [1]. While at moderate exposures to electrons in a scanning electron microscope (10^12 e/m^2), no changes were observed, intense electron exposure led to irreversible damage with reversible alterations occurring at intermediate conditions. To better understand the conductive mechanism and how these layers react to the presence of excess electrons, ionic liquid nano-films on interdigitated electrodes were prepared and a voltage applied between them. The monitored currents indicated that charges were permanently transferred into the sample. Atomic force microscopy revealed changes to the film*s morphology as well as shifts in dynamic mode phase, indicating trapping of charges. These findings are compatible with theoretical studies, suggesting additional electrons in this particular ionic liquid do neither pair with cations nor form cation shells, but further reduce anions into a doubly negative charge state [2]. [1] Wendt et al., J. Space Weather Space Clim. 2024, 14, 18 [2] Xu et al., J. Phys. Chem. B 2015, 119, 2, 532-542

O 69: Nanostructures at surfaces:1D, 2D, networks – Poster

Time: Wednesday 18:00–20:00 Location: P2

O 69.1 Wed 18:00 P2

Study of different structural phases of Ni-DCA networks on graphene/Ir(111) — •Ayesha Jabeen[1], Dominik Hrůza[1], Zdeněk Jakub[1], Jakub Planer[1], Anna Kurowska[1], Pavel Procházka[1], and Jan Čechal[1,2] — [1]CEITEC - Central European Institute of Technology, Brno University of Technology, Czech Republic — [2]Faculty of Mechanical Engineering, Brno University of Technology, Czech Republic

2D metal-organic frameworks (MOFs) represent a promising class of two-dimensional nanomaterials with tunable electronic and magnetic properties, which could have potential applications in catalysis and spintronics. In this

study, we investigate the structural phases and thermal stability of Ni-DCA (9,10-dicyanoanthracene) networks supported on graphene/Ir(111). Employing Low-Energy Electron Microscopy (LEEM), Scanning Tunnelling Microscopy (STM), and X-ray Photoemission Spectroscopy (XPS), we identified three distinct structural phases: two phases composed of isolated $Ni_1(DCA)_3$ coordination complexes coexisting with hydrogen-bonded DCA molecules, and one extended metal-organic framework with $Ni_2(DCA)_3$ stoichiometry. Despite their different long-range order, all three phases have the same local Ni coordination environment. Thermal annealing reveals that the $Ni_2(DCA)_3$ network is the least stable of the three, dissociating into the individual complex phases upon mild annealing around 80 °C. These findings elucidate the polymorphic nature and thermal limitations of Ni-DCA networks supported on graphene/Ir(111), contributing to the understanding of DCA-based MOFs.

O 69.2 Wed 18:00 P2

Examining the character of coordination bonding in two-dimensional MOFs by photoemission tomography — •Dominik Brandstetter[1], Simone Mearini[2], Andreas Windischbacher[1], Yan Yan Grisan Qiu[2], Daniel Baranowski[2,3], Vitaliy Feyer[2,4], Claus Micheal Schneider[2,4,5], and Peter Puschnig[1] — [1]University of Graz, Graz, Austria — [2]Jülich Research Centre, Jülich, Germany — [3]Present address: Pacific Northwest National Laboratory, Richland WA, USA — [4]University of Duisburg-Essen, Duisburg, Germany — [5]UC Davis, Davis CA, USA

We investigate the nature of the coordination bonds in 2D MOFs by examining a well-ordered nickel tetracyanoquinodimethane (Ni-TCNQ) monolayer on a Ag(100) substrate. Notably, photoemission data shows a splitting of the valence band into bonding and anti-bonding states, resulting from the interaction between the Ni d-states and the ligand orbitals. By making use of the energy-resolved photoemission momentum maps, we are able unambiguously reveal signatures of covalent bonding between the organic ligands and the transition metal d-states by identifying fingerprints of the involved orbitals in momentum space. These hybridized states are crucial in understanding the MOF's electronic structure, which is a determining factor for their electronic and magnetic properties. Our results are concrete evidence of the covalent character within 2D MOFs, offering a deeper understanding of their fundamental electronic properties.

O 69.3 Wed 18:00 P2

Superconducting quantum corrals — •Divya Jyoti[1] and Nicolás Lorente[2] — [1]Christian-Albrechts-Universität zu Kiel, Kiel, Germany — [2]Centro de Fisica de Materiales (CFM), Donostia - San Sebastian, Spain

Quantum corrals enable atomically precise control of electronic confinement on surfaces, and their extension to superconductors opens new possibilities for manipulating in-gap Bogoliubov quasiparticles. In this work, we develop a microscopic Bogoliubov-de-Gennes Green-function framework [1-2] for multiple δ-like impurities on 2D superconducting lattices. As a benchmark, the method reproduces the superconducting mirage associated with Yu-Shiba-Rusinov states in elliptical corrals. By tuning the corral geometry, and material parameters, the spatial structure and spectral evolution of in-gap quasiparticle states is determined. We further explore the effect of confinement on engineered topological phases by placing a Majorana-hosting ferromagnetic spin chain inside an elliptical corral and showing that geometric confinement strongly hybridizes its zero-energy modes, redistributing their spin texture and shifting spectral weight to finite energies. These confined in-gap states offer a new route to engineer topological features, linking atomically crafted quantum matter to emerging platforms for topological quantum computation. [1] Morr et al., Phys. Rev. Lett. 92, 107006 (2004) [2] Flatté et al., Phys. Rev. B 56, 11213 (1997)

O 69.4 Wed 18:00 P2

Cooperative Rotation and Spin Switching of Molecules in Artificial Arrays — •Niklas Ide, Arnab Banerjee, Richard Berndt, and Alexander Weismann — IEAP, Kiel, Germany

Artificial arrays of tin phthalocyanine (SnPc) molecules on Pb(100) substrate are investigated using a low-temperature scanning tunneling microscope. Switching the central SnPc molecule between its two out-of-plane configurations (SnPc↑ → SnPc↓) triggers a collective rotation of all surrounding molecules in the array. This correlated structural response is accompanied by a change of the molecular spin states. A model of the intermolecular and molecular substrate interactions reproduces the experimental observations.

O 69.5 Wed 18:00 P2

Nonalternant Carbon Nanoribbon with 4-5-6-8 Topology via Indenofluorene Polymer Fusion — •Dong Han[1], Tim Naumann[1], Faming Kang[1], Alexandr Oshchepkov[2], Mikhail Kalinin[2], Ye Liu[1], Zilin Ruan[1], Konstantin Y. Amsharov[2], and J. Michael Gottfried[1] — [1]Philipps-Universität Marburg, Fachbereich Chemie, Hans-Meerwein-Str. 4, 35032 Marburg, Germany — [2]Martin-Luther-Universität Halle-Wittenberg, Institut für Chemie, Organische Chemie, 06120 Halle (Saale), Germany

Carbon nanoribbons (CNRs) with nonhexagonal rings constitute a fascinating class of low-dimensional carbon materials exhibiting tunable chemical and physical properties distinct from those of conventional graphene nanoribbons (GNRs). Here, we report the on-surface synthesis and characterization of a nonalternant 4-5-6-8 CNR. This nanoribbon is obtained via lateral fusion of cis-linked indeno[2,1-a]fluorene (IF) polymer chains, formed by sequential debrominative and dehydrogenative C-C coupling reactions of a halogenated arene. Bond-resolved scanning tunneling microscopy (BR-STM) confirms the atomic structure of the resulting CNR. Scanning tunneling spectroscopy (STS) and density functional theory (DFT) calculations reveal its distinct electronic properties arising from the nonhexagonal rings. Notably, the 4-5-6-8 CNR exhibits a bandgap of 1.13 eV, highlighting the critical role of ring topology in modulating quantum confinement. X-ray photoelectron spectroscopy (XPS) further elucidates reaction pathways and intermediate species. This study establishes a controlled on-surface synthetic route towards structurally complex CNRs.

O 69.6 Wed 18:00 P2

Tuning electronic properties in 2D Covalent Organic Frameworks via on-surface chemistry — •Mira Sophie Arndt[1], Christoph Wachter[2], Roman Pallach[3], Yan Yan Grisan Qiu[4], Simone Mearini[4], Vitaliy Feyer[4], Sebastian Henke[3], Oliver T. Hofmann[2], Mirko Cinchetti[1], and Giovanni Zamborlini[5] — [1]Departement of Physics, TU Dortmund, Otto-Hahn-Straße 4, 44227 Dortmund, Germany — [2]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria — [3]Department of Chemistry, TU Dortmund, Otto-Hahn-Straße 6, 44227 Dortmund, Germany — [4]Peter Grünberg Institute (PGI-6), Forschungszentrum Jülich GmbH, 52428 Jülich, Germany — [5]Institute of Physics, NAWI Graz, University of Graz, Universitätsplatz 5, 8010 Graz, Austria

Two-dimensional covalent organic frameworks (2D COFs) arranging in a Kagome lattice exhibit intriguing electronic properties, like flat bands and Dirac cones. We investigate the carbonyl-bridged aza-triangulene (P^2TANGO), which assembles into a Kagome lattice on Au(111). Inspired by reports that deoxygenation of the precursor induces an open-shell triplet ground state, we explore hydrogen-assisted deoxygenation to tune the COF's electronic properties. Our angle-resolved photoemission measurements reveal changes in the electronic structure upon oxygen removal, including energy shifts of the dispersive valence band features. DFT confirms that the shift grows with the deoxygenation, and that, in case of a complete deoxygenation, the degeneracy between the flat bands and the Dirac-dispersing bands is lifted.

O 69.7 Wed 18:00 P2

On-surface Synthesis of Aza-Coronoids — •Tim Naumann[1], Zilin Ruan[1], Olaf A. Kleykamp[1], Linus Pohl[2], Anton Nizovtsev[2,3,4], Alix Kaczmarek[2], Eugen Sharikow[1], Jörg Sundermeyer[1], Doreen Mollenhauer[2,3,4], and J. Michael Gottfried[1] — [1]Marburg University, Hans-Meerwein-Str. 4, 35032 Marburg, Germany — [2]Justus Liebig University Giessen, Heinrich-Buff-Ring 17, 35392 Giessen, Germany — [3]Helmholtz Institute for Polymers in Energy Applications Jena, Lessingstr. 12-14, 07743 Jena, Germany — [4]Institute for Technical and Environmental Chemistry, Friedrich-Schiller-Universität Jena, Philosophenweg 7a, 07743 Jena, Germany

Chemical reactivity and electronic properties of nanographenes are tailored by functionalization, edge topology and doping. A versatile sub-class within the nanographenes are coronoids, defined as benzenoids featuring a cavity. π-extended coronoids possess low solubility and are challenging target molecules for in-solution chemistry. However, reliable access via on-surface synthesis was demonstrated. Here, we combined in-solution and on-surface techniques to gain access to various aza-coronoids. Besides planar armchair-edge and zigzag-edge terminated coronoids, a curved coronoid was synthesized. Nitrogen functionalization of the inner cavity allows for hosting a metal atom and yields coronoid-metal complexes. In contrast, nitrogen core-doping significantly alters the electronic properties. Low-temperature scanning tunneling microscopy/spectroscopy (STM/STS), non-contact atomic force microscopy (nc-AFM) and DFT calculations were performed.

O 69.8 Wed 18:00 P2

Bottom-up fabrication of molecular islands utilizing an SPM-based manipulation approach — •Mong-Wen Gu[1,2], Ruslan Temirov[1,2,3], F. Stefan Tautz[1,2,4], and Christian Wagner[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Jülich, Germany — [2]Jülich Aachen Research Alliance, Fundamentals of Future Information Technology, Germany — [3]II. Physikalisches Institut, Universität zu Köln, Cologne, Germany — [4]Institut für Experimentalphysik IV A, RWTH Aachen, Aachen, Germany

The scanning probe microscope (SPM) allows single molecules to be manipulated with very high precision. SPM-based manipulation provides an opportunity for the fabrication of nanostructures through bottom-up construction. One critical challenge is using molecules other than conventional CO molecules as building blocks. Here, we explore the parameter space of the manipulation process in which a single PTCDA (3,4,9,10-perylene tetracarboxylic dianhydride) molecule bridges the SPM junction. We demonstrate the bottom-up construction of artificial PTCDA islands on Ag(111). These islands reproduce the native monolayer lattice structure, can be customized in size and shape and thus allow studying their electronic properties in a systematic way.

O 69.9 Wed 18:00 P2

Effect of the catalytic-substrate and graphene-films on the growth and physical properties of non-stoichiometric silicon-oxide nanoparticles — •Mehmet Selim Imamoglu, Cem Kincal, and Oguzhan Gürlü — Istanbul Technical University, Istanbul, Turkey

It is well known that silicon-oxide particles form during the growth of graphene by chemical vapor deposition (CVD) in a quartz furnace. Our studies showed that the creation and structure of these particles is mostly governed by the hydrogen flow rate during growth. Moreover, we have proven that they can be covered by graphene films depending on their morphology; showing that graphene growth during CVD process can continue over a non-catalytic substrate. In this work we have further investigated the formation and physical properties of such nanoparticles. Our results indicated that CVD grown silicon-oxide nanoparticles have non-stoichiometric nature leading to photoluminescent behavior. In this presentation their structure and physical properties as a function of the growth substrate (Ni and Cu foils) and the existence or in-existence of graphene films will be discussed. We will also present the methodology to transfer these nanoparticles on to random substrates.

O 69.10 Wed 18:00 P2

Towards on-surface synthesis of helicene chains — •Jung-Ching Liu[1], Miguel Gavara[1], Kévin Martin[2], Narcis Avarvari[2], Karl-Heinz Ernst[3,4,5], and Johannes Barth[1] — [1]Department of Physics, Technical University of Munich, James-Franck-Str. 1, 85748 Garching, Germany — [2]University of Angers, CNRS, MOLTECH-Anjou, SFR MATRIX, 49000 Angers, France — [3]Empa, Swiss Federal Laboratories for Materials Science and Technology, Überlandstrasse 129, 8600 Dübendorf, Switzerland — [4]Institute of Physics, Czech Academy of Sciences, Cukrovarnická 10, 16200 Prague 6, Czech Republic — [5]Department of Chemistry, University of Zurich, Winterthurerstrasse 190, 8057 Zürich, Switzerland

Helicenes are polycyclic aromatic helical compounds which have been investigated at surfaces regarding their spin selectivity due to their chirality and potential use in organic spintronics. To enhance chirality-induced spin selectivity, extended helicene chains are of interest. However, fabrication of such helicene chains has not yet been reported. Here, we present atomically precise dibromohexahelicene chain formations on Au(111). Investigated by STM and bond-resolving nc-AFM at 4K, we found self-assembled supramolecular clusters at low coverage. Coupling reactions occur as the annealing temperature reaches 330C. By further annealing to 380C, short segments of planar structures are found along with 3D chains. The findings indicate potential nanographenes formation, tentatively ascribed to a Diels-Alder pathway. Our study provides insights into extended on-surface synthesis using non-planar molecular precursors.

O 69.11 Wed 18:00 P2

Orthogonally oriented molecular motors assembled on the surface: from liquid-solid to ultrahigh vacuum — •Robby Reynaerts[1], Cosima Stähler[2], Steven De Feyter[3], Ben L. Feringa[2], and Leonhard Grill[1] — [1]Department of Chemistry, Division of Physical and Theoretical Chemistry, University of Graz, Heinrichstraße 28, 8010 Graz, Austria — [2]Stratingh Institute for Chemistry, University of Groningen, 9747 AG Groningen, The Netherlands — [3]Department of Chemistry, Division of Molecular Imaging and Photonics, KU Leuven, Celestijnenlaan 200F, B-3001 Leuven, Belgium

Molecular motors continue to attract wide interest, due to their capability to convert energy into uni-directional rotary motion at the nanoscale. Immobilization of molecular motors on a solid surface through molecular self-assembly could amplify their nanoscale motion. Applying specific molecular design such controlled assembly of molecular motors was achieved at the liquid-solid (LS) interface under ambient conditions and studied using scanning tunnelling microscopy (STM). However, the dynamics inherent to ambient conditions were inseparable from the response of the molecular motors to external stimuli. Bringing the system over to low temperature and ultra-high vacuum (LT-UHV) conditions would rid any inherent dynamics from those ambient conditions. In this contribution I will discuss the controlled self-assembly of molecular motors on a solid surface achieved through molecular design under ambient and LT-UHV conditions and the experimental transition between these conditions. References: Chem. Rev. 2005, 105, 1281; Chem. Eur. J. 2024, e202303994.

O 69.12 Wed 18:00 P2

Manipulation of Atomically Precise Nanostructures from Single Atoms and Molecules — •Nikita Osipov, Christophe Nacci, Grant J. Simpson, and Leonhard Grill — Physical Chemistry Department, University of Graz, Heinrichstrasse 28, 8010 Graz, Austria

Quantum corrals are of particular interest in surface science as they can be used to investigate quantum phenomena, such as quantum mirage [1] or function as quantum simulators that mirror the electronic properties of real atoms or molecules [2]. Currently, investigating these prominent structures requires researchers to manually assemble the objects on a surface using atomic manipulation techniques, a process that is extremely time-consuming. Our work aims to solve this critical bottleneck and save valuable research time. A primary goal of our project is to create an instrument for automatic and autonomous atomic manipulation. We are developing this system using machine learning algorithms to enable the careful, precise positioning of atoms or molecules [3]. This novel instrument will facilitate the assembly of large-scale objects or complex compositions of multiple smaller ones with high precision, thereby enabling the collection of significantly more data. In this work, we present our current status of assembled quantum corrals on noble metal surfaces. First results of manually assembled nanostructures will be presented together with the computational algorithm in the automated construction. [1] Li, Q. et al., Nat. Commun. 11 (2020) 1400. [2] E. Sierda et al., Science 380 (2023) 1048-1052. [3] B. Ramsauer et al., J. Phys. Chem. A 127 (2023) 2041.

O 69.13 Wed 18:00 P2

Atomic-Scale Sequencing of Biomolecules with nc-AFM — •Benjamin Mallada[1], Alejandro Lynch-Gonzalez[1], Marko Grabarics[1], Pavel Jelinek[2], Bruno de la Torre[3], and Stephan Rauschenbach[1] — [1]Department of Chemistry, University of Oxford, Oxford, UK — [2]Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic — [3]Nanomaterials and Nanotechnology Research Center (CINN-CSIC) , Mieres, Spain

Glycans, peptides, and cyclodextrins present major challenges for structural analysis due to branching, heterogeneous modifications, and stereochemical diversity. Conventional tools such as MS and NMR often fail to resolve these features at the single-molecule level. Non-contact AFM, combined with STM and KPFM under cryogenic UHV conditions, has recently demonstrated chemical sensitivity sufficient to discriminate functional groups and stereochemical arrangements by probing electrostatic and non-covalent interactions. Applications include the direct visualization of glycans in protein and lipid conjugates [1], submolecular resolution of cyclodextrins [2], and progress toward sequencing of complex carbohydrates and peptides. These results underline the potential of nc-AFM to expand the scope of SPM from imaging and identification toward true atomic-scale sequencing of biomolecules.

O 70: 2D materials: Stacking and heterostructures – Poster (joint session O/TT)

Time: Wednesday 18:00–20:00 Location: P2

O 70.1 Wed 18:00 P2

Unexpected Ordered Interfaces in WSe_2-$MoSe_2$ Lateral Interfaces Observed by STEM — •Matvei Kislitsyn[1], Max Bergmann[1], Julian Picker[2], Jürgen Belz[1], Robin Günkel[1], Badrosadat Ojaghi Dogahe[1], Shamail Ahmed[1], Andrey Turchanin[2], and Kerstin Volz[1] — [1]mar.quest | Marburg Center for Quantum Materials and Sustainable Technologies, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Faculty of Chemistry and Earth Sciences, Friedrich-Schiller-Universität, 07743 Jena, Germany

Two-dimensional WSe_2-$MoSe_2$ lateral heterostructures offer a platform for engineering band alignment and excitonic behavior through atomic-scale control of composition, making this material attractive for use in 2D optoelectronic devices. In this contribution, we present a systematic scanning transmission electron microscopy (STEM) study of monolayer WSe_2-$MoSe_2$ heterostructures synthesized by chemical vapor deposition (CVD) directly on SiO_2 TEM grids. While some investigated 2D flakes show atomically sharp interfaces with minimal intermixing, we also observe a highly ordered and unexpected interface configuration consisting of alternating Mo and W atomic rows. By comparing experimental observations with STEM image simulations and theoretical predictions, we analyze the structural origins of both interface types and discuss the mechanisms that may give rise to this unusual ordering. These results provide insight into interface formation mechanisms in lateral transition-metal dichalcogenide heterostructures and their potential impact on material properties.

O 70.2 Wed 18:00 P2

Superdomains and Strain Localization in Twisted Two Dimensional Transition Metal Dichalcogenides — •Riya Patel[1], Daniel Wolf[1], Kristina Weinel[1,2], Silke Hampel[1], and Axel Lubk[1,2] — [1]IFF, IFW Dresden, 01069 Dresden — [2]Faculty of Physics, Technical University Dresden, 01069 Dresden

Bilayers of 2D transition metal dichalcogenides (TMDCs) exhibit special structural and electronic phenomena when stacked with a low-twist-angle. Particularly, they undergo lattice reconstruction, forming large triangular stacking domains, separated by domain walls that concentrate strain (soliton regime), which

was shown in simulations. However, direct experimental quantification of these strain features and their correlation with electronic properties remains limited. Here we investigate low-twist-angle TMDCs using high-resolution transmission electron microscopy to visualize the reconstructed super lattice and identify the resulting superdomains structure. We employ geometric phase analysis to quantitatively map the strain distribution at the domain walls with nanometer resolution, revealing spatial maps of different strain components. We use Electron Energy Loss Spectroscopy to further probe the electronic properties of the reconstructed system. The understanding of strain localization in superdomain structures and the related electronic properties in such systems facilitate strain-engineered electronic properties in twisted TMDCs.

O 70.3 Wed 18:00 P2

Pseudomonolayer TMDCs via organic intercalation — •Katharina Steinkirchner[1,2], Jakob Dilling[1,2], Matthias Kalläne[1,2,3], Tim Riedel[1,2], Markus Scholz[4], and Kai Rossnagel[1,2,3,4] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [4]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany

Transition metal dichalcogenides (TMDCs) are a versatile class of layered materials with tuneable electronic properties. One approach to tailoring these properties is to manipulate the material's effective dimensionality. Specifically, intercalating cationic organic molecules with different alkane carbon chain into the van der Waals gaps between the layers increases the interlayer distance of the TMDC host material. This transforms the crystal from a bulk state to a monolayer-like state, thereby altering the electronic structure [1]. Here, we present a comprehensive study of the geometric and electronic structures of intercalated and non-intercalated TMDCs, such as $NbSe_2$, using SEM, EDS, and 11eV laser-based ARPES.

[1] H. Zhang *et al.*, Nat. Phys. **18**, 1425 (2022).

O 70.4 Wed 18:00 P2

Preparation of quasi-freestanding few-layer samples of 2D materials — •Seyedeh Helya Alaei, Hanna Shirin Pulikkal Hamza, Mashood Tariq Mir, Lukas Nöding, Ahmed Hassanien, Arne Senftleben, Jochen Mikosch, and Thomas Baumert — University of Kassel, Institute of Physics, 34132 Kassel, Germany

Two-dimensional (2D) materials have garnered significant attention in the last two decades and have been analyzed using various methods in the fields of materials science and physics. To study the dynamic behavior of 2D materials upon irradiation with femtosecond laser pulses using ultrafast electron diffraction, it is necessary to isolate few-layer structures from bulk crystals and prepare them in a quasi-freestanding manner. Due to the weak van-der-Waals forces between the layers relative to the in-plane forces of the structure, mechanical exfoliation is a commonly used method. However, the transfer is challenging, due to the thinness of the flake and the adhesive force between the flake and the surface. Our preparation involves three major steps: (1) exfoliation using adhesive tape and viscoelastic gel, (2) isolation of 2D material nanosheets with thicknesses ranging from 3 to 50 nm, and (3) transfer onto a standard sample mesh of transmission electron microscopy with a high success rate. The transfer exploits liquid-solid phase transitions of a soluble wax-like material. In this ongoing study, the 2D ferromagnetic material Fe_5GeTe_2 has been of interest. We will discuss the different steps in detail and the challenges associated with the preparation of this material, including the fragility of the crystals due to oxidation and the partially covalent out-of-plane forces.

O 70.5 Wed 18:00 P2

Ordering Phenomena in MoS_2 Nanocrystals on Graphite — •Lukas Nöding[1], Ahmed Hassanien[1], Mashood Tariq Mir[1], Hanna Shirin Pulikkal Hamza[1], Seyedeh Helya Alaei[1], Thomas Baumert[1], Jochen Mikosch[1], Florian Grassme[2], Claudia Backes[2], and Arne Senftleben[1] — [1]University of Kassel, Institute of Physics, Kassel, Germany — [2]University of Kassel, Institute of Chemistry, Kassel, Germany

Two-dimensional transition-metal dichalcogenides (TMDCs) such as MoS_2 offer a platform for tailoring electronic and optical properties through controlled stacking and orientation. Achieving ordered assemblies of MoS_2 nanocrystals on crystalline substrates is, therefore, of considerable interest. In this work, we study the crystallographic alignment of MoS_2 nanocrystals on a graphite substrate. The samples were prepared using the Langmuir-Schäfer technique, enabling the reproducible deposition of nanocrystals with controlled density. To probe the crystallographic alignment of the deposited nanocrystals with respect to the graphite lattice, we performed wide field static electron diffraction measurements at an acceleration voltage of 35 kV, complemented by selected area electron diffraction at 200 kV.

Our preliminary analysis reveals a pronounced localized and short-range ordered crystallographic alignment of the MoS_2 nanocrystals, extending over at least a few micrometers. A quantitative evaluation of the global ordering behavior, as well as its dependence on crystal size and deposition parameters, is currently underway and will be discussed.

O 70.6 Wed 18:00 P2

Multiferroic Two-Dimensional Cu(CrX2)2 (X = S, Se, and Te) as Anode Materials for Lithium-Ion Batteries: A First-Principles Study — •Muhammad Fayaz[1] and Zijing Lin[2] — [1]Department of Physics, University of Science and Technology of China, Hefei 230026, China — [2]Department of Physics, University of Science and Technology of China, Hefei 230026, China

Identifying two-dimensional (2D) materials with the desired electrochemical performance for lithium-ion batteries is of great interest in developing next-generation energy devices. Motivated by the successful synthesis of multiferroic 2D materials, Cu(CrX2)2 (X = S, Se, and Te), which exhibit simultaneous ferroelectricity and ferromagnetism, we performed first-principles calculations to investigate their potential as anodes for lithium-ion batteries. We comprehensively investigate the electrochemical properties of the predicted systems and demonstrate that lithium exhibits sufficient mobility on their surface, with appreciable stability. For instance, the binding energy (Eb) of the lithium adatom on Cu(CrS2)2 is -4.034 eV, with a diffusion barrier as low as 0.212 eV. As a consequence, the maximum theoretical specific capacity for lithium adatoms reaches as high as 1089 and 666 mAhg-1, respectively, for Cu(CrS2)2 and Cu(CrSe2)2, which can be attributed to a much higher storage capacity of lithium adatoms compared to previously identified 2D anode materials. All of these remarkable properties, including high binding energy (Eb), low diffusion barrier, high specific capacity, and good electrical conductivity.

O 70.7 Wed 18:00 P2

Valence-Band Renormalization and Spin Splitting in a Monolayer WTe2/WSe2 Heterostructure — •Daiyu Geng, Natalie Lehmann, Jiabao Yang, and Niels Schröter — Max Planck Institute of Microstructure Physics, Weinberg 2, Halle (Saale), Germany

Monolayer WTe2 (1L-WTe2) hosts a variety of broken-symmetry phases, including a quantum spin Hall insulator, a topological excitonic insulator, and several intriguing spin-ordered states. The dielectric environment and charge-carrier density play crucial roles in the competition among these electronic phases. In this work, we investigate the band structure of 1L-WTe2 interfaced with semiconducting WSe2 using laser- and synchrotron-based micro-ARPES. We observe strong valence-band renormalization accompanied by pronounced spin splitting in 1L-WTe2. Additionally, multiple replica pockets emerging in the Fermi surface indicate a substantial moiré effect in this heterostructure.

O 71: 2D Materials: Electronic structure, excitations, etc. – Poster (joint session O/TT)

Time: Wednesday 18:00–20:00 Location: P2

O 71.1 Wed 18:00 P2

Observation of many-body-localization in substituted $1T$-TaS_2 — •Jesumony Jayabalan[1], Gael Reecht[1], Ricards Kristers Knipšis[2], Florian K Diekmann[3], Friedemann Queisser[2], Walter Schnelle[4], Ping Zhou[1], Kai Rossnagel[3], Ralf Schützhold[2], Manuel Gruber[1], and Uwe Bovensiepen[1] — [1]Uni. of Duisburg-Essen, Fakultät für Physik and CENIDE — [2]HZ Dresden-Rossendorf, — [3]CAU of Kiel and DESY — [4]MPI for Chemical Physics of Solids, Dresden

Random modulations in the potential landscape are known to localize a single quantum particle, the Anderson localization leads, to stable non-thermalizing states. Adding interaction is expected to cause delocalization and a quick thermalization of such single particles, but in a strongly disordered system, the many-body quantum state itself becomes localized, known as the Many-Body Localization (MBL). Using time-resolved photoelectron spectroscopic measurements, we show that it is possible to realize MBL states in a Tungsten substituted $1T$-TaS_2 material. Electrons are excited by using a 1.51 eV, 50 fs pulses and a 6 eV probe pulse was used to photoemit electrons. In contrast to ultrafast (<20 fs) decay of doublons in pristine $1T$-TaS_2 [1], we observe that some of the doublons decay in hundreds of femtosecond time scale, while the rest lasts for more than few microseconds. This observation is supported by scanning tunneling micro-

scopic measurements and Fermi-Hubbard model calculations. Funding by DFG through QUAST-FOR5249 and SFB 1242 is acknowledged. [1] M. Ligges et al., Phys. Rev. Lett., 120, 166401 (2018).

O 71.2 Wed 18:00 P2

Exciton Transport in Monolayer TMDs — •Lifeng Ou, Alejandro Molina-Sánchez, and Alberto García-Cristóbal — ICMUV, University of Valencia, Valencia, Spain

Atomically thin transition metal dichalcogenides semiconductor emerges as promising candidates for novel optoelectronic application, displaying weak dielectric screening due to its truly two-dimension character. The optical properties are mostly related to inter-band transitions between valence and conduction bands, also called the strongly binding electron hole pair, exciton. Strain is expected to impact spatiotemporal distribution of excitons, e.g. spatially inhomogeneous strain acts as a driving force for exciton/carrier funneling, similarly to bias fields for charged particles. In this work we demonstrate the capability to manipulate exciton motion via spatially modulated strain fields, where excitonic energy especially its bandgap is largely tunable and the effective mass of electronic valleys is modified resulting in a qualitative change of the excitonic landscape and efficiency of exciton-phonon scattering channels. These transport properties are represented by the coupled two equations, continuity equation and drift-diffusion equation, which derive from zero-order and first-order moment of Boltzmann equation, respectively. In addition, the simulation diffusion coefficient and mobility in latter equation are evaluated by first-principle and experiment qualitatively, as the function of strain fields.

O 71.3 Wed 18:00 P2

trARPES investigation electron-phonon coupling in CrSBr — •Maurits Houmes, Karl Schiller, Lasse Sternemann, Jonah Nitschke, and Mirko Cinchetti — Departement of Physics, TU Dortmund University, 44227 Dortmund, Germany

CrSBr is a magnetic, semiconducting van der Waals material that has recently attracted significant interest. It hosts both localized Frenkel excitons and delocalized Wannier-Mott-like excitons, and its excitonic properties are strongly influenced by magnetic ordering and lattice distortions. [1,2,3] These features make CrSBr a compelling platform for exploring correlated phenomena in condensed matter systems.

To advance our understanding of the interplay between excitons, magnetism, and lattice dynamics in this material, a more complete characterization is essential. In this work, we present time- and angle-resolved photoemission spectroscopy (trARPES) measurements performed on CrSBr, with particular emphasis on quantifying the electron-phonon coupling. Aiming to provide a previously missing component needed to build a comprehensive picture of the interactions in CrSBr, offering a foundation for future studies and potential technological applications of this promising material.

1. Smiertka, M. et al. Preprint at ArXiv:2506.16426 (2025). 2. Lin, K. et al. ACS Nano 18, 2898-2905 (2024). 3. Bork, S. et al. Preprint at ArXiv:2511.20268v1 (2025).

O 71.4 Wed 18:00 P2

Probing defect-induced wave patterns and superconductivity in $2H$-NbS_2 — Werner M.J. van Weerdenburg, •Margarete Huisinga, Constantin Flommersfeld, Lisa M. Rütten, and Katharina J. Franke — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Transition metal dichalcogenides (TMDCs) host a variety of electronic phases, including superconductivity and charge-density-wave (CDW) order. Recent reports on $2H$-NbS_2 have added a coexisting pair-density-wave (PDW) order to this set, inspiring new questions about the coexistence and driving mechanisms of these phases [1]. In contrast, the closely-related superconducting compound $2H$-NbS_2 lacks a CDW phase, but has been suggested to be close to a CDW instability and sensitive to the presence of defects [2,3].

Using low-temperature scanning tunneling microscopy and spectroscopy, we probe the electronic, phononic and superconducting properties of $2H$-NbS_2. We observe wave-like modulations around intrinsic defects in differential-conductance maps and compare them to band-structure calculations. To assess the nature of these modulations, we probe the modulated regions and characterize the superconductivity spatially. These observations add to the ongoing exploration of superconducting, CDW, and PDW phases in TMDC materials.

[1] Liu et al., Science 372,1447-1452 (2021); [2] Heil et al., PRL 119, 087003 (2017); [3] Wen et al., PRB 101:241404, 6 (2020)

O 71.5 Wed 18:00 P2

Theory of few- and many-body excitations in carbon nanotubes — •Maurice Beringuier[1,2] and Richard Schmidt[1,2] — [1]Institut für Theoretische Physik, Philosophenweg 16, 69120 Heidelberg — [2]Universität Heidelberg, Grabengasse 1, 69117 Heidelberg

Even decades after their discovery, some properties of Carbon Nanotubes (CNTs) are still not fully understood. One of the phenomena still lacking a satisfying explanation is the behaviour of the absorption spectrum of semiconducting CNTs under doping. A resonance in these spectra appears only in the presence of additional charge carriers.

This has in the past been described with phenomenological models or few body physics (using trions and excitons), but experimental data (e.g. time resolved measurements of the spectra) hint at potential signatures of many-body physics. Inspired by their abundance in 2D or 3D semiconductors and cold quantum gases, we investigate whether quasiparticles like Fermi polarons could be responsible for the observations in CNTs, which due to their interesting geometry exhibit aspects of both 1D and 2D materials.

We tackle these questions by modeling charge carriers and excitons on CNTs interacting using a combination of exact diagonalization and variational techniques to gain insight into the interplay of few- and many-body physics in these systems.

O 71.6 Wed 18:00 P2

Spin-orbit coupling in non-van der Waals 2D materials — •Mani Lokamani[1], Gustav Bihlmayer[2], Gregor Michalicek[2], Daniel Wortmann[2], Stefan Blügel[2], and Rico Friedrich[1,3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [2]Forschungszentrum Jülich — [3]TU Dresden

In recent years, the rising class of non-van der Waals 2D materials [1] has garnered substantial attention for their distinctive electronic and magnetic properties. In this contribution, we explore the impact of spin-orbit coupling (SOC) on the properties of these non-van der Waals 2D systems and its potential to induce topological properties. Given the presence of heavy elements like Bi and Tl in several 2D candidates, SOC effects notably influence the electronic structure. In our approach, we utilize AFLOW's standardized workflows [2] for initial screening. Subsequently, we extract metadata using AFLOW and tailor the parameters with an AiiDA-plugin [3] for precise electronic structure calculations employing the full-potential all-electron program FLEUR [4] within AiiDA. We analyze the influence of SOC on band structures and densities of states, with a particular focus on topologically protected 1D conduction edge channels.

[1] R. Friedrich *et. al.*, Nano Lett. **22**, 989 (2022).
[2] Divilov *et. al.*, High Entropy Alloys Mater. **3**, 178 (2025).
[3] G. Pizzi *et al.*, Comput. Mater. Sci. **111**, 218 (2016).
[4] The FLEUR project: https://www.flapw.de.

O 71.7 Wed 18:00 P2

Strain Engineering Single Photon Emission in hBN and MoS2 Monolayers using First Principles — •Paulina Chodyra, Chengcheng Xiao, Johannes Lischner, and Arash Mostofi — Departments of Physics and Materials and the Thomas Young Center for Theory and Simulation of Materials, Imperial College London, London SW7 2AZ, U.K

Point defects in monolayer hexagonal boron nitride (hBN) and molybdenum disulphide (MoS_2) are promising single-photon emitters (SPEs) for quantum technologies due to their potential for room-temperature operation and high photon emission efficiency. In this work we use density-functional theory calculations to investigate the nitrogen antisite-vacancy complex (N_BV_N) and boron vacancy (V_B) in hBN, and the sulphur vacancy (V_S) in MoS_2. We calculate the defect formation energy of different charge states of these defects as a function of biaxial strain and electronic chemical potential. For the charge states that are likely candidates for SPE, we find that their stability can be enhanced via application of biaxial strain. Furthermore, the range of electronic chemical potential over which these charge states are stable can also be increased. These findings can provide predictive design rules for strain-engineered SPEs with improved resilience against electrostatic fluctuations. It also establishes our first steps toward an accelerated discovery of stable SPEs across 2D materials, where DFT-derived stability criteria combined with optical absorption and emission spectra could enable a deeper understanding of SPE operation under realistic conditions.

O 71.8 Wed 18:00 P2

Beyond the Gamma point: Scanning tunneling spectroscopy on MoS_2/graphene/Ir(111) — Borna Pielić[1,2], Dino Novko[2], Nina Girotto Erhardt[2], Vito Despoja[2], Alice Bremerich[1], Sumanasa Begur Prakash[1], •Robin Ohmann[1], and Carsten Busse[1] — [1]Universität Siegen, Walter-Flex-Str. 3, 57068 Siegen, Germany — [2]Institute of Physics, Bijenička cesta 46, 10000 Zagreb, Croatia

Scanning tunneling spectroscopy (STS) reveals information about the band structure of surfaces by measuring the local density of states, and it also allows detection of quasiparticles. For semiconducting transition-metal dichalcogenides the conduction- and valence-band edges have been readily explored with this method. However, STS studies at higher energies than the Γ-point are limited. Here, we investigate epitaxially grown monolayer islands of MoS_2 on graphene/Ir(111) using STS at low-temperature (T=10 K). Specifically, we employ the constant-current STS method, which enables easier access to spectroscopic features with higher energies, than the more commonly used constant-height STS. We find several peaks a few hundred meV above the Γ-point. We do not see them on graphene, allowing us to exclude substrate- or tip-related effects. When measured near the step edge of an island, these peaks bend closer to the Fermi level, similar to the peak at the Γ-point. Their appearance also varies

depending on tip condition and intercalation. Our observations cannot be explained in a single-particle picture. Possible many-body models, such as phonon assisted inelastic tunneling or plasmarons are discussed.

O 71.9 Wed 18:00 P2

Band structure and Work Function in Ultrathin HfSe2 — •Young Jun Chang — University of Seoul, Seoul, Republic of Korea

Two-dimensional (2D) transition metal dichalcogenides (TMDs) exhibit significant modifications in their electronic structures when reduced from bulk to monolayer thickness. In this study, we investigated the thickness-dependent electronic properties of epitaxial 1T-HfSe2 thin films. The films were grown via molecular beam epitaxy (MBE) and monitored in situ by reflection high-energy electron diffraction (RHEED). Scanning tunneling microscopy (STM) revealed atomically flat surfaces with well-defined 1T hexagonal lattices, while scanning tunneling spectroscopy (STS) measured a bandgap of ~1.1 eV for the monolayer. Angle-resolved photoemission spectroscopy (ARPES) revealed thickness-induced band splitting in the valence band, while the valence band maximum (VBM) remained pinned regardless of thickness. In contrast, the work function increased monotonically with film thickness. Density functional theory (DFT) calculations reproduced the observed band structures and attributed the thickness-dependent work function to the screening effect of the underlying graphene substrate. These findings provide key insights into band alignment and interface engineering in 2D semiconductor-based electronic and optoelectronic devices. (RS-2023-00220471, RS-2023-00284081, RS-2024-00334854)

O 71.10 Wed 18:00 P2

Exciton and trion dynamics of 2D transition metal dichalcogenides — •Seawoo Moon[1], Alessandro De Vita[1], Lawson T. Lloyd[2], Tania Mukherjee[1], Anh T. Nguyen[3], Dong-Wook Kim[3], Martin Wolf[2], Ralph Ernstorfer[1,2], and Tommaso Pincelli[1] — [1]Institute for Physics and Astronomy, TU Berlin, Germany — [2]Fritz Haber Institute of the Max Planck Society, Germany — [3]Department of Physics, Ewha Womans University, South Korea

Key functionalities of transition metal dichalcogenides (TMDs) are determined by excitons whose behaviour can be tweaked by interface–induced external perturbation such as proximity effects, charge transfer and local electromagnetic fields. Excitonic behaviors and band alignment of TMDs with interfacing materials are explored. We studied the band alignment of monolayer WS_2 on nanostructured Ag by Kelvin probe force microscope, a tool that can map electrical potential of sample surface. By this method, the exciton–to–trion conversion mechanisms in WS_2 could be explained, including the role of the localized surface plasmons. For a more direct approach, time and angle–resolved photoemission spectroscopy (TrARPES) with pump–probe technique is employed to directly map the equilibrium and non–equilibrium electronic structure of TMD–metal and TMD/TMD interfaces. In–situ and ex–situ techniques are required to achieve pristine TMD surfaces and interfaces, since TrARPES is a highly surface sensitive technique.

O 71.11 Wed 18:00 P2

Ultrafast Photocarrier-Induced Ionic Rearrangement in Monolayer ReS_2 Probed with Femtosecond Electron Diffraction — •Victoria C. A. Taylor[1], Yoav W. Windsor[1,2], Samuel Lai[3], Hyein Jung[1,2], Martin Wolf[1], Fang Lui[3], and Ralph Ernstorfer[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany — [2]Technische Universität Berlin, 10623 Berlin, Germany — [3]Stanford University, Stanford, CA 94305, USA

Rhenium disulphide (ReS_2) exhibits a distorted crystal structure compared to prototypical hexagonal transition metal dichalcogenides. This Peierls-like distortion results in quasi-1D chains of Re ions running in plane through each layer of ReS_2, which give rise to prominent anisotropic properties, such as polarization dependent optical absorption and anisotropic effective carrier masses.

We investigate the ultrafast lattice dynamics of monolayer ReS_2 with femtosecond electron diffraction (FED). Leveraging the strength of FED as a direct and quantitative measurement of the crystal lattice, we fit the intensities of many hundreds of Bragg peaks at each time delay to extract time resolved crystallographic information.

With this method, we not only resolve the increase in the incoherent phonon population (Debye-Waller), but also reveal a concerted atomic rearrangement within the lattice, with the ions rapidly (< 1 ps) moving away from their equilibrium atomic coordinates and returning on timescales of a few picoseconds. We associate this response with the aforementioned distortion, and discuss the physical origin.

O 71.12 Wed 18:00 P2

Exploring Zincblende (100) Semiconductor Surfaces as Platforms for Correlated Adatom Lattices — •Olga Kashirina, Niklas Enderlein, and Philipp Hansmann — Friedrich-Alexander-Universität Erlangen-Nürnberg

Adatom lattices on (111) surfaces of zincblende structured semiconductors have proven to be versatile, experimentally realizable platforms for hosting strong electronic correlations and associated emergent behavior near the Fermi energy (see [1] and references therein). Our recent study [2] reveals transition metals adatom lattices on 3C-SiC(111) surfaces to be intriguing candidates for strongly correlated material design. In the present contribution we continue this strategy by leaving the hexagonal/triangular lattices. Specifically, we explore the (100) surfaces of silicon, diamond, and 3C-SiC which in the infinite bulk exhibit a fourfold rotoinversion symmetry enabling square/rectangular adatom lattices. As the (100) surface is prone to dimerization, an additional complication arises from dimer-derived electronic states inside the bulk gap, which - depending on the chosen adatom and substrate combination - may or may not hybridize with the adatom states. In this context, the adatom coverage is another crucial parameter as it directly influences the nature of surface reconstructions and dimerizations. To assess the structural stability of our candidate systems, we employ phonon calculations based on density-functional perturbation theory as well as molecular-dynamics simulations. [1] X. Cao, et al., PRB 97, 155145 (2018). [2] H. Menke, N. Enderlein, et al., arXiv:2410.17165.

O 71.13 Wed 18:00 P2

Engineering correlated electrons in adatom lattices on semiconductors — •Tim Kullick[1], Niklas Enderlein[1], Henri Menke[1,2], Giorgio Sangiovanni[3], and Philipp Hansmann[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Max Planck Institute for Solid State Research, Stuttgart — [3]Julius-Maximilian-Universität of Würzburg

Adatom lattices on (111) surfaces of zinc-blende structured semiconductors have proven to be versatile, experimentally realizable platforms for hosting flat bands with strong electronic correlations near the Fermi energy. A recent study [1] revealed transition metals on 3C-SiC(111) surfaces to be intriguing adatom systems, showcasing the diverse nature of strongly correlated systems. Together with earlier theoretical and experimental studies on adatom lattices on the Si(111) surfaces, this recent work underlines the great potential of this material family. In the present project, we explore promising adatom lattices on semiconducting/insulating substrates such as SiC and cubic BN in order to realize one-, two-, and three-band Hubbard models at different fillings. Combined with estimates of the quasiparticle interaction via cRPA, we point out new material directions in this increasingly vivid field. [1] H.Menke, N.Enderlein, *et al.*, arXiv:2410.17165.

O 71.14 Wed 18:00 P2

Investigation of the atomic and electronic structures of WSe2-xTex — •Ganbat Duvjir[1], Nguyen-Hoang Dang[2], Younghun Hwang[1], and Jungdae Kim[1] — [1]Department of Semiconductor Physics and Engineering, University of Ulsan, Ulsan 44610, Republic of Korea — [2]Electricity and Electronics and Semiconductor Applications, Ulsan College, Ulsan 44610, Republic of Korea

Ternary transition metal dichalcogenides (TMDs) exhibit diverse crystal structures and electronic properties depending on their composition. In this study, we systematically investigate the atomic and electronic structure of ternary WSe2-xTex as a function of Te concentration using scanning tunneling microscopy/spectroscopy (STM/S). Notably, STM topography indicates that increasing the Te content induces structural deformation of the hexagonal lattice of WSe2-xTex. This deformation manifests as the stretching of 2H structure along the zigzag direction and compression along the armchair direction. STS measurements reveal a significant reduction in the band gap of WSe2-xTex with increasing Te concentration. While the valence band maximum shifts toward the Fermi level, the conduction band minimum remains relatively unchanged.

O 71.15 Wed 18:00 P2

STM study on tuning the Fermi level of transition metal dichalcogenides — •Nguyen-Hoang Dang[1], Mincheol Kim[2], Ganbat Duvjir[1], Young Jun Chang[2,3], and Jungdae Kim[1] — [1]Department of Semiconductor Physics and Engineering, University of Ulsan, Ulsan 44610, Republic of Korea — [2]Department of Physics, University of Seoul, Seoul 02504, Republic of Korea — [3]Department of Smart Cities, University of Seoul, Seoul 02504, Republic of Korea

Controlling the Fermi level is essential for tailoring the electronic properties of semiconductors. Here, we investigate two routes of chemical doping and defect control using scanning tunneling microscopy and spectroscopy. For V-doped $MoSe_2$, we study how substitutional V atoms influence its electronic structure. Although STM primarily probes the top Se layer and the dopants are not directly imaged, the topography exhibits defect-like features whose contrast reverses with the bias polarity: dark at positive sample bias and bright at negative bias. This is characteristic of negatively charged acceptor states, consistent with V substituting Mo. STS spectra show a Fermi-level shift toward the valence band, indicating that V doping drives $MoSe_2$ from intrinsic n-type toward p-type. For $HfSe_2$, we study defect control via thermal annealing. STS measurements under different annealing conditions show Fermi level shifts toward the conduction band, suggesting that prolonged annealing enhances Se-vacancy formation, which acts as an electron donor. These results highlight how STM/STS links local defects with electronic properties, offering microscopic insight into Fermi level tuning through doping and defect engineering.

O 71.16 Wed 18:00 P2

Impact of Mo doping on the charge density wave in 1*T*-TaS_2 studied by laser-ARPES and LEED — •Adina Timm[1,2], Finja Schillmöller[1,2], Florian K. Diekmann[1,2], Jana Kähler[1,2], Matthias Kalläne[1,2,3], Tim Riedel[1,2], and Kai Rossnagel[1,2,3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Controlling charge density waves (CDWs) in quantum materials enables the fine-tuning of their electronic properties, paving the way for future electronic and optoelectronic devices. The layered compound 1*T*-TaS_2 exhibits various temperature-dependent CDW phases that we aim to modify through doping. We introduced the dopant molybdenum during crystal growth via the chemical vapor transport method. Using 11-eV laser-based angle-resolved photoelectron spectroscopy (ARPES), we comparatively measured the electronic band structures of pristine and Mo-doped 1*T*-TaS_2 crystals. Complementary low-energy electron diffraction (LEED) measurements revealed the structural rearrangements during the CDW transitions and partial CDW suppression at specific doping levels. Our results suggest that modest Mo doping allows for subtle adjustments to the CDW landscape of 1*T*-TaS_2, yielding different transition temperatures while preserving the underlying electronic-structural order.

O 71.17 Wed 18:00 P2

Probing Electronic Structure Modulation in WSe_2 and $MoTe_2$ under Out-of-Plane Electric Fields via ARPES and XPS — •Sonja Reinheimer[1,2], Lukas Bruckmeier[1,2], Jakob Dilling[1,2], Jens Buck[1,2], Matthias Kalläne[1,2,3], Chithra Sharma[1,2,4], Markus Scholz[5], and Kai Rossnagel[1,2,3] — [1]IEAP, CAU Kiel, 24098 Kiel, Germany — [2]RHL, DESY, 22607 Hamburg, Germany — [3]KiNSIS, CAU Kiel, 24098 Kiel, Germany — [4]Universität Hamburg, 22761 Hamburg, Germany — [5]DESY, 22607 Hamburg, Germany

Transition metal dichalcogenides (TMDCs) are quantum materials that exhibit a broad spectrum of emergent electronic phenomena, arising from layer-dependent band structures. Owing to their tunable (opto-)electronic properties, TMDCs are promising candidates for next-generation photovoltaic devices and highly integrated electronic components. A key challenge is to systematically control charge transport and band alignment in these layered systems. Here, we investigate vertically stacked 2*H*-WSe_2/2*H*-$MoTe_2$ heterostructures using angle-resolved photoemission spectroscopy (ARPES) and X-ray photoelectron spectroscopy. By performing in-operando ARPES on a sample with an applied out-of-plane electric field during the measurements, we can directly probe field-induced modifications to the electronic band structure and the density of states. This approach enables us to identify electric-field-driven changes in the electronic and lattice structure and contribute to a deeper understanding of electric control mechanisms in TMDC heterostructures.

O 71.18 Wed 18:00 P2

Many-body localisation in the Fermi-Hubbard model? — •Ričards Kristers Knipšis[1], Jesumony Jayabalan[2], Gael Reecht[2], Vivek Mondal[2], Florian Konstantin Diekmann[3], Friedemann Queisser[1], Ping Zhou[2], Walter Schnelle[4], Kai Rossnagel[3,5], Ralf Schützhold[1,6], Manuel Gruber[2], and Uwe Bovensiepen[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg, Germany — [3]Institute of Experimental and Applied Physics, Christian-Albrechts-University of Kiel, Kiel, Germany — [4]MPI for Chemical Physics of Solids, Dresden, Germany — [5]Ruprecht-Haensel-Laboratory, DESY, Hamburg, Germany — [6]Institute of Theoretical Physics, Dresden University of Technology, Dresden, Germany

Motivated by recent experimental results, we study the 2D Fermi-Hubbard model in the Mott insulator state under the influence of a disorder potential. Special emphasis is placed on signatures of many-body localisation.

Using the hierarchy of correlations, we find that the disorder potential can localise the effective quasi-particle wavefunctions, resulting in their spatial separation. This, in turn, can be used to explain the drastic increase in the quasi-particle lifetimes observed in experiment.

Funding by the DFG through the SFB 1242 is gratefully acknowledged.

O 71.19 Wed 18:00 P2

Magnetic properties of V-doped WSe2 — •Jules M. Knebusch[1,2], Jana Kähler[1,2], Matthias Kalläne[1,2,3], Robert Zierold[4], Tim Riedel[1,2], Adina Timm[1,2], Robert H. Blick[4], and Kai Rossnagel[1,2,3] — [1]IEAP, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]RHL, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [4]CHyN, Universität Hamburg, 22761 Hamburg, Germany

Spintronics holds promise for highly efficient classical and quantum computing and is therefore considered a key technology for future innovation. Pristine tungsten diselenide (WSe_2), known as a semiconductor with a quasi-two-dimensional hexagonal 2*H* structure, is expected to transform into a room-temperature dilute ferromagnetic semiconductor upon vanadium doping. This makes it a highly attractive candidate for spintronic applications. Density functional theory calculations and scanning transmission electron microscopy studies support this assumption, and RKKY interactions are predicted to be the driving mechanism. Pristine WSe_2 and vanadium-doped WSe_2 crystals were synthesized in separate in-house batches using the chemical vapor transport (CVT) method. The doped samples were grown with varying nominal concentrations of V intended to induce substitutional doping at the tungsten sites. The samples were investigated using a vibrating-sample magnetometer (VSM). The results provide insight into the magnetic characteristics of the doped material compared to the pristine reference crystal.

O 71.20 Wed 18:00 P2

Coexistence of a fully metallic antiphase boundary and the semiconducting charge density wave phase in 1T-TaS_2 — •Georg A. Traeger[1], Kai Rossnagel[2,3], and Martin Wenderoth[1] — [1]IV. Institute of Physics, University of Göttingen, Göttingen, Germany — [2]Institute of Experimental and Applied Physics, Kiel University, Kiel, Germany — [3]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Transition metal dichalcogenides are an ideal platform for studying the interplay between charge density waves (CDWs), electronic correlations, and defect states. Using scanning tunneling microscopy and spectroscopy, we investigate a new type of intrinsic antiphase boundary (APB) in the commensurate CDW phase of 1T-TaS_2. In contrast to previous studies, we find a metallic APB extending laterally across several nanometers. We observe evanescent states spilling out from the defect into the metallic region and find that the fingerprint of the semiconducting system gradually disappears within the APB, without signs of strong interactions, suggesting the orthogonality of the two systems wave functions. Our findings highlight the crucial role of domain boundaries in the interpretation of other, especially conductivity-based, measurements. Furthermore, we propose this new type of metallic APB as a model system to study interlayer coupling in correlated layered materials.

O 71.21 Wed 18:00 P2

Temperature-dependent VUV-ARPES of 1*T*-$Mo_xTa_{1-x}S_2$ — •Torben Petersen[1,2], Matthias Kalläne[1,2,3], Adina Timm[1,2], Tim Riedel[1,2], and Kai Rossnagel[1,2,3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Examining the charge density wave (CDW) phase transitions of transition metal-substituted transition metal dichalcogenides (TMDCs) provides insight into tuning transition behavior by doping. To this end, we use the 1*T*-$Mo_xTa_{1-x}S_2$ reference system, comparing the pristine sample with two doped samples (x = 0.5% and x = 1%) using 11 eV laser-based VUV-ARPES. We investigate work function changes alongside doping-induced band structure changes in the temperature range of 60 K to 370 K. This allows us to observe the high- and low-temperature CDW phase transitions known from the pristine material and determine how the CDW-induced band structure changes vary with doping.

O 71.22 Wed 18:00 P2

STM/STS Studies of Single-Atom Fe Inclusions in MBE-grown Monolayer MoS_2/Gr/Ir(111) — •Alina Drechsler, Marta Przychodnia, Maciej Bazarnik, and Anika Schlenhoff — Institute of Physics, University of Münster, Germany

Transition metal dichalcogenides (TMDs) exhibit thickness-dependent electronic properties and are highly sensitive to structural defects, which can strongly modify their density of states even at low concentrations. Defect engineering has therefore become an important route to tailor their electronic, magnetic, optical, and catalytic behaviour. While most of the current research focuses on naturally occurring defects in chemical vapour-deposited TMDs, we focus on intentional single-atom inclusions in TMDs grown by molecular beam epitaxy (MBE) to improve control in defect engineering.

We present scanning tunneling microscopy and spectroscopy (STM/STS) studies of Fe-doped monolayer MoS_2 on Gr/Ir(111), achieved by co-evaporation Fe during MBE growth. By comparing to undoped MoS_2 grown under identical UHV conditions, we identify the Fe-related defects and measure their electronic signatures. STS reveals in-gap states associated with single-atom Fe inclusions, whose spatial distributions are resolved via differential conductance mapping. Additionally, resonant tunneling spectroscopy shows that Fe inclusions modify the image potential states by locally shifting their energetic positions. Our work demonstrates the potential of single-atom substitutions for tailoring the electronic properties of two-dimensional TMDs.

O 71.23 Wed 18:00 P2

Layer thickness dependent band gap of MBE grown single- to few-layer MoS_2 — •Maciej Bazarnik[1], Marta Przychodnia[1,2], Thorsten Deilmann[3], and Anika Schlenhoff[1] — [1]Institute of Physics, University of Münster, Germany — [2]Institute of Physics, Poznan University of Technology, Poland — [3]Institute of Solid State Theory, University of Münster, Germany

In light of the rise of transition metal dichalcogenides as 2D semiconductors for device applications, band engineering becomes very important from an application point of view. In many of these materials, such as the canonical example of MoS_2, the semiconductor band gap depends on the layer number. There is a transition from an indirect band gap semiconductor in bulk to a direct band gap for a monolayer. Interestingly, it was predicted and experimentally confirmed that, by thinning the material from bulk to a bilayer, the indirect transition blue-shifts.

Here, we present the results of scanning tunnelling spectroscopy measurements on MoS_2 that has been grown in situ via molecular beam epitaxy (MBE) on graphene on Ir(111) at thicknesses ranging from 1 to 6 layers. We observe a decrease in the band gap with increasing layer number. We also find a pinning of the conduction band, which vanishes for layer thicknesses beyond 4 layers. Comparing our experimental data with DFT and GW calculations indicates that a screening in addition to that of the substrate needs to be introduced to explain the experimentally obtained relation. We discuss possible sources of this additional screening in light of our findings.

O 72: 2D Materials beyond graphene: Growth, structure and substrate interaction – Poster (joint session O/TT)

Time: Wednesday 18:00–20:00 Location: P2

O 72.1 Wed 18:00 P2

In-Situ CVD growth of vertical Heterostructures of Borophene and Hexagonal Boron Nitride — •Niels Ganser[1], Marko Kriegel[1], Smruti Ranjan Mohanty[1], Karim Omambac[1], Marin Petrovic[2], Christian Brand[1], Steffen Franzka[3], Birk Finke[1], Tobias Hartl[4], Thomas Michely[4], Frank-Joachim Meyer zu Heringdorf[1,3], and Michael Horn-von Hoegen[1] — [1]Universität Duisburg-Essen — [2]Institute of Physics, Zagreb — [3]ICAN, Duisburg — [4]Universität zu Köln

Intrinsic segregation provides a promising and scalable route for the in situ fabrication of 2D heterostructures. Using UHV chemical vapor deposition (CVD) of a single borazine ($B_3N_3H_6$) precursor [1], we demonstrate the growth of an hBN/borophene heterostructure on Ir(111). At high temperatures and low precursor pressures, boron dissolves into the Ir subsurface region, creating a boron reservoir below the surface [2]. Largely increasing the precursor dosing pressure shifts the chemical potential toward the formation of a complete hBN layer. Upon cooldown, the decreasing boron solubility of the Ir substrate drives segregation to the surface, where a borophene layer forms underneath the hBN overlayer and thus completing the heterostructure. The resulting structure and its growth kinetics were investigated using a combined low energy electron diffraction (SPA-LEED) and microscopy (LEEM) approach.

[1] K. Omambac et al., ACS Nano 17 (2023) 17946
[2] K. Omambac et al., ACS Nano 15 (2021) 7421

O 72.2 Wed 18:00 P2

Growth of 2D molecular networks on graphene — •Haruto Shibahara and Toyo Kazu Yamada — Dept. Materials Science, Chiba Univ., Chiba, Japan

We demonstrate the engineering of qubits on solid surfaces using organic molecules and transition-metal magnetic atoms. Atomically flat and clean graphene (Gr) grown on an Ir(111) substrate was selected as the platform. Scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED) revealed the characteristic moiré pattern, while scanning tunneling spectroscopy (STS) and angle-resolved photoemission spectroscopy (ARPES) confirmed the presence of Dirac bands. Although single atoms can in principle serve as qubits, they tend to thermally diffuse on surfaces and their energy levels may remain degenerate. To overcome these issues, it is necessary to coordinate the atoms with organic ligands, whose ligand fields can lift the degeneracy. As a first approach, we attempted to employ 1,3,5-tris(4-bromophenyl)benzene (TBB) molecules to form a two-dimensional (2D) covalent organic framework. However, on the Gr surface we found that thermal activation desorbed the TBB molecules before they could undergo Ullmann coupling. As a second approach, we attempted to grow a 2D metal organic framework (MOF) on Gr. The details of this effort will be discussed.

O 72.3 Wed 18:00 P2

Probing the Electrostatic Potential of hBN by AFM with Oxygen-Terminated Copper Tips — •Jan ter Glane[1,2], Philipp Wiesener[1,2], Thorsten Deilmann[3], Milena Merkel[1,2], Maciej Bazarnik[2], Anika Schlenhoff[2], and Harry Mönig[1,2] — [1]Center for Nanotechnology, University of Münster, Germany — [2]Institute of Physics, University of Münster, Germany — [3]Institute of Solid State Theory, University of Münster, Germany

Monolayer hexagonal boron nitride (hBN) hosts point defects with promising optoelectronic properties, yet their atomic structure remains unclear [1]. Conventional scanning tunneling (STM) and atomic force microscopy (AFM) lack elemental contrast, making it difficult to reliably distinguish B and N sites. Non-contact AFM with oxygen-terminated copper tips (CuOx-tips) has previously enabled elemental discrimination and defect identification on metal oxides [2].

Using CuOx-tip AFM, we demonstrate elemental contrast on NaCl thin films, suggesting its broad applicability to polarized surfaces. Leveraging this capability, we investigate its application to monolayer hBN. DFT-optimized electrostatic potential calculations predict clear B-N contrast. To realize these measurements, we employ in-situ chemical vapor deposition growth procedures for high-quality hBN on single-crystalline substrates. We outline the benefits of CuOx-tip AFM and present initial results towards correlating STM/STS measurements, aiming to enable atom-specific defect identification in hBN.

[1] Grosso *et al.*, Nat. Commun. **8**, 705 (2017)
[2] Wiesener *et al.*, ACS Nano **18**, 21948 (2024)

O 72.4 Wed 18:00 P2

Pt-doped borane nanomembranes — •Martha Frey[1], Julian Picker[1], Christof Neuman[1], Jan Macháček[2], Tomáš Baše[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, Lessingstraße 10, 07743 Jena, Germany — [2]The Czech Academy of Sciences, Institute of Inorganic Chemistry, 250 68 Husinec Rez, 1001, Czech Republic

Boranes are clusters of boron and hydrogen atoms that form three-dimensional, cage-like molecules. We have recently employed them as convenient starting precursors for synthesising two-dimensional (2D) carbon-free nanomembranes. In this study, we present the preparation and characterisation of the self-assembled monolayers (SAMs) of two thiolated *syn*-$B_{18}H_{22}$ clusters on silver substrates. Subsequently, these SAMs were cross-linked laterally to form boron nanomembranes (BNMs) via low-energy electron irradiation under ultra-high vacuum (UHV) conditions. We investigated the structural and chemical properties of these 2D nanomembranes using surface-sensitive techniques such as X-ray photoelectron spectroscopy (XPS) and scanning tunnelling microscopy (STM). Both the starting SAMs and the resulting boron nanomembranes exhibited reactivity toward Pt-containing complexes. While such reactivity was expected for the SAMs, it was particularly noteworthy that the BNMs also enabled the insertion of Pt atoms. This Pt-doping positions borane-derived SAMs and BNMs as a promising 2D platform for nanoscale catalytic studies.

O 72.5 Wed 18:00 P2

Defects and Initial Approaches to TMDC Heterostructure Growth on Pt_xTe_y films — •Isabella Stollberg, Andreas Raabgrund, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Transition-metal dichalcogenides (TMDCs) can generally be synthesised either by co-evaporating the metal and chalcogen onto a suitable substrate [1] or by depositing only the chalcogen onto the desired metal surface. Using STM, STS, and DFT, we investigate Pt_xTe_y films on Pt(111) prepared via the latter approach. With increasing Te content, different initial growth surface telluride structures are observed, followed by the formation of Pt_2Te_2 and $PtTe_2$ layers [2]. This contribution focuses on STM and spatially resolved STS analyses of point defects in $PtTe_2$, as well as domain boundaries within a $PtTe_2$ or Pt_2Te_2 layer. Furthermore, we evaluate the suitability of these telluride films as substrates for TMDC heterostructure growth. First results on attempting to grow $TiTe_2$ and $PdTe_2$ demonstrate considerable intermixing. While $TiTe_2$ islands can be identified by their apparent height and other lattice constants, $PdTe_2$ islands cannot be distinguished from $PtTe_2$ based on topography due to their similar vertical and lateral lattice parameters.

[1] K. Lasek et al., Nano Lett. **22**, 23 (2022)
[2] T. Kißlinger et al., Phys. Rev. B **108**, 205412 (2023)

O 72.6 Wed 18:00 P2

Boosting the Efficiency of Quantum Replica-Exchange Molecular Dynamics — •Jan-Niklas Mohr, Shubham Sharma, and Mariana Rossi — MPI for the Structure and Dynamics of Matter, Hamburg, Germany

Replica exchange molecular dynamics can be combined with path-integral techniques in order to incorporate quantum statistics in the sampled ensembles [1].

However, the efficiency in swapping replicas is decreased to a point that makes simulations extremely inefficient at lower temperatures.

We propose a new acceptance criterion for path-integral replica-exchange molecular dynamics (PI-REMD) that incorporates the path-integral spring term in the Hamiltonian and rescales it consistently. As a result, the acceptance probability is only sensitive to potential-energy differences, and the efficiency of the method is thus increased. Benchmarking on several test systems, including asymmetric double wells and glassy-like potentials, shows that our method outperforms standard PI-REMD in sampling efficiency and exchange frequency. We also show improvements for realistic materials, such as monolayer 1H-TaS_2 [2], where it is paramount to obtain an accurate description of the charge-density-wave phase transition. Our acceptance criterion therefore provides an efficient and reliable tool for studying quantum phase transitions and exploring thermodynamic ensembles under challenging conditions.

[1] Kapil *et al.*, Comput. Phys. Commun. 236, 214-223 (2019).
[2] Schobert *et al.*, SciPost Phys. 16, 046 (2024)

O 73: Graphene: Growth, structure and substrate interaction – Poster

Time: Wednesday 18:00–20:00 Location: P2

O 73.1 Wed 18:00 P2

Towards enhanced spin-orbit coupling in epitaxial graphene via Pb intercalation — •Markus Gruschwitz[1], Sergii Sologub[1,2], Hoyeon Jeon[3], Saban Hus[3], An-Ping Li[3], and Christoph Tegenkamp[1] — [1]Institut für Physik, TU Chemnitz, Germany — [2]Institute of Physics, NAS of Ukraine, Kyiv, Ukraine — [3]CNMS, ORNL, Oak Ridge, USA

The design of noval quantum phases by combining low dimensional materials poses the next evolution step of electronics. Intercalated epitaxial graphene on SiC embodys a van-der-Waals heterostack with well defined lattice arrangement. Stabilizing monolayers of heavy elements in proximity to graphene, potentially enhances the spin-orbit interaction (SOI) in graphene. Using Pb as intercalant, we reliably decouple and neutralize graphene by minimizing the substrate influence. At the interface coexisting striped and hexagonal superstructures emerge from local strain and density variations in the Pb monolayer. [1] Multi-probe transport measurements, assisted by finite element simulations, revealed a temperature dependent resistance. This emergent behavior was attributed to a gap opening in graphene in the order of 3-5 meV. [2] Tip–sample spacing dependent spectroscopy supports this finding by a clearly reduced density of states at the Dirac point. The desired enhanced intrinsic SOI competes with Rashba-SOI and modulations of the sublattice potential by the Pb superstructure. Although the nature of this gap was not revealed yet, it has potential to stabilize a quantum spin Hall state.

[1] Adv. Mater. Interfaces 12, 21: e00617 (2025)
[2] Phys. Rev. B 109, 245430 (2024)

O 73.2 Wed 18:00 P2

Graphene-Based Coatings on Titanium Alloy for Implants — •Franziska Gladitz[1], Christof Neumann[1], Guobin Jia[2], Jonathan Plentz[2], and Andrey Turchanin[1] — [1]Friedrich-Schiller-University Jena, Institute of Physical Chemistry, Jena, Germany — [2]Leibniz-Institut of Photonic Technology (Leibniz-IPHT), Jena, Germany

Titanium alloy implants are essential for bone replacement surgeries; however, they are susceptible to infection. To improve their antimicrobial properties, we develop graphene-based coatings on the implant substrates (alloy Ti6Al4V), taking advantage of the antibacterial and biocompatible properties of graphene (G) or graphene oxide (GO). For this purpose, the titanium alloy is coated with G or GO nanosheets using different coating techniques like double self-assembly procedure and electrochemical deposition. The coatings are characterized using complementary characterization techniques including scanning electron microscopy (SEM), X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, atomic force microscopy (AFM) and optical microscopy. The morphological and chemical properties of the obtained graphene coatings are analyzed in respect to their growth conditions to elucidate influences on the quality, uniformity, and possible biofunctional performance.

O 73.3 Wed 18:00 P2

Graphene on 4H-SiC and 6H-SiC: The Influence of the SiC-Polytype onto the Local Transport Properties of Graphene — •Simeon Bode[1], Benno Harling[1], Klaus Pierz[2], Teresa Tschirner[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August-Universität Göttingen — [2]Physikalisch-Technische Bundesanstalt (PTB), Braunschweig

Studies of Graphene on silicon carbide have shown a strong dependence of the surface termination of the SiC substrate on the local transport properties. In this study, we investigate the influence of the polytype of the substrate SiC onto the local properties of Polymer Assisted Sublimation Growth (PASG) graphene. It is known that graphene on 6H-SiC displays two distinct surface terminations [1], while on 4H-SiC it is only one dominant surface termination. Here, local characterization is done by AFM and STM, while the local electronic properties are investigated by STS. Graphene on both polytypes present a similar characteristic in multibias topographies. To gain access to local transport properties, we utilized Scanning Tunneling Potentiometry (STP), which revealed two distinct sheet resistances attributed to the different surface terminations. Although PASG graphene on 4H-SiC shows only one surface termination, the spread of the sheet resistance is much larger than the difference of the two distinct sheet resistances on 6H-SiC. This work was financially supported by the DFG through the FOR5242. [1] Sinterhauf et al., Nat Commun 11, 555, 2020

O 73.4 Wed 18:00 P2

Sn intercalation of Zero-Layer Graphene — •Jan-Lucas Hornbostel, Benno Harling, and Martin Wenderoth — IV. Physikalisches Institut, Georg-August Universität Göttingen

Graphene is a 2D material with a wide range of potential applications. Our research area is the intercalation of epitaxial graphene with tin, a system that has recently shown interesting phenomena such as Mott states [1]. To achieve such systems, zero-layer graphene (ZLG) as starting point is intercalated. Tin binds to the SiC substrate transforming the ZLG into quasi-freestanding monolayer graphene. ZLG graphene can be epitaxially grown on SiC using various methods. The intercalation of Sn on polymer assisted sublimation growth (PASG) samples has shown to be strongly influenced by substrate steps [2]. In this study, we grow ZLG samples using resistive heating under UHV conditions on 6H-SiC. Compared to PASG, AFM and KPFM reveal a weakness of UHV growth for producing high quality ZLG samples, namely a generally disorder structure and depressions within the terraces. This type of defects disappears at higher temperatures. After ZLG growth and verification, Sn is deposited. We focus specifically on the influence of sample temperature (120-1000 K) during deposition. These are analyzed using AFM and KPFM. [1] Ghosal et al, Phys. Rev. B 111, 235426, 2025 [2] Harling et al, Carbon 244, 120711, 2025

O 73.5 Wed 18:00 P2

Ca-intercalation of epitaxial monolayer graphene — Luqman Mahdi Syed[1,2], Niclas Tilgner[1,2], •Philip Schädlich[1,2], and Thomas Seyller[1,2] — [1]Institut für Physik, Technische Universität Chemnitz — [2]Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Technische Universität Chemnitz

Realizing proximity-induced correlation effects, such as superconductivity, in graphene is a major challenge in the field of research on two-dimensional (2D) materials. Among the graphite intercalation compounds (GICs), the Ca-GICs exhibit the highest critical temperature with T_c=11.5 K, where the electron doping from the Ca atoms may be a crucial factor. Hence, expanding this superconducting phase into the 2D limit of epitaxial monolayer graphene (EMLG) on SiC(0001) requires precise control over the arrangement of the intercalated Ca atoms. However, several structural models have been proposed for Ca-intercalated EMLG, and in particular, the vertical position - i.e., the gallery - in which Ca resides remains unresolved (S. Ichinokura et al. 2016 ACS Nano 10 2761, J.C. Kotsakidis et al. 2020 Chem. Mater. 32 (15) 6464). Here, we investigate Ca-intercalation into EMLG grown by polymer-assisted sublimation growth. Using x-ray and angle-resolved photoemission spectroscopy, we monitor the intercalation process and quantify the doping level. Our results indicate the saturation of the SiC interface by Ca. We observe the low-energy bands of the resulting intercalated bilayer graphene, and more interstingly regarding the superconducting state, a highly doped graphene π-band, which may point towards the presence of calcium in the upper gallery.

O 73.6 Wed 18:00 P2

Porphyrin derivatives on Graphene/Cu(111) — •Asma Khizar, Christophe Nacci, and Leonhard Grill — Department of Physical Chemistry, University of Graz, Heinrichstrasse 28, 8010 Graz, Austria

Molecules as well as their assemblies and reactions have been widely investigated on single-crystal metal samples, which represent a highly defined flat support for efficient diffusion and high-resolution imaging by scanning probe microscopy (STM). However, the interaction between the metal and the molecule can alter the intrinsic properties of the molecules, making a decoupling layer essential to understand the pristine molecular properties. Graphene, with its two-dimensional structure and weak interaction with adsorbates, serves as an excellent decoupling layer for molecules. On epitaxial graphene, the reduced molecule-metal interaction allows molecules to retain their intrinsic electronic features while still sensing the underlying metal, which influences adsorption energy and selective interactions. In this study, we use Cu(111) as a substrate for

graphene growth, due to its cleanliness and minimal lattice mismatch. Our focus is on chemical reactions of porphyrin derivatives on the graphene layer, thus at a distance from the copper catalyst. Various stimuli are used to controllably dissociate side groups from the molecules and induce covalent coupling to get better insight into the chemical reactions.

O 74: Graphene: Electronic structure, excitations, etc. – Poster (joint session O/TT)

Time: Wednesday 18:00–20:00 Location: P2

O 74.1 Wed 18:00 P2

Strong-Field Bloch Electron Interferometry for Band-Structure Retrieval — •Tamara Pröbster, Tobias Weitz, Christian Heide, and Peter Hommelhoff — Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Physik, Staudtstr. 1, 91058 Erlangen

Strong optical fields drive electrons in solids far from equilibrium, enabling access to ultrafast quantum dynamics that directly reflect the underlying band structure. When Bloch electrons in graphene are exposed to an intense few-cycle laser field, they undergo coherent intraband motion during which they accumulate a quantum phase determined by the local band curvature. If this laser-driven trajectory encounters an avoided crossing between the valence and conduction bands, the electron wave packet can coherently split via a Landau-Zener transition. In our work, we exploit pairs of such transitions to realize strong-field Bloch electron interferometry, forming an interferometric sequence fully embedded in the electronic band structure. The resulting interference encodes band information in the phase-dependent photocurrent. We retrieve the Fermi velocity of graphene near the K points as 1.07 ± 0.04 nm·fs^{-1}, in excellent agreement with theoretical expectations. Our results establish strong-field Bloch electron interferometry as a general and versatile approach for band-structure reconstruction under ambient conditions. Because the method relies solely on ultrafast optical driving and detection, it is naturally suited for tracking light-induced modifications of electronic structure with femtosecond temporal resolution.

O 74.2 Wed 18:00 P2

Folding the electronic band structure of graphene-Bi and graphene-Pb heterobilayers — •Johanna Schurr, Alexander Korn, Andres Unigarro, Sibylle Gemming, and Nebahat Bulut — Institute of Physics, TU Chemnitz, Germany

Translational and rotational degrees of freedom in 2D material stacks open up a wealth of tunable materials properties, such as electrical conductivity, magnetism, or optical properties, in particular if heavy intercalant atoms are present. In this study, the band structure of the two hexagonal hetero-bilayer systems bismuthene-graphene and plumbene-graphene were investigated, because experiment gives evidence for a large number of structural varieties especially for plumbene.

The aim was to identify and characterise the influence of bismuthene and plumbene layers on the band structure of graphene. For this purpose a code was generated to correlate the k-path of the band structures calculated for supercells and primitive cells within their respective Brillouin zones. Subsequent folding back of the bands into the first Brillouin zone of the supercell, while maintaining the information of the original k-path in the primitive cell, provided an overview of all existing bands and the origin of their Brillouin zone.

O 74.3 Wed 18:00 P2

A tool for folding and unfolding of electronic band structures applying it to graphene and the gold(111)-surface — •Alexander Korn, Nebahat Bulut, and Sibylle Gemming — Institute of Physics, TU Chemnitz, Germany

The electronic band structure is an important property of materials. For comparison with experiments and other studies, as well as for better readability, it is useful to display and analyse the band structure of the primitive cell rather than a supercell. Studying more complex materials with dopants or adatoms is only possible using a supercell instead. Therefore, one must unfold the band structure of the supercell into the primitive cell.

For this purpose, we offer a tool for abinit (www.abinit.org) that can be used to unfold all possible supercells. The unit vectors of the supercell can be stretched and also rotated relative to the unit vectors of the primitive cell. We also offer an additional qualitative tool for band folding that also tracks the origin of the Brillouin zone of each band at each k-point. We provide a practical example of folding and unfolding using the gold(111) surface with sulfur as an adatom.

O 74.4 Wed 18:00 P2

Enhanced Screening in Indium Intercalated Graphene Enabled by 2D Nearly Free Electron States — •Lukas Gehrig[1,2], Cedric Schmitt[1,2], Kilian Strauss[1,2], Jonas Erhardt[1,2], Stefan Enzner[2,3], Martin Kamp[1,4], Timur Kim[5], Giorgio Sangiovanni[2,3], Jörg Schäfer[1,2], Simon Moser[6], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Universität Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [4]Röntgen Center for Complex Material Systems, Würzburg, Germany — [5]Diamond Light Source, Harwell Science and Innovation Campus, Didcot, United Kingdom — [6]Experimentalphysik IV - AG Oberflächen, Ruhr-Universität Bochum, Germany

Intercalation of epitaxial graphene on SiC has been intensively explored to modify graphene's electronic properties, but previous intercalants provide only weak screening, leading to pronounced electron-plasmon coupling and the appearance of plasmaron bands in ARPES [1]. Here, we demonstrate that intercalated bilayer indium exhibits strongly Rashba-split bands, which acquire nearly free-electron-like character at the Fermi level. This induces exceptionally strong screening in graphene, significantly reducing many-body renormalization effects in the graphene bands, which arise from plasmaron coupling. This approach opens new opportunities to explore and control many-body interactions in graphene-based heterostructures.

[1] Bostwick A et al., Nat. Phys. 3, 36-40 (2007)

O 74.5 Wed 18:00 P2

Terbium intercalation as a route to n-doping of graphene past the van Hove singularity — •Bharti Matta[1], Philipp Rosenzweig[1], Craig Polley[2], Kathrin Küster[1], and Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]MAX IV Laboratory, Lund, Sweden

Exotic ground states driven by many-body interactions, such as unconventional chiral superconductivity and spin-density waves, were theoretically predicted more than a decade ago for heavily n-doped graphene near the van Hove singularity (VHS). In recent years, achieving such high doping levels in epitaxial graphene on SiC via intercalation has attracted considerable interest. Intercalation of rare-earth elements such as Gd, Yb, and Er has already proven promising in reaching these regimes. Here, we demonstrate that intercalation of Tb atoms at the graphene/SiC interface provides access to extreme n-doping levels beyond the π^* VHS, without requiring any adsorbates on the graphene surface. The extended VHS is shifted by 0.07 eV below the Fermi level (E_F) as seen in angle-resolved photoemission spectroscopy. From the area enclosed by the giant hole pocket around Γ, we extract an electron density of $\approx 5{\times}10^{14}$ cm^{-2}. Strong renormalization of the graphene bands leads to a Dirac point about 1.55 eV below E_F, indicating that the doping cannot be described by a rigid single-particle band shift. Based on these experimental parameters, theoretical calculations predict the emergence of topological superconductivity with a critical temperature up to 600 mK (S. A. Herrera *et al.*, *ACS Nano 18* (51), 34842–34857 (2024)).

O 74.6 Wed 18:00 P2

Vanishing Fermi velocity in Periodically Strained Graphene — •Leo-Malik Benneka[1], Taher Rhouma[2], Guy Trambly de Laissardière[2], Clemens Winkelmann[1], Mark Zelsmann[3], and Vincent Renard[1] — [1]Université Grenoble Alpes, CEA-IRIG-PHELIQS, 38000 Grenoble, France — [2]CNRS-LPTM, CY Cergy Paris Université, 95302 Cergy-Pontoise, France — [3]CNRS-LTM, 38000 Grenoble, France

Intense research has been made in engineering flat bands in twisted bilayer graphene, leading to various correlated phases [1]. An alternative route to realizing similar flat bands involves a monolayer graphene strained by a periodic triangular superlattice induced by a corrugated substrate. The height modulation h and the superlattice periodicity L serve as tuning parameters for controlling band flattening and the Fermi velocity v_F near the Dirac cones [2, 3]. Tight-binding calculations were performed by explicitly accounting for relative rotations between the graphene lattice and the superlattice, as would occur in an experimental device. These calculations not only reproduce the known decrease of the Fermi velocity with increasing h [4], but also reveal a renormalization of v_F that depends on the specific ratio $\sqrt{a_C C\ L}/h$ and on the relative lattice orientation. Remarkably, this behavior is universal for any superlattice size L. These predictions may assist in the design of experimental devices aimed at engineering flat bands. [1] Cao et al., Nature, 556 (2018) 43-50 ; [2] Mao et al., Nature, 7820 (2020) 215-220 ; [3] Yuan et al., Phys. Rev. B, 24 (2024) 245408 ; [4] S. P. Milovanović et al., Phys. Rev. B, 24 (2020) 245427.

O 74.7 Wed 18:00 P2

Optimizing the excitation cross section for graphene phonons in inelastic electron tunnelling via intercalation. — Karl Rothe[1], •Nicolas Néel[1], Mads Brandbyge[2], and Jörg Kröger[1] — [1]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany — [2]Center of Nanostructured Graphene, Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

Platinum-intercalated graphene on a (111)-oriented iridium surface gives rise to a variety of rotational domains, which exhibit characteristic moiré patterns. Independent of the twist angle subtended by the graphene and substrate lattice, inelastic electron tunnelling spectroscopy reveals elevated graphene phonon excitation only on the intercalated phases. Combining spatially resolved spectroscopy of the electronic structure with non-equilibrium Green's function simulations highlights the relevance for effective phonon creation of the balance between elastic and inelastic electron transport. The intercalation-induced shift of electron density of states from the Brillouin zone centre to its boundary enhances the inelastic channel at the expense of the elastic channel and thereby increases the phonon excitation cross section. Financial support by the Deutsche Forschungsgemeinschaft through KR 2912/18-1 is acknowledged.

O 74.8 Wed 18:00 P2

Se-intercalation of graphene on SiC(0001) — •Susanne Wolff[1,2] and Thomas Seyller[1,2] — [1]Institut für Physik, Technische Universität Chemnitz — [2]Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Technische Universität Chemnitz

The epitaxial growth of graphene on SiC in an argon atmosphere is a well-established method to produce homogeneous, high quality carbon layers. The first-grown carbon layer exhibits a $\left(6\sqrt{3}\times 6\sqrt{3}\right)R30^{\circ}$ periodicity and is partially covalently bound to the SiC substrate. Therefore, this so-called buffer layer lacks the typical electronic properties of graphene. One pathway to decouple the buffer layer from the substrate and obtain graphene-like electronic properties is intercalation, which involves introducing a certain element at the buffer layer/SiC interface. Furthermore, the choice of intercalant influences the electronic properties of the decoupled graphene.

In this study, we investigated the intercalation of a buffer layer with selenium (Se). This process was carried out in a two-zone tube furnace, with the selenium precursor $SnSe_2$ and the buffer layer positioned in different temperature zones. The samples were characterized using X-ray photoelectron spectroscopy (XPS) and angle-resolved photoelectron spectroscopy (ARPES). XPS revealed successful decoupling of the buffer layer with intercalated Se at the interface and not-intercalated Se on the surface. ARPES measurements in the vicinity of the Dirac point of graphene showed a p-type doping of the decoupled carbon layer.

O 74.9 Wed 18:00 P2

Mesoscopic Lateral Intercalation Dynamics of Indium Between the Epitaxial Zero-Layer of Graphene and SiC — •Benno Harling[1], Zamin Mamiyev[2], Narmina Balayeva[2], Dietrich R.T. Zahn[2], Christoph Tegenkamp[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August-Universität, Friedrich-Hund-Platz 1, 37077, Göttingen, Germany — [2]Institut für Physik, Technische Universität Chemnitz, Reichenhainer Str. 70, 09126, Chemnitz, Germany

Intercalation, the process of diffusing a material species in-between layered materials, can be utilized for both bulk and 2D systems to achieve tailored electronic properties. [1] For the 2D limit, this work investigates the lateral diffusion dynamics of indium intercalation into the epitaxial zero-layer of graphene on SiC using Kelvin Probe Force Microscopy (KPFM). For tin, material transfer across surface substrate steps is observed at local sites at the mesoscopic scale. [2] With the used experimental parameters, we find that this is not the case for indium intercalation. Instead, only terrace transport is observed. The KPFM measurements were complemented by micro-Raman spectroscopy, assessing the extent and uniformity of In intercalation. Remarkably, intercalation through the carbon layer seems to be dependent on the graphene or substrate properties that still need to be further resolved. This leads to a situation where just some of the terraces are observed to be intercalated. Financial support by the DFG within Research Unit FOR5242 is acknowledged. [1] Stark et al., Adv. Mater. 2019, 31, 1808213 [2] Harling et al., Carbon 244 (2025) 120711

O 75: Topical Talk Bibes (joint session O/TT)

Time: Thursday 9:30–10:15 Location: TRE/PHYS

Topical Talk O 75.1 Thu 9:30 TRE/PHYS

Oxide interfaces as platforms for emergent quantum phenomena — •Manuel Bibes — Laboratoire Albert Fert, CNRS, Thales, U. Paris-Saclay, Palaiseau (France)

Oxide surfaces and heterointerfaces host electronic phases that emerge from the combined effects of broken inversion symmetry, orbital reconstruction, and electrostatic boundary conditions. In this overview, I will discuss how two-dimensional electron gases (2DEGs) formed at oxide surfaces and interfaces give rise to large and tunable spin-orbit interactions, interfacial magnetism, and ferroic control of transport properties.

The focus will be on Rashba-type spin-orbit coupling in oxide 2DEGs and its interplay with ferromagnetism and ferroelectricity, leading to effects such as electrically tunable Anomalous Hall effect, spin and orbital Edelstein effects, and spontaneous non-reciprocal charge transport. Angle-resolved photoemission spectroscopy (ARPES) and X-ray photoelectron spectroscopy (XPS) play a central role in elucidating the electronic structure, orbital character, and electrostatic landscape underlying these phenomena, and in establishing clear links between interface chemistry, symmetry breaking, and transport behavior.

Finally, I will discuss how these engineering 2DEGs enables new routes toward low-power spin-orbitronic and ferroelectric device concepts compatible with silicon technology. The talk will highlight open challenges and opportunities at the interface between surface science, correlated electron physics, and oxide electronics.

O 76: Electronic structure of surfaces: Spectroscopy, surface states II

Time: Thursday 10:30–12:15 Location: HSZ/0201

O 76.1 Thu 10:30 HSZ/0201

Angle-resolved photoemission spectroscopy study on AgTe/Ag/Au(111) heterostructures. — •Muthu P. T. Masilamani, Sophia Munne, Begmuhammet Geldiyev, Maximilian Ünzelmann, and Friedrich Reinert — Experimental Physics VII and Würzburg-Dresden Cluster of Excellence ctd.qmat, Universität Würzburg, Germany

We report a comprehensive angle-resolved photoemission spectroscopy (ARPES) study on the electronic band structure of AgTe/Ag/Au(111) heterostructures. We systematically explore the interplay between Rashba-like spin-split surface states (SS) of AgTe [1] and quantum well states (QWS) of Ag/Au(111) [2] by epitaxially varying the Te coverage and the Ag spacer-layer thickness. This allows us to address the influence of epitaxial composition on the electronic structure. Our measurements reveal decoupling of the Rashba-like SS and QWS, with no observable hybridisation, attributed to their distinct orbital symmetries. Furthermore, we investigate the emergence of moiré reconstruction in the AgTe/Ag/Au(111) heterosystem.

[1] Ünzelmann, M. et al. PRL. 124, 176401 (2020)
[2] Forster, F. et al. PRB. 84, 075412 (2011)

O 76.2 Thu 10:45 HSZ/0201

One-step investigation of the electronic tapestry of 2H-WSe2 — •Ridha Eddhib[1], Samuel Beaulieu[2], Aki Pulkkinen[1], and Jan Minar[1] — [1]New Technologies Research Centre, University of West Bohemia, 301 00 Pilsen, Czechia — [2]Université de Bordeaux-CNRS-CEA, CELIA, UMR5107, F33405 Talence, France.

Angle-resolved photoemission spectroscopy (ARPES) is a powerful tool for unraveling the electronic band structure of crystalline solids. However, the intricate and multifaceted electronic structures of complex materials often require complementary measurement strategies and careful experimental design. In our research, we employed the one-step model of photoemission, as implemented in the SPRKKR code[1], supported by experimental studies. We combined circular dichroism in photoelectron angular distributions (CDAD) with the layer-dependent symmetry properties of 2H-WSe2, which enables a time-reversal operation (TRCDAD)[2]. This approach quantifies the modulation of photoemission intensity across a wide energy range, providing detailed insight into the material's fine electronic structure while suppressing extrinsic contributions to the photoemission cross section to some extent. We present the monolayer, bilayer, and trilayer contributions to the photocurrent alongside the bulk response, while accounting for final-state effects using both time-reversed low-energy electron diffraction and a free-electron-gas final-state. [1]Ebert, H., Koedderitzsch, D., & Minar, J. (2011). Reports on Progress in Physics, 74(9), 096501. [2]Beaulieu, S., Schusser, ... & Ernstorfer, R. (2020). Physical Review Letters, 125(21), 216404.

O 76.3 Thu 11:00 HSZ/0201

Spin-orbital signatures and topological evolution in the $Mo_xW_{1-x}Te_2$ alloy — •Sarath Sasi[1], Aki Pulkkinen[1], Raphaël Salazar[1], Jakub Schusser[1], Laurent Nicolaï[1], Christine Ritcher[2,3], and Karol Hricovini[2,3] — [1]New Technologies Research Centre, University of West Bohemia, Pilsen, Czech Republic — [2]LPMS, CY Cergy Paris Université, Neuville-sur-Oise, France — [3]Université Paris-Saclay, CEA, CNRS, LIDYL, Gif-sur-Yvette, France

We examine how compositional disorder modifies the electronic structure of the transition-metal dichalcogenide alloy $Mo_xW_{1-x}Te_2$[1], with particular attention to the evolution of band topology and the persistence of Type-II Weyl features. Using high-resolution spin-polarized ARPES and circular-dichroism ARPES provides complementary insights into the spin and orbital character of the electronic states. These measurements give insight into its intrinsic spin-orbital properties compared to WTe_2[2], and for identifying how alloying is affecting its properties, like Berry curvature. Together with fully relativistic one-step photoemission calculations within the SPR-KKR[3] framework, we yield a detailed picture of how alloying tunes the electronic structure and topological responses in this family of quantum materials.

[1] Belopolski, I., Sanchez, D., Ishida, Y., et al. Nat. Commun. 7, 13643 (2016).

[2] Heider, T., Bihlmayer, G., Schusser, J., et al. Phys. Rev. Lett. 130, 146401 (2023).

[3] Braun, J., Minar, J., Ebert, H. Physics Reports, 740 (2018).

O 76.4 Thu 11:15 HSZ/0201

electronic properties observation of kagome lattice Nb3X8 by angle-resolved photoemission spectroscopy — •Xiaojing Liu[1], Antonija Grubisic-cabo[1], Joost aretz Aretz[2], Sergii Grytsiuk[2], Marco Bianchi[3], Malte Rosner[2,4], Mazhar Ali[5], Philip Hofmann[3], Zhiying Dan[1], Giovanna Feraco[1], Chrystalla Knekna[1,6], Muhammad Waseem[1], and Mikhail Katsnelson[2,7] — [1]University of Groningen, Groningen, The Netherlands — [2]Radboud University, Nijmegen, The Netherlands — [3]Aarhus University, Aarhus, Denmark — [4]Bielefeld University, Bielefeld, Germany — [5]Delft University of Technology, Delft, the Netherlands — [6]University of Amsterdam, Amsterdam, The Netherlands — [7]Constructor University, Bremen, Germany

The Nb3X8 family (X=Cl, Br, I) is a novel group of breathing kagome materials. Despite interest in these materials, their electronic properties are still unclear and are likely to differ among the family members. For instance, they could exhibit characteristics of either a strongly correlated Mott insulator or a weakly correlated obstructed atomic insulator. Moreover, the kagome lattice can naturally host flat bands, which give rise to exotic properties such as spin-liquids and high-temperature superconductivity. Here, I will present our recent experimental investigation of the band structure in bulk Nb3X8 kagome materials by means of angle-resolved photoemission spectroscopy (ARPES). With ARPES we directly image the flat bands in the Nb3X8 systems, and are able to verify their strong correlation character with the support of theoretical calculations.

O 76.5 Thu 11:30 HSZ/0201

Studying the polar surfaces of MAX and MAB phases using μ-ARPES — •Gesa Siemann[1], Gianmarco Gatti[1], Amalie Svaneborg[5], Wu Bing[4], Anders S. Mortensen[1], Charlotte Sanders[2], Naina Kushwaha[2,6], Jenny Rigden[2], Yu Zhang[2], Matthew D. Watson[3], Kristian Thygesen[5], Zdeněk Sofer[4], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Aarhus University, DK — [2]Central Laser Facility, Harwell, UK — [3]Diamond Light Source, UK — [4]University of Chemistry and Technology Prague, CZE — [5]Department of Physics, Technical University of Denmark, Lyngby, DK — [6]School of Physics and Astronomy, St Andrews University, UK

Natural heterostructures with interlayer charge transfer in the bulk can exhibit distinctive surface effects when this transfer is interrupted, such as Rashba splitting and itinerant ferromagnetism, both absent in the bulk. These layered systems therefore provide a platform to study how charge redistribution and symmetry breaking shape the emerging surface electronic structure. Here, we introduce MAX and MAB phases as a promising material family to host similar effects due to their alternating MX and A layers. After cleaving the samples, we used photoemission experiments with a micrometer-scale light spot (μ-ARPES), allowing us to reliably distinguish different surface terminations and their electronic structures. This work furthermore explores how covalency and metallicity govern charge transfer, and thus the surface electronic properties, in layered compounds.

O 76.6 Thu 11:45 HSZ/0201

Spin-resolved momentum microscopy of BiX_2 surface alloys on Cu(111) and Ag(111) using a 2D imaging spin-filter — •Fabian Göhler, Stefanie Suzanne Brinkman, Xin Liang Tan, Anders Christian Mathisen, Chul-Hee Min, and Hendrik Bentmann — Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, 7491 Trondheim, Norway

Despite the rapid development of angle-resolved photoelectron spectroscopy (ARPES), measurements of the electron spin over wide regions in momentum space remain challenging with single-channel spin detectors. In this contribution, we present spin-resolved ARPES measurements from a momentum microscope, which gives the photoelectron momentum distribution over the full half-sphere above the sample surface. When combined with a 2D imaging spin filter [1], this allows parallel measurement of the in-plane spin polarization for full constant energy cuts $E(k_x, k_y)$. We acquired data on BiX_2/X(111) surface alloys - formed by 1/3 monolayer of Bi atoms arranged in a $(\sqrt{3}\times\sqrt{3})R30^\circ$ periodicity on Cu(111) or Ag(111) - which are well established model systems for spin-orbit effects and (spin-dependent) photoemission from surfaces [2-4]. Using linearly polarized ($h\nu$ = 6.0 eV) and unpolarized ($h\nu$ = 21.2 eV) light sources, we probe the spin polarization in these systems for varying experimental conditions.

[1] C. Tusche et al., Ultramicroscopy 159, 520 (2015)

[2] R. Noguchi et al., Phys. Rev. B 95, 041111 (2017)

[3] H. Bentmann et al., Phys. Rev. Lett. 119, 106401 (2017)

[4] A. Winkelmann et al., New J. Phys. 14, 083027 (2012)

O 76.7 Thu 12:00 HSZ/0201

Distinguishing bulk vs surface states from designed cleaving planes in ruthenium dioxide with ARPES — •Maria Visscher[1,2], Lea Richter[1], Sebastian Buchberger[2], Shu Mo[2], Bruno Saika[2], Mats Leandersson[3], Craig Polley[3], Andrew Mackenzie[1,2], and Phil King[2] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]University of St Andrews, St Andrews, UK — [3]Max IV, Lund, Sweden

Ruthenium dioxide has a rich band structure, giving rise to phenomena like superconductivity under strain and hosting a Dirac nodal line network. Recent studies also found that the material hosts flat band surface states and unusual spin-polarisations. These phenomena motivate the need for more detailed studies into its electronic structure. ARPES would be an ideal probe for this, and there have been several pioneering studies to date. However, the material's strongly three-dimensional structure makes these experiments challenging because of difficulties both in preparing the required atomically flat and clean surfaces, and in disentangling bulk from surface states in the electronic structure. Here, we exploit a fabrication method based on Focused Ion Beam (FIB) structuring to stimulate cleaving along desired crystallographic planes. With this method, we obtained high quality surfaces in two distinct orientations, allowing high-resolution ARPES experiments. From this, and supporting density-functional calculations, we identify a rich hierarchy of bulk and surface states in this system and uncover a strong influence of structural relaxations and surface stoichiometry on the electronic states that form.

O 77: Nanostructures at surfaces:1D, 2D, networks II

Time: Thursday 10:30–12:15 Location: HSZ/0204

O 77.1 Thu 10:30 HSZ/0204

Interplay of flexibility, coverage, and host-guest interaction in the self-assembly of Tris(4-carboxyphenyl)amine (TCA) on Au(111) — Vishakya Jayalatharachchi[1], •Paul Philip Schmidt[1], Roberto Robles[2], Nicolas Lorente[2], Meike Stöhr[1,3], and Sabine Maier[1] — [1]Department Physik, FAU Erlangen-Nürnberg, Erlangen, Germany — [2]CFM/MPC (CSIC-UPV/EHU), Donostia-San Sebastián, Spain — [3]University of Applied Sciences of the Grisons, Switzerland

Triphenylamine derivatives are attractive building blocks for molecular architectures owing to their strong electron-donating properties, structural versatility, and ability to form highly ordered structures. Here, we explore how the non-planar and conformationally flexible arms of the unbridged threefold-symmetric TCA influence its self-assembly on Au(111), with particular emphasis on the formation and stability of porous networks. Using a combination of STM, LEED, and DFT, we show that RT deposition of TCA on Au(111) produces a coexistence of hexagonal porous domains and close-packed structures. Upon subsequent annealing, well-ordered porous networks emerge, stabilized by the dimeric carboxylic acid bonding motif. At higher coverage, this motif persists but instead directs the formation of close-packed assemblies. These findings provide insights into the interplay between molecular flexibility, intermolecular interactions, and coverage in directing supramolecular architectures of unbridged triphenylamines on metal surfaces. In addition, we show on the example of molecular rotors the hosting properties of the porous TCA network.

O 77.2 Thu 10:45 HSZ/0204

Revealing and manipulating correlated protons in one-dimensional hydrogen-bonded chains at the atomic scale — •Yiqi Zhang — Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

Hydrogen-bonded systems such as water and ice exemplify highly cooperative proton dynamics, where covalent bonds are broken and formed in a concerted fashion. Yet directly probing and controlling many-body proton configurations at the atomic scale remains challenging. Here, using bond-resolved atomic force microscopy and spectroscopy, we reveal multistate proton ordering in self-assembled one-dimensional chains of an imidazole derivative on a noble metal surface. In as-grown chains of varying length, we consistently identify an interior species bonded to an extra proton, forming a localized imidazolium cation (state 1). Selective removal of a single proton from either chain end triggers a collective rearrangement of protons, yielding unidirectional hydrogen-bonding along the entire chain (states 2 or 3). Further deprotonation creates a proton vacancy, enabling reversible switching of hydrogen-bonding directionality (states 4 and 5) via collective proton hopping above a threshold bias voltage. In conjunction with density functional theory calculations, we elucidate the microscopic origin of complex proton ordering in hydrogen-bonded chains and the correlated motion of multiple protons.

O 77.3 Thu 11:00 HSZ/0204

On-Surface Synthesis of a Janus Polyazaacene — •Faming Kang, Tim Naumann, Zilin Ruan, Ye Liu, and J. Michael Gottfried — Fachbereich Chemie, Philipps-Universität Marburg, Hans-Meerwein-Str. 4, 35032 Marburg, Germany

Acenes are a fascinating class of polycyclic aromatic hydrocarbons that have gained considerable research interest due to their potential application in organic electronics as well as their role in advancing fundamental knowledge about conjugated aromatic systems. Isosteric exchange of CH units of the acenes by nitrogen atoms formally gives azaacenes. The nitrogen substitution pattern, i.e., the number, position, and type of nitrogen atoms enables topological design of azaacenes, which facilitates precise tuning of frontier orbital energy level alignment and radical characters. Guided by topological considerations, introducing distinct edge structures on either side further creates Janus azaacenes. Here, we successfully synthesized a Janus polyazaacene on the Au(111) surface, in which one edge was decorated by nitrogen atoms while the other edge keeping unchanged. The length of such a polymer chain can reach up to 50 rings. Using scanning tunneling microscopy, we characterized its geometric structure and electronic property on Au(111), as well as its stability in air.

O 77.4 Thu 11:15 HSZ/0204

Modeling the Registry of Molecular Adsorbates on Solid Surfaces — •David Ari Hofmeister[1], Christian Erik Selzer[2], Laura zur Horst[1], Simon Christian Rickert[1], Julia Kohn[2], Andreas Hansen[2], Stefan-Sven Jester[1], and Sigurd Höger[1] — [1]Kekulé-Institut für Organische Chemie und Biochemie, Rheinische Friedrich-Wilhelms-Universität Bonn, Bonn (Germany) — [2]Mulliken Center for Theoretical Chemistry, Rheinische Friedrich-Wilhelms-Universität Bonn, Bonn (Germany)

Rationalizing the adsorption behavior of large organic molecules on crystalline substrates is crucial for the design of functional surfaces in supramolecular chemistry, catalysis, and electronics. Conventional quantum-chemical approaches often fail for large π-conjugated systems due to their size and conformational flexibility. Here, we present a physically intuitive and generalizable method that overcomes these limitations by optimizing the molecular registry through a geometry-based strategy: maximizing the overlap between surface-oriented hydrogen atoms ("spikes") and the periodic "pockets" defined by the hexagon centers of HOPG. Inspired by the Groszek alkane-on-graphite model, our approach extends to structurally complex architectures and assigns adsorption geometries with high resolution without costly computations. Combining registry scoring with STM data allows the determination of absolute atropisomer conformations, demonstrating that geometric registry is a broadly applicable metric for predicting the surface arrangements of large molecules.

O 77.5 Thu 11:30 HSZ/0204

Low Dimensional Assemblies of Endohedral Fullerenes on Surfaces — •Lukas Emanuel Spree[1,2], Caroline Hommel[1,2], Pierre Josse[1,2], Justyna Piwowar[1,2], Robert Ranecki[1,2], and Andreas Heinrich[1,3] — [1]IBS Center for Quantum Nanoscience, Seoul, South Korea — [2]Ewha Womans University, Seoul, Republic of Korea — [3]Department of Physics, Ewha Womans University, Seoul, Republic of Korea

Scanning probe microscopy techniques like STM and AFM facilitate the characterization of atoms and molecules on flat substrates with nearly unrivaled spatial resolution. Utilizing the strengths of these techniques, our team is looking to build custom molecular structures in a bottom-up manner and characterize their physical properties.

The main focus of this work is on endohedral fullerenes, a class of compounds that facilitate the stabilization of exotic configurations of few-atom structures within a carbon cage. Among them are some of the best single molecule magnets discovered to date, as well as promising candidates for spin-qubits. These desirable traits are combined with very high chemical stability. Utilizing the physical properties of these fascinating compounds is limited by two main issues: synthetic yield and, to a lesser degree, crystalline order. Both can be addressed elegantly by focusing on their properties in low dimensional arrangements, like monolayers or single molecules on ultraflat surfaces.

In this presentation we will detail our ongoing efforts of utilizing a broad range of deposition techniques, molecule manipulation on the surface, and chemical self-assembly approaches.

O 77.6 Thu 11:45 HSZ/0204

Electronic Modulation by the Sc3N Cluster in Endohedral Fullerene Sc3N@C80 — •Seong-Hyun Hong[1,4], Dmitriy Borodin[1,2], Lukas Spree[1,2], Andrés Pinar Solé[1,2], Caroline Hommel[1,2], Merve Ercelik[1,2], Shinjae Nam[1,2], Robert Ranecki[1,2], Fabio Donati[1,3], Se-Jong Kahng[4], and Andreas Heinrich[1,3] — [1]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS) — [2]Ewha Womans University — [3]Department of Physics, Ewha Womans University — [4]Department of Physics, Korea University

Endohedral fullerenes such as Sc3N@C80 present a unique platform to study confined molecular systems, where the behavior of an enclosed cluster can strongly influence the properties of the surrounding cage. Understanding how the Sc3N cluster interacts with the carbon framework at the submolecular level is essential, but direct observation of these interactions remains challenging due to existence of carbon cage.

Here, we combine low-temperature scanning tunneling microscopy (STM) and atomic force microscopy (AFM) with a CO-functionalized tip to investigate Sc3N@C80. Using scanning tunneling spectroscopy (STS) and Kelvin probe force microscopy (KPFM), we map the charge distribution across the fullerene with submolecular resolution, revealing how the Sc3N cluster modulates the electronic structure of the cage. This approach provides significant insight into the interplay between core position and molecular charge distribution, uncovering details of the inner cluster that were previously unclear.

O 77.7 Thu 12:00 HSZ/0204

Ferroelectric vortices in elemental Bismuth square islands — •Shasha Xue and Hao Zheng — Tsung-Dao Lee Institute, Shanghai Jiao Tong University, Shanghai, China

Ferroelectric vortices, with their unique topological polarization patterns, show great potential for next-generation electronics. Although they have been observed in compounds, their realization in single-element materials has remained elusive. Here, we experimentally prepare three-bilayer Bi(110) square-shaped islands on high-T_C superconductor ($Bi_2Sr_2CaCu_2O_{8+\delta}$) substrates by molecular beam epitaxy. Scanning tunneling microscopy/spectroscopy combined with first-principal calculations verify in-plane polarization and a ferroelectric vortex state in our islands, as well as reveals exceptional vortex stability against electric-field-driven switching. This work pioneers single-element ferroelectric vortices, advances topological ferroelectrics design and expands the understanding in related fundamental physics.

O 78: Vacuum Science & Technology: Theory and Applications I

Time: Thursday 10:30–12:15 Location: HSZ/0401

Invited Talk O 78.1 Thu 10:30 HSZ/0401

The Wendelstein 7-X plasma vessel vacuum system from a scientific perspective — •Georg Schlisio[1], Torsten Bräuer[1], Stylianos Varoutis[1], Paul McNeely[1], Dirk Hartmann[1], Chandra Prakash Dhard[1], Dirk Naujoks[1], Victoria Hak[1], and the W7-X team[2] — [1]Max-Planck-Institut für Plasmaphysik, Teilinstitut Greifswald — [2]See author list of O. Grulke et al. Nuclear Fusion, 64(11), 112002 (2024)

Wendelstein 7-X (W7-X) is the world's most advanced stellarator, a long-overlooked concept for magnetic confinement fusion. Fusion devices require excellent vacuum conditions to minimize impurity influx and charge-exchange losses during high-temperature plasma operation. The W7-X plasma vessel vacuum system comprises the main vessel, 254 vacuum ports, and several auxiliary diagnostic vacuum systems, the largest of which is the Neutral Beam Injection (NBI) system.

We describe the W7-X plasma vessel vacuum system and its instrumentation for total and partial pressure measurements. A key parameter for valve and gauge calibration, as well as for exhaust quantifi- cation, is the effective plasma-vessel volume; we outline an approach for determining this volume with sufficient pre-

cision. We also report experimentally derived pumping speeds of the turbomolecular pumps (TMPs) and cryo vacuum pumps (CVPs), which are essential inputs for modelling and exhaust analysis.

As an application of these capabilities, a recent study of gas-species transport in the sub-divertor region is shown, comparing experimental measurements with modelling results.

O 78.2 Thu 11:00 HSZ/0401

Pulsed Molecular Beam Reactive Scattering for Investigation of Surface Chemical Reactions — •Oleksandr Arsatiants, Tobias Hinke, Kevin Bertrang, and Ueli Heiz — Chair of Physical Chemistry, Technical University of Munich, Lichtenbergstr. 4, 85748 Garching, Germany

Molecular beam reactive scattering (MBRS) is a powerful technique for investigating surface reactions on defined surfaces in UHV, providing complementary results to single-cycle experiments like thermal desorption spectroscopy (TDS) [1]. Pulsed MBRS is especially promising, as it can be used to investigate surface reaction kinetics under quasi steady-state conditions [2-5]. For molecules with complex MS fragmentation patterns, however, the short time scales present a challenge due to mass switching delays. Ongoing work on automation of p-MBRS measurements for rapid mass switching will be presented.

[1] F. Zaera, Surf. Sci. Rep. 72 (2), 59-104 (2017).

[2] P. N. Brier, J. N. Fletcher and P. A. Gorry, Surf. Sci. 365 (2), 525-534 (1996).

[3] P. Bond, P. N. Brier, J. Fletcher, P. A. Gorry and M. E. Pemble, Chem. Phys. Lett. 208 (3-4), 269-275 (1993).

[4] P. Bond, P. N. Brier, J. Fletcher, W. J. Jia, H. Price and P. A. Gorry, Surf. Sci. 418 (1), 181-209 (1998).

[5] M. D. Rötzer, M. Krause, T. Hinke, K. Bertrang, F. F. Schweinberger, A. S. Crampton and U. Heiz, Phys. Chem. Chem. Phys. 26 (18), 13740-13750 (2024).

O 78.3 Thu 11:15 HSZ/0401

Advancing Ultra-Clean Deposition of Fragile Molecular Building Blocks via Electrospray-Based Controlled Ion Beam Deposition — •Andreas Walz[1,2], Annette Huettig[1,2], Michael Walz[1,2], Hartmut Schlichtung[1,2], Patrick Lawes[2], and Johannes V. Barth[2] — [1]pureions GmbH, Gilching, Germany — [2]Technical University of Munich, Physics E20, Garching, Germany

The fabrication of functional nanostructures from organic, inorganic, or biorelevant molecular building blocks regularly requires clean and gentle deposition in vacuum. Conventional approaches such as thermal evaporation (MBE, OMBE) are restricted to volatile species, while solution-based deposition techniques offer versatility but frequently suffer from impurities.

Controlled Ion Beam Deposition (CIBD) in UHV, equipped with an electrospray ionization (ESI) source overcomes these limitations by granting access to a broad class of large, reactive, and fragile species including functionalized organic molecules, graphene nanoribbons, proteins, and DNA. Efficient ion transfer and mass selection is ensured through fully digitally driven ion guides and a digital quadrupole mass filter (dQMF) with "virtually unlimited" mass range. Control over kinetic energy and dose allow for soft-landing or, when desired, reactive landing of the building blocks.

We present advances in ES-CIBD instrumentation and exemplary STM/AFM characterization of depositions. The technology provides a high degree of control during depositions, clean layers of mass selected molecules and access to otherwise low processability material.

O 78.4 Thu 11:30 HSZ/0401

Temperature-Programmed Spectroscopy: A Novel Tool for Kinetic and Mechanistic Studies for Processes on Surfaces — •Robert Bavisotto and Wilfred Tysoe — Department of Chemistry and Biochemistry, University of Wisconsin-Milwaukee, Milwaukee, WI 53211, USA

Advances in computational chemistry have facilitated the integration of theoretical calculations to complement experimental findings. However, since computational methods depend on many approximations and variables, they require careful validation, which in the case of experimental validation can be challenging or unfeasible. For example, activation barriers are often predicted using climbing nudged elastic band calculations, whose benchmarking has traditionally relied on temperature-programmed desorption, a technique inherently sensitive only to processes that produce gas-phase products. To establish a surface-selective experimental approach capable of probing kinetic processes directly on surfaces without requiring gas-phase products, a suite of innovative spectroscopic techniques is introduced. These methods, collectively referred to as temperature-programmed spectroscopy (TPS), rely on precise control of sample conditions, enabling surface spectroscopic data to be collected quasi-continuously. These novel analytical tools can be easily combined with existing spectroscopic methods, such as IR or XPS, without the need for new capital equipment. This capability enables the detection of subtle changes over short time intervals, thereby facilitating kinetic measurements of surface-based processes that were previously unverifiable.

O 78.5 Thu 11:45 HSZ/0401

Traceable outgassing rate measurements of sticky gases — •Matthias Bernien[1], Annas bin Ali[1], Janez Šetina[2], and Karl Jousten[1] — [1]Physikalisch-Technische Bundesanstalt (PTB), Berlin, Germany — [2]Inštitut za kovinske materiale in tehnologije (IMT), Ljubljana, Slovenia

In the semiconductor industry, the outgassing of components in vacuum must be well controlled. These contaminants are monitored using quadrupole mass spectrometry. However, quantitative measurements of the amount of contamination are challenging as quadrupole mass spectrometers (QMSs) inherently lack stability of their sensitivity. To provide comparability and traceability of outgassing rate measurements, processes and transfer standards must be established. PTB together with IMT and industrial partners have developed and characterized outgassing reference samples for dodecane and water. These reference samples consist of a reservoir sealed with an elastomer through which the liquids permeate into vacuum. The reference samples provide well-defined outgassing rates that are used to calibrate QMSs in situ for water and hydrocarbon contaminants. When using sticky gases like water and dodecane, a significant amount of gas molecules adsorbs on the inner surfaces of the vacuum chamber. A numerical model is utilized to simulate the dynamics of the adsorbed phase and the gas phase.

O 78.6 Thu 12:00 HSZ/0401

A dynamic analysis of the static friction in microscopic Hertzian contacts: Size effects and 2D-material assisted superlubricity — •Ahmed Uluca[1,2], Pierce Sinnott[1,2], and Graham Cross[1,2] — [1]School of Physics, Trinity College Dublin, Dublin, Ireland — [2]CRANN, Trinity College Dublin, Dublin, Ireland

Friction governs how objects start to move, yet our understanding still relies on empirical laws that vary across materials and length scales. To build a more fundamental picture, we focus on the interfacial shear strength (ISS)-a concept adapted from fracture mechanics that describes friction in terms of shear stress over the contact area.

We developed a mesoscale dynamic analysis method capable of probing contact radii from tens of nanometers to micrometers with sub-nanometer displacement and 10-nanonewton force resolution. Starting from static contact, we gradually increase lateral oscillation amplitude while tracking contact radius and laterally stuck zone radius. This enables us to monitor the transition from sticking to sliding in real time while simultaneously measuring contact radius.

Using diamond-fused silica pairs, we map ISS across pressures from tens of MPa to several GPa and compare the results with theoretical models spanning from the Peierls (lattice) stress to the upper bound of a perfectly commensurate interface. Our findings reveal a pressure and scale dependent shear strength that is consistent with the dislocation emission models, extended to include the effects of deformation mode, nanoroughness, junction growth and interfacial modification by graphene layers.

O 79: Plasmonics and nanooptics: Light-matter interaction, spectroscopy III

Time: Thursday 10:30–12:15 Location: HSZ/0403

O 79.1 Thu 10:30 HSZ/0403

Cavity control of multiferroic order in the single-layer NiI_2 — •Chongxiao Fan[1,2], Emil Viñas Boström[1], Xinle Cheng[1], Lukas Grunwald[1], Dante Kennes[2], and Angel Rubio[1,3] — [1]Max Planck Institute for the Structure and Dynamics of Matter — [2]Institute for Theory of Statistical Physics, RWTH Aachen University — [3]Initiative for Computational Catalysis, Flatiron Institute

Controlling materials in thermal equilibrium, through their interactions with quantum fluctuations of the electromagnetic field, is a promising new frontier in material engineering. Although recent experiments have demonstrated cavity effects in charge density wave, quantum Hall systems and superconducting systems, a smoking gun experiment is lacking for magnetic systems. To a large extent this comes from the focus on discontinuous phase transitions (e.g. from antiferro- to ferromagnetic), where a large light-matter coupling is required for cavity modifications to be observable. Here, we instead propose spiral magnets as a promising platform to explore cavity effects, where even a small cavity-mediated change in magnetic interactions is directly reflected in a change of the spiral wavelength. For concreteness we focus on the single-layer multiferroics NiI_2 and $NiBr_2$, with the surface phonon polaritons of the paraelectric substrate $SrTiO_3$ acting as the cavity. We show that the surface cavity suppresses the ratio J_3/J_1 of the third nearest and next nearest neighbor exchange interactions,

leading to a increase of the spiral wavelength and the eventual transition into a ferromagnetic state. Our work proposes a realistic platform to observe cavity renormalization effects in magnetic systems.

O 79.2 Thu 10:45 HSZ/0403

Compressing few-cycle optical near fields in the tip-sample junction of a scanning probe microscope — •Sam S. Nochowitz, Tom Jehle, Juanmei Duan, and Christoph Lienau — Institute of Physics, University of Oldenburg, 26129 Germany

Plasmonic nanogaps confine light to dimensions in the nanometer or even subnanometer range while simultaneously enhancing the local electromagnetic field strength. This spatial confinement of light led to dramatic advances in nanosensing (1) and tip-enhanced Raman Spectroscopy. So far, the time dynamics of the fields emitted from such nanocavities have achieved little attention. Here, we introduce a broadband interferometric scattering-type SNOM technique to reconstruct amplitude and phase of light scattered from a sharp gold taper acting as a near-field probe. We isolate the near-field that is scattered from the apex and quantitatively measure its time structure (2). The apex field decays within 6 fs, a decay time mainly given by the radiative damping of the apex mode. Upon approaching the tip to a gold surface, the coupling of the apex field to its image dipole results in 2-fold reduction in the decay time to less than 2.7 fs, caused by phase shifts in the apex response, predicted in FDTD simulations (3). Our results pave the way towards linear and nonlinear ultrafast oscilloscopy with nm/fs resolution. (1) R. J. Chikkardy et al., Nature 535, 127 (2016); (2) T. Jehle, submitted (2025). (3) S. Thomas et al. New J. Phys. 17 (2015).

O 79.3 Thu 11:00 HSZ/0403

Symmetry Guidelines of Vacuum Cavity Material Engineering — •Jingkai Quan[1], Chongxiao Fan[1], Benshu Fan[1], I-Te Lu[1], and Angel Rubio[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761, Hamburg, Germany — [2]Center for Computational Quantum Physics, Flatiron Institute, Simons Foundation, New York City, New York, 10010, USA

Cavity material engineering, which manipulates material properties by exploiting vacuum-fluctuating photon modes in dark cavities, is a rapidly advancing field. Despite significant progress, most studies focus on isolated combinations of materials and cavity modes. In this study, based on a comprehensive group theory analysis, we develop a general framework for cavity material engineering with linearly polarized vacuum photon modes. We analyze the symmetry of the effective photon-free Hamiltonian inside dark cavities and establish a complete symmetry-breaking characterization induced by cavity photon modes across all 32 crystalline point groups. Building on this analysis, we predict phenomena such as the degeneracy lifting and emergence of new infrared and Raman spectral features induced by cavity modes. More intriguingly, we reveal a previously overlooked effect: cavity-induced polarization in non-polar crystals, and derive the corresponding tensor forms. These predictions are validated through advanced quantum-electrodynamical density-functional theory (QEDFT) calculations. Our work uncovers the fundamental symmetry principles governing light-matter interactions in the dark cavity and provides a systematic roadmap for future researches in cavity material engineering.

O 79.4 Thu 11:15 HSZ/0403

Low temperature near-field fingerprint spectroscopy of 2D electron systems in oxide heterostructures and beyond — Julian Barnett[1], Konstantin Wirth[1], Richard Hentrich[2], Yasin C. Durmaz[2], Felix Gunkel[3], Marc-Andre Rose[3], and •Thomas Taubner[1] — [1]I. Institute of Physics (IA), RWTH Aachen University — [2]Attocube Systems AG, Munich — [3]PGI-7, Forschungszentrum Jülich

Scattering-type scanning near-field optical microscopy (s-SNOM) is a useful tool for the non-destructive investigation of buried confined electron systems with nanoscale resolution, however, a clear separation of carrier concentration and mobility was often not possible. Here, we predict a characteristic fingerprint response of the LaAlO3/SrTiO3 2DEG in the mid-infrared spectral range, which was not experimentally accessible in the past, and verify this using a state-of-the-art tunable narrow-band laser in cryo-s-SNOM at 8 K [1]. Our modeling allows us to separate the influence of carrier concentration and mobility on fingerprint spectra and to characterize 2DEG inhomogeneities on the nanoscale. We show that our fingerprint spectra are a universal feature and generally applicable to confined electron systems, like topological insulators or stacked van-der-Waals materials.

[1] J. Barnett et al., Nat. Comm. 16, 4417 (2025).

O 79.5 Thu 11:30 HSZ/0403

Tunable skyrmion, meron, and skyrmion bag topologies in surface phonon polariton lattices — •Julian Schwab[1], Florian Mangold[1], Bettina Frank[1], Timothy J. Davis[1,2], and Harald Giessen[1] — [1]4th Physics Institute, Research Center SCoPE, and Integrated Quantum Science and Technology Center, University of Stuttgart, Germany — [2]School of Physics, University of Melbourne; Parkville Victoria 3010, Australia

Surface phonon polaritons (SPhPs) enable nanoscale manipulation of mid-infrared light via deeply subwavelength topological vector textures, such as skyrmions. Achieving dynamic, real-time control over these topological features remains challenging. Here, we theoretically propose and numerically demonstrate an actively tunable platform on a silicon carbide membrane that creates diverse topological lattices, including skyrmions, merons, and skyrmion bags. By exploiting the sublinear SPhP dispersion, we dynamically adjust the excitation wavelength to tune the topological character of the lattices. This allows for the tunability between bubble-type and Néel-type configurations in the electric field and the spin angular momentum. Furthermore, we identify a novel singularity-type meron arising from the interplay of electric and magnetic spin components. This texture exhibits topological charge conservation in moiré superlattices and a spatially confined spin reversal with tunable lateral sizes as low as $\lambda_{SPhP}/29$. These findings provide a versatile framework for on-chip, reconfigurable topological photonic devices with potential applications in high-resolution imaging and precision metrology.

O 79.6 Thu 11:45 HSZ/0403

Raman Studies of Proximity Effects in Epitaxial Graphene: Emphasis on Strong Light-Matter Coupling — •Zamin Mamiyev, Narmina O.Balayeva, Dietrich R.T. Zahn, and Christoph Tegenkamp — Institut für Physik, Technische Universität Chemnitz

Proximity engineering provides a route to tailor the electronic and vibrational properties of epitaxial graphene without introducing structural disorder. Because phonons and electronic states in graphene are strongly coupled, Raman spectroscopy provides a reliable approach to studying the quasiparticle dynamics and their modification in graphene.

In this work, we investigate how Sn and In intercalation, their nanoscale distributions, and the resulting interfacial reconstructions modify the phonon dynamics of quasi-free monolayer graphene on SiC(0001), particularly focusing on the plasmonically enhanced light-matter interaction regimes, such as in surface- (SERS) and tip- (TERS) enhanced Raman spectroscopies. Using resonance μ-Raman and TERS, we map the charge doping, electron-phonon coupling, and anharmonicities with high spectral and spatial resolution. Combined with electron diffraction, scanning tunneling microscopy (STM), and atomic force microscopy (AFM), our measurements allow us to study the optical fingerprints of strain, charge transfer, and symmetry-breaking that originate from distinct metal-intercalated interfaces and confined 2D metallic layers [1-2]. [1] Z. Mamiyev et.al., Adv. Optical. Mat. e00979 (2025); [2] Z. Mamiyev et.al., Carbon 234, 120002 (2025)

O 79.7 Thu 12:00 HSZ/0403

Inelastic electron-light interaction probed by holographic scanning transmission electron microscopy — •Tim Dauwe[1,2], Nora Bach[1,2], Murat Sivis[1,2], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Germany

Ultrafast Transmission Electron Microscopy (UTEM) is a unique tool to study inelastic electron-light scattering (IELS). Photon-Induced Near-Field Electron Microscopy (PINEM) can now routinely image optical fields at laser-excited nanostructures in magnitude. Phase-resolved imaging is enabled by sequential interactions [1,2]. However, this requires an elaborate geometry with multiple optical interaction stages and offers only limited variability in tailoring the interaction. In this work, we combine IELS with a STEM holography approach, using two spatially separated, coherent electron probes [3]. By recording the interference pattern in the far field behind an electron spectrometer, we get simultaneous access to the energy of the electrons and the phase imprinted during the inelastic interaction. Our results from two interfering quantum walks reveal exotic electron states governed by interaction strengths and relative phase differences. Our approach further enhances the UTEM near field imaging capabilites and enables tailoring of electron states by multiple parallel electron-light interactions.

[1] D. Nabben et al., Nature 619 (2023)
[2] J.H. Gaida et al., Nat. Photon. 18 (2024)
[3] F.S. Yasin et al., J. Phys. D: Appl. Phys. 51 205104 (2018)

O 80: Gerhard Ertl Young Investigator Award Competition

Time: Thursday 10:30–13:00 Location: TRE/PHYS

O 80.1 Thu 10:30 TRE/PHYS

Surface chemistry of silicate minerals at the atomic scale — Luca Lezuo[1], Andrea Conti[1], Alexander Hoheneder[1], Elena Vaníčková[2], Domitilla Aloi[1], Rainer Abart[3], Florian Mittendorfer[1], Michael Schmid[1], Ulrike Diebold[1], and •Giada Franceschi[1] — [1]Inst. Appl. Phys., TU Wien, Austria — [2]CEITEC, Brno, Czechia — [3]Dept. Lithospheric Res., Uni Wien, Austria

Silicate minerals underpin key processes in geochemistry, atmospheric science, and materials technology, yet their atomic-scale surface chemistry remains insufficiently understood. Their intrinsic heterogeneity and electrical insulation have limited experimental characterization, leaving most mechanistic insight to simulations. Here, we extend the capabilities of noncontact atomic force microscopy (ncAFM) in ultrahigh vacuum to achieve atomic and chemical resolution on natural silicates such as muscovite mica,[1,2] feldspar microcline[3] and wollastonite.[4] Our measurements provide direct evidence for processes central to mineral reactivity, such as ion hydration, ice nucleation, and carbonation reactions. They demonstrate that ncAFM affords fundamental insights previously restricted to theory and offer benchmark data to guide and challenge emerging computational models of mineral-gas interactions.

[1]G.F. *et al.*, *Nat. Commun.* **14**, 208 (2023); [2]G.F. *et al.*, *Faraday Discuss.* **249**, 84 (2024); [3]G.F. *et al.*, *JPCL* **15**, 15 (2023); [4]Conti *et al.*, *submitted* (2025).

O 80.2 Thu 11:00 TRE/PHYS

First Principles Investigations of Energy Dissipation Processes during Atom-Surface Collisions — •Nils Hertl[1,2] and Reinhard J. Maurer[1,2,3] — [1]Department of Chemistry, University of Warwick, Coventry, UK — [2]Department of Physics, University of Warwick, Coventry, UK — [3]Department of Physics, University of Vienna, Vienna, Austria

H atom scattering experiments have emerged as a powerful tool for selectively probing the energy transfer mechanisms between adsorbate and surface, which are relevant for adsorption—the first elementary step in heterogeneous catalysis. This typically includes both phonon and electron excitation in the substrate. Yet, the latter is challenging to model with molecular dynamics because it requires simulation techniques that go beyond the Born-Oppenheimer approximation. In this talk, I will demonstrate how combining electronic structure theory, machine learning, and non-adiabatic molecular dynamics enables a quantitative study of energy transfer between H atoms and surfaces across diverse material classes. I will show that the computed energy loss spectra agree well with experimental findings, enabling detailed characterisation of individual energy transfer channels as well as processes that are experimentally inaccessible, such as adsorption. Based on these findings, I will present a conceptual framework that links adsorbate and surface electronic structure to the probability for non-adiabatic effects to occur in gas-surface collisions.

O 80.3 Thu 11:30 TRE/PHYS

Exchange-driven magnetoelastic coupling in a correlated itinerant ferromagnet — •Carolina A. Marques[1], Luke C. Rhodes[1], Weronika Osmolska[1], Harry Lane[1], Izidor Benedičič[1], Masahiro Naritsuka[1], Siri A. Berge[1], Rosalba Fittipaldi[2], Mariateresa Lettieri[2], Antonio Vecchione[2], and Peter Wahl[1,3] — [1]SUPA, School of Physics and Astronomy, University of St Andrews, UK — [2]CNR-SPIN, c/o Università di Salerno, Italy — [3]Physikalisches Institut, Universität Bonn, Germany

The electronic properties of materials are the result of the complex relationship between lattice and electronic degrees of freedom. In magnetic materials, exchange interactions leads to magnetoelastic coupling, whose effect can be enhanced by the presence of electronic correlations. In the itinerant ferromagnet $Sr_4Ru_3O_{10}$, its magnetic and electronic properties are strongly influenced by electron correlations driven by Van Hove singularities close to the Fermi level. Here, we detect changes to the electronic structure, magnetic ground state and lattice in $Sr_4Ru_3O_{10}$ using scanning tunneling microscopy and spectroscopy (STM/STS). By switching between ferromagnetic and anti-ferromagnetic alignment of the magnetization of the surface and subsurface layers, we study the impact of exchange interaction on the electronic structure and detect jumps in the interlayer spacing, revealing giant exchange magnetostriction in $Sr_4Ru_3O_{10}$. Our measurements reveal a direct link between exchange interaction, electronic and crystal structures, providing a platform to test theoretical descriptions of strongly correlated electron materials.

O 80.4 Thu 12:00 TRE/PHYS

Effect of atomic-scale defects on light-matter interaction in transition-metal dichalcogenides — •Vibhuti N. Rai, Junyoung Sim, Florian Faaber, Sergey Trishin, Nils Bogdanoff, Paul Wiechers, Caroline Firschke, Tom S. Seifert, Tobias Kampfrath, Christian Lotze, and Katharina J. Franke — Freie Universität Berlin, Department of Physics, Arnimallee 14,14195 Berlin, Germany

Defects crucially affect the physical properties of (quasi-) two-dimensional materials, such as transition metal dichalcogenides (TMDCs). Here, by using THz scanning tunneling microscopy [1], we excite and detect long-range coherent in-plane shear and out-of-plane breathing modes on the surface of 2H-$MoTe_2$. We find that atomic-scale intrinsic defects influence their relative excitation efficiency. We attribute this response to local tip-induced band bending [2].

In the monolayer limit, where quantum confinement enhances defect sensitivity, we further show ultrafast charge modulation in defect sites of quasi-freestanding nanopatches of a monolayer MoS_2 on Au(111) driven by THz pulses. These insights into defect-mediated phonon excitation and charge transfer provide a pathway toward future ultrafast electronics.

[1] Cocker et al., Nature Photonics 7, 620-625 (2013)
[2] Rai et al. arXiv:2506.08219v2 (2025)

O 80.5 Thu 12:30 TRE/PHYS

Topological Dirac Quasiparticles Tailored by Moiré Engineering — •Maximilian Ünzelmann, Romana Ganser, Muthu Masilamani, Begmuhammet Geldiyev, and Friedrich Reinert — Exp. Physik VII and Würzburg-Dresden Cluster of Excellence ctd.qmat, Universität Würzburg, Germany

Moiré heterostructures have become a promising platform for tailoring electronic states in a highly controllable manner. The emergent superlattice potential gives rise to band gaps in the folded moiré band structure, which lead to a quenching of kinetic energy and thus increase of electron-electron interactions. Emergent flat bands have been observed in nano-focused angle-resolved photoemission spectroscopy (ARPES) experiments and demonstrated to trigger correlation-driven phenomena. Here, we go beyond the mere creation of flat bands and demonstrate that surface moiré engineering allows transforming a 'simple' epitaxial monolayer-substrate heterostructure into topological Dirac matter. In particular, using ARPES experiments, we will (i) prove the existence of one-dimensional Dirac fermions in the moiré-driven band structure, (ii) show that those are robustly protected by the emergent superlattice symmetry, and (iii) demonstrate how the entire mini-band structure can be controlled by epitaxial manners and sample temperature. Overall, this expands the potential of moiré materials by shifting the focus from almost exclusively flat bands to the creation of new, highly controllable Dirac quasiparticles.

O 81: Catalysis and surface reactions II

Time: Thursday 10:30–12:15 Location: TRE/MATH

O 81.1 Thu 10:30 TRE/MATH

Pd/Cu single atom alloys for selective alcohol dehydrogenation: from single crystalline to nanostructured model catalysts — •Philipp Alexander Fredersdorff[1], Jan Smyczek[1], Carsten Schroeder[1], Paul Froehlich[1], Paul Kohlmorgen[1], Stephan Appelfeller[2], Konstantin Neyman[3], and Swetlana Schauermann[1] — [1]Institute of Physical Chemistry, University Kiel, 24118 Kiel, Germany — [2]MAX IV Laboratory, Lund University, 22100 Lund, Sweden — [3]Departament de Ciència de Materials i Química Física & Institut de Química Teòrica i Computacional (IQTC-UB), Universitat de Barcelona, Barcelona 08028, Spain

Single-atom alloy (SAA) catalysts offer atomic-level control of selectivity, yet structure reactivity relationships in realistic systems remain insufficiently understood. Here, we report the first preparation of well-defined Pd/Cu single-atom alloy nanoparticles under UHV on Al2O3/NiAl(110) and investigate their properties using IRAS CO titration, STM, and TPD. Temperature-dependent Pd de-aggregation shows the same behaviour as on Pd/Cu(111), with optimal incorporation at 550 K. Both de-aggregated materials catalyze the non-oxidative dehydrogenation of butanol, but only the nanostructured Pd/Cu-NP SAA achieves 100 percent selectivity, completely suppressing CO formation. A Pd-coverage-dependent analysis reveals that cluster formation rapidly decreases aldehyde selectivity on single-crystal Pd/Cu(111), whereas the newly developed nanostructured SAA catalysts maintain full selectivity across a wide Pd range.

O 81.2 Thu 10:45 TRE/MATH

Acetylene Cyclotrimerization to Aromatic Products on Coinage Metal Surfaces — Nipun T. S. K. Dewage[1], •Dennis Meier[1], Santu Biswas[2], Matthew M. Montemore[2], and E. Charles H. Sykes[1] — [1]Department of Chemistry, Tufts University, Medford, Massachusetts 02155, USA. — [2]Department of Chemical and Biomolecular Engineering, Tulane University, New Orleans, Louisiana 70118, USA.

Benzene and toluene are indispensable chemical feedstocks used in products ranging from pharmaceuticals to building materials. They are primarily produced through petroleum cracking and reforming, which require high energy input, severe operating conditions, and lack 100% selectivity. As the chemical industry transitions from oil to shale gas as its primary hydrocarbon feedstock, interest is growing in alternative routes to synthesize aromatics. One promising approach is the cyclotrimerization of acetylene, which uniquely yields benzene with 100% selectivity on Ag(111) in ultra-high vacuum. However, this reaction requires more than a monolayer of acetylene to initiate benzene formation, necessitating high pressures that may limit industrial viability. In this work, we investigate strategies to enhance the activity of this reaction on coinage metal surfaces.

O 81.3 Thu 11:00 TRE/MATH

Automated Workflow for Kinetic Modeling in Heterogeneous Catalysis: A Case Study of the Ammonia Oxidation Reaction — •Emanuel Colombi Manzi, Hyunwook Jung, Hendrik H. Heenen, Vanessa J. Bukas, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin

Developing reliable kinetic models in computational catalysis is a big challenge, especially when involving large reaction networks with complex intermediates. Atomistic models built upon first-principles energetics, typically density-functional theory (DFT), are widely used today for elucidating catalytic mechanisms and trends. The cost of DFT calculations, however, makes these models far too expensive to thoroughly sample the many structural configurations that are possible for all relevant surface-bound intermediates. As a result, assumptions on the preferred geometry or surface binding site are commonly adopted based on chemical intuition. Here, we present a fully automated workflow that derives an entire microkinetic model without any *a priori* knowledge or heuristics about the preferred binding configurations. The approach is demonstrated on the kinetics of NH_3 oxidation over selected metal surfaces and alloys. Enabled by an efficient DFT-trained machine learned interatomic potential, an ensemble of low-energy adsorbate structures is identified through global optimization and all process barriers between them are systematically computed. Our simulations provide chemical insight beyond the limitations of standard DFT models and open the road for large-scale screening studies without the need of simplifying assumptions like scaling relations.

O 81.4 Thu 11:15 TRE/MATH

Adsorption of CO and CO_2 on MgO(100) single-crystal surfaces investigated by polarization-resolved IRRAS — •Wangtao Li, Zairan Yu, Alexei Nefedov, Christof Wöll, and Yuemin Wang — Institue of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen, Germany

MgO, a low-cost alkaline metal oxide material, is widely used in heterogeneous catalysis. Comprehensive understanding of MgO-based catalysts requires reliable reference data from surface science studies on MgO model systems. Here, we present polarization-resolved reflection absorption spectroscopy (IRRAS) data obtained for CO and CO_2 adsorption on MgO(100) single-crystal surfaces using a sophisticated UHV apparatus (THEO). The low-temperature (67 K) and temperature-dependent IRRAS results provide deep insights into the interaction of CO and CO_2 with MgO(100). The p- and s-polarized IRRAS data enable detailed analysis of vibrational frequencies, adsorption configurations, and binding energies of different species bound to distinct surface sites including defects. This work was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - Project-ID 426888090 - SFB 1441.

O 81.5 Thu 11:30 TRE/MATH

Experimental Modelling of Ti-based (Photo-)Catalysts for the Activation of Greenhouse Gasses — •Lars Mohrhusen — Carl von Ossietzky Universität Oldenburg, Germany

Sustainable catalysts are key materials for future energy technologies and the activation of greenhouse gasses via thermal and photo-catalysis. To replace critical raw materials such as (noble) metals in (photo-)catalysts, we combine low-dimensional (semi-)metallic structures such as point defects or 2D materials with oxides to hybrid materials. Combined insights from spectroscopy, microscopy and reactivity studies on well-defined model systems under UHV or so-called operando conditions gains a comprehensive atomistic picture.[1–3]

Selected examples for such Ti-based materials relevant for solar photocatalysis will be presented. Therein, the activation of greenhouse gas molecules (esp. N_2O and CO_2) on Ti^{3+} and Ti^{2+} defects will be illuminated.[3,4] While such gases interact weakly with defective rutile TiO_2 in UHV, higher pressures of CO_2 combined with the presence of water as an H donor were found to enable a rich reduction chemistry along multiple parallel pathways in operando-XPS.[4] In addition to oxides, nanostructured 2D titanium disulphide (TiS_2) as well as conjugated organic polymers on metal and oxide surfaces represent potential candidates for photocatalytic applications.[5]

[1] L. Mohrhusen et al., J. Phys. Chem. C 2022, 126, 48, 20332. [2] L. Mohrhusen et al., Small 2024, 2405715. [3] L. Mohrhusen K. Al-Shamery, Catal. Lett. 2023, 153, 2, 321. [4] J. Klimek, et al. under review [5] N. Kruse et al. Small 2025, 38, e06023.

O 81.6 Thu 11:45 TRE/MATH

Studying low surface area photocatalysts at ambient pressure in a microreactor — •Paula Neumann[1], Clara Aletsee[2], Martin Tschurl[1], and Ueli Heiz[1] — [1]Chair of Physical Chemistry, School of Natural Sciences & Catalysis Research Center, Technische Universität München, Lichtenbergstr. 4, 85748 Garching, Germany — [2]SurfCat Section for Surface Physics and Catalysis, Department of Physics, Technical University of Denmark, 2800 Kgs Lyngby, Denmark

While driving reactions with solar light is an ambitiously pursued goal, current approaches often suffer from low efficiencies due to missing knowledge about reaction dynamics on the catalysts surface. Here, the application of highly defined photocatalysts may allow deeper mechanistic insight but their low surface area imposes high demands on detection sensitivity for studying reactions at ambient conditions. Our gas-phase microreactor enables time-resolved investigation of planar photocatalysts by mass spectrometry in a well-defined reaction environment. Using the photo-oxidation of alcohols on a titania photocatalyst as a model system we show how reaction mechanisms first established in the ultra-high vacuum transfer to conditions of 1000 mbar. Disentangling the mechanistics of alcohol photochemistry might be a crucial step towards improving hydrogen formation as an important energy carrier as well as opening up pathways for the production of higher-value chemicals.

O 81.7 Thu 12:00 TRE/MATH

Model-Free Reconstruction of Local Kinetic Information on Catalytic Surfaces from Operando Profile Measurements — •Jinyi Zhou[1], Mishai Avila[2], Daniel Runge[3], Lukas Thum[4], Heinz Junkes[1], Michael Geske[2], Christian Merdon[3], Frank Rosowski[2,5], Karsten Reuter[1], Christoph Scheurer[1], and Sebastian Matera[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]BasCat - UniCat BASF JointLab, TU Berlin — [3]Weierstraß-Institut, Berlin — [4]Helmholtz-Zentrum Berlin — [5]BASF SE, Catalysis Research, Ludwigshafen, Germany

Operando characterization experiments are typically strongly affected by transport effects, which can cause strong local variations of reactivity and concentration on the catalytic surface. We present a framework that allows one to obtain this local kinetic information from a measured concentration profile away from the active surface, without assuming any specific kinetic model. Utilizing Green's functions of the transport operator and a function space formulation of the inverse problem, the approach allows robust reconstruction from finite, noisy data. We apply this approach to a compact profile reactor, where concentration is measured along the axis of a channel flow with catalyst deposited on the channel walls. Using synthetic data, we demonstrate that the approach has the potential to resolve sub-millimeter variations in surface reactivity with modest computational and experimental footprints. Additional challenges that need to be overcome in order to fully exploit this potential for high accuracy when using experimental data will be discussed.

O 82: Focus Session: Unoccupied States by Inverse Photoemission III

The Other Half of the Picture: 50 Years of Direct Access to Unoccupied States by Inverse Photoemission

In 1981, J. Pendry evaluated the experimental access to electron states in solids: "Currently only half of the picture can be seen with photoemission. Inverse photoemission provides the other half." A complete picture of electron states needs both occupied and unoccupied states in order to describe, understand, and finally tailor macroscopic material properties. In 1976, V. Dose had submitted a first paper on Bremsstrahlung Isochromat Spectroscopy in the VUV range: "The physics involved may be most simply described as an inverse photoelectric effect." The first experiments provided surface-sensitive information on the density of unoccupied states. Later, momentum and spin resolution were added to investigate the spin-dependent E(k) dispersion of unoccupied electron states. During five decades, the technique was further developed by several groups worldwide to enhance the intensity and improve the resolution in energy, momentum, and spin. A wealth of information was gained about metals, semiconductors, ultrathin films as well as adsorbate systems. The experimental studies were accompanied by several theoretical approaches, which are able to accurately describe the unoccupied electronic structure and model the inverse photoemission process. In 2012, H. Yoshida extended the energy range to the near-UV range (low-energy inverse photoemission), which is especially suited to study organic samples due to a lower damage risk caused by the exciting electron beam.

Current research fields for inverse photoemission are, e.g., spin textures of exchange- and/or spin-orbit-induced influenced systems and topological insulators, gap structures in transition metal dichalcogenides, LUMO levels in semiconductors for photovoltaic applications, electronic structure of atomic-layer and quantum materials. This focus session will highlight recent advances obtained by inverse photoemission in different fields and material systems. Also, it will bring together researchers from different areas for addressing current trends and future applications of inverse photoemission from experimental as well as theoretical perspective.

Organized by Markus Donath, Fabian Schöttke and Peter Krüger (U Münster).

Time: Thursday 10:30–12:30 Location: WILL/A317

Invited Talk O 82.1 Thu 10:30 WILL/A317

Low-energy inverse photoelectron spectroscopy (LEIPS): probing unoccupied states and conduction band structure in functional materials — •Hiroyuki Yoshida — Chiba University, Chiba, Japan

We developed low-energy inverse photoelectron spectroscopy (LEIPS) in 2012 [1] to enable damage-free probing of functional materials such as organic semiconductors, polymers and hybrid perovskites. By reducing the incident electron energy below the damage threshold (about 5 eV), LEIPS allows damage-free measurements while simplifying operation and improving energy resolution. By incorporating an electron energy analyzer [2], we achieved an energy resolution of 98 meV. LEIPS enables determination of electron affinity with an uncertainty of 0.1 eV. These precise values provide access to key parameters including band gaps, exciton binding energies, polarization energies, and electron injection barriers. The technique has been commercialized, and more than 100 systems are now in operation worldwide. We further developed angle-resolved LEIPS (AR-LEIPS) [3], enabling for the first time direct observation of conduction band structure in organic semiconductors [4]. The measured band structures yield insight into electron-phonon coupling and polaron formation relevant to carrier transport. [1] Chem. Phys. Lett. 539-540, 180 (2012). [2] Rev. Sci. Instrum. 94, 043908 (2023). [3] Rev. Sci. Instrum. 94, 063903 (2023). [4] Nat. Mater. 21, 910 (2022).

Invited Talk O 82.2 Thu 11:00 WILL/A317

Enhanced Sensitivity in Low-Energy Inverse Photoemission Spectroscopy with an Off-Axis Parabolic Mirror for Efficient Light Collection — •Yongsup Park[1,2], Jong-Am Hong[1], Kyu-Myung Lee[1], and Min-Jae Maeng[1] — [1]Dept. of Physics, Kyung Hee University, Seoul, Republic of Korea — [2]Dept. of Information Display, Kyung Hee University, Seoul, Republic of Korea

Inverse photoemission spectroscopy (IPES) is a powerful tool for studying unoccupied electronic states but suffers from low sensitivity due to the low photon emission probability during free electron transitions. To improve sensitivity via better photon collection, an off-axis parabolic (OAP) mirror was designed and built for low-energy IPES (LEIPS). Optical simulations showed the OAP mirror raised photon collection efficiency from 3.06% to 63.3%, confirmed experimentally through LUMO spectra of C60 thin films. The OAP mirror-LEIPS system was applied to study energy level alignment (ELA) of pentacene films on substrates with different work functions (WF). By measuring HOMO and LUMO levels, the changes in transport gaps and the ELA with respect to the Fermi level were analyzed. Pentacene showed n-type behavior on low WF substrate (Cs2CO3) and p-type on high WF substrate (ITO). This OAP mirror-enhanced LEIPS system significantly shortened experiment times, enabling efficient and reliable measurements.

O 82.3 Thu 11:30 WILL/A317

Development of angle resolved low energy inverse photoelectron spectroscopy for conduction band structure measurements of functional materials — •yuki kashimoto[1], satoshi ideta[1], haruki sato[1], keita kawamura[1], hibiki orio[1], and hiroyuki yoshida[1,2] — [1]chiba university, chiba, japan — [2]chiba university MCRC, chiba, japan

Understanding the energy band structure is essential for clarifying charge-transport behavior in solids. Although angle-resolved inverse photoelectron spectroscopy (ARIPES) can measure conduction bands, it is unsuitable for emerging materials such as organic semiconductors due to their narrow bandwidths and electron irradiation damage. Low-energy inverse photoelectron spectroscopy (LEIPS)[1] overcame these issues by reducing the electron kinetic energy. In this study, we advanced LEIPS and enabled band-structure measurements by introducing angle-resolved detection. Stray electric and magnetic fields were suppressed, and a dedicated low angular spread, energy-scannable electron source was implemented. This enabled angle-resolved LEIPS (AR-LEIPS) with 0.23 eV energy resolution and 0.94 nm^{-1} momentum resolution[2]. Using AR-LEIPS, we determined the conduction band structure of pentacene, the first such measurement for an organic semiconductor[3] and revealed the conduction-band dispersion of the photovoltaic perovskite $CH_3NH_3PbI_3$. [1] H.Yoshida, Chem. Phys. Lett. 539-540, 180 (2012). [2]Y.Kashimoto, H.Yoshida et al, Rev. Sci. Instrum. 94, 063903 (2023) [3] H. Sato, H. Yoshida et al, Nature Mat. 21,910 (2022).

O 82.4 Thu 11:45 WILL/A317

Observation of conduction band structure of conductive polymer PBTTT — •Taichi Suruga[1], Shunichiro Ito[2], Taishi Takenobu[2], and Hiroyuki Yoshida[1,3] — [1]Chiba University, Chiba, Japan — [2]Nagoya University, Nagoya, Japan — [3]Chiba University MCRC, Chiba, Japan

The most fundamental information regarding the electron transport mechanism of these polymers is the conduction-band structure. However, until now, we did not have the appropriate methods to measure it. In 2020, we developed angle-resolved low-energy inverse photoelectron spectroscopy (ARLEIPS) [1] and successfully measured the conduction band structure of small-molecule organic semiconductors for the first time [2]. In this study, we applied ARLEIPS to a conductive polymer. Fabricating crystalline thin films with well-aligned molecular orientation is essential for the ARLEIPS measurement. We fabricated thin films using the blade-coating method [3]. Using ARLEIPS, we observed the conduction-band structure of a conductive polymer, PBTTT-C14 [4,5], in oriented films. As predicted by the DFT calculations, the bands split into two and exhibited large dispersion along the Γ-Z direction. These results demonstrate the first observation of conduction-band in a conductive polymer. [1] Y. Kashimoto, H. Yoshida et al., Rev. Sci. Instrum, 94, 043908 (2023) [2] H. Sato, H. Ishii, H. Yoshida et al., Nat. Mater. 21, 910 (2022). [3] D. Delongchamp et al., ACS Nano. 3, 780 (2009). [4] H. Tanaka, K. Kanahashi, T. Takenobu et al., Sci. Adv., 6,

eaay8065 (2020) [5] S. Ito, H. Tanaka, T. Takenobu et al., Appl. Phys. Express 18, 021002 (2025)

O 82.5 Thu 12:00 WILL/A317

Effects of Crystallization on the Electronic Structure of Discrete Oligomers — •Alexander Ehm[1], Rukiya Matsidik[2], Michael Sommer[2], and Dietrich R. T. Zahn[1] — [1]Semiconductor Physics and Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), TU Chemnitz, Chemnitz, Germany — [2]Polymer Chemistry, TU Chemnitz, Chemnitz, Germany

Recently, organic photovoltaic cell efficiency surpassed the 20 % landmark, thanks to the development and improved crystallinity of non-fullerene acceptor (NFA) molecules and suitable polymer donors [1]. Low exciton binding energies (EBE), measured by the difference of the transport gap and the optical bandgap, were attributed as key factors in such improvements [2].

Photoemission and low-energy inverse photoemission spectroscopy (PES and LEIPES) in combination directly measure the transport gap. However, challenges are posed by their surface sensitivity in conjunction with the solution processing, low conductivity and radiation sensitivity of thin films of large organic molecules.

Here, we address strategies to avoid surface contamination and charging effects, while investigating the interfacial electronic structure of conjugated discrete oligomer films [3] spin-coated on Ag substrates. Their thermal crystallization reduced their bulk EBE to < 0.1 eV.

[1] F. Furlan, N. Gasparini, Nat. Mater. 24, 336 (2025)
[2] A. Sugie *et al.*, J. Phys. Chem. Lett. 14, 11412 (2023)
[3] R. Matsidik *et al.*, J. Am. Chem. Soc. 145, 8430 (2023)

O 82.6 Thu 12:15 WILL/A317

Development of near-ambient-pressure low-energy inverse photoelectron spectroscopy enabling measurement under the water vapor pressure — •Mihiro Kubo[1], Gaku Yokogawa[1], Hitoshi Tomizuka[2], and Hiroyuki Yoshida[1] — [1]Chiba University, Chiba, Japan — [2]TOYAMA Co., Ltd., Kanagawa, Japan

Inverse photoemission spectroscopy has evolved over fifty years, providing essential insight into the unoccupied electronic structure. In 2012, Dr. Yoshida developed low-energy inverse photoelectron spectroscopy (LEIPS[1]). This technique enables the measurement of organic materials without damaging the sample by reducing the kinetic energy below 5 eV, their typical damage threshold. To further extend the applicability of LEIPS, we are developing near-ambient-pressure LEIPS (NAP-LEIPS) capable of measurement under the vapor pressure of water (10^3 Pa). NAP-LEIPS will allow measurements of volatile samples, biomaterials, and catalysis with the introduction of reactive gases. To realize NAP-LEIPS, we use an electron gun with a yttria-coated disc cathode and an electrostatic energy analyzer. Because the electron source operates at pressures better than 10^{-5} Pa, a differential pumping system is installed between the electron source chamber and the main chamber (10^3 Pa). Electrons travel about 300 mm through the differential pumping section using an electrostatic transfer lens. Photons emitted from the sample are focused by a mirror, passed through a band-pass optical filter, and detected with a photomultiplier tube. The apparatus has been constructed and is currently in the start-up phase. [1] H. Yoshida, Chem. Phys. Lett. 539-540, 180 (2012).

O 83: Organic molecules on inorganic substrates: electronic, optical and other properties III

Time: Thursday 15:00–17:30 Location: HSZ/0201

O 83.1 Thu 15:00 HSZ/0201

Spin-Crossover and Structural Correlation in Surface Confined Indigo-Based Fe-Coordination Polymers — •Mohammad Salehi[1], Aliki Soufla[2], Hongxiang Xu[1,5], Fulden Eratam[3], David A. Duncan[3,4], Tien-Lin Lee[3], Joachim Reichert[1], Johannes V. Barth[1], and Anthoula C. Papageorgiou[2] — [1]Technical University of Munich, DE — [2]National and Kapodistrian University of Athens, GR — [3]Diamond Light Source, UK — [4]University of Nottingham, UK — [5]Peking University, CN

Surface confined coordination polymers (CPs) exhibiting spin-crossover (SCO) behavior hold promise for molecular spintronics. By harnessing the natural dye indigo as a molecular building block, we investigated $[\text{Fe-indigo}]_n$ CPs on Ag(111). Sub-molecular resolution scanning tunnelling microscopy (STM) and atomic force microscopy (AFM) confirmed well-defined CPs. We employed Fe *L*-edge X-ray absorption near-edge spectroscopy and high-resolution Fe 2*p* soft X-ray photoelectron spectroscopy to probe the spin states of Fe-indigo CPs at different temperatures. The data analysis supports thermally activated spin-crossover behavior, as predicted by density functional theory calculations. Normal incidence X-ray standing wave analysis yielded varying adsorption heights of Fe centers. We correlate the spin state with structural variations, revealing the interplay between ligand fields and magnetic properties.

O 83.2 Thu 15:15 HSZ/0201

Probing pi-conjugation in functionalized pentacene via photoemission orbital tomography — Felix Otto[1], Andrei Matestskii[2], Maximilian Schaal[1], Elise Fürch[1], Jonas Brandhoff[1], Roman Forker[1], François C. Bocquet[2], Michael G. Ramsey[3], Serguei Soubatch[2], •Peter Puschnig[3], Frank Stefan Tautz[2], and Torsten Fritz[1] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Germany — [2]PGI-3, FZ Jülich & RWTH Aachen University, Germany — [3]Institute of Phyics, University of Graz, Austria

Tuning the electronic structure of polycyclic aromatic hydrocarbons is an effective route to control their physical and chemical properties. Here, we present an experimental approach that enables direct assessment of how chemical functionalization modifies the conjugation length of adsorbed molecules. We demonstrate the method using pentacenequinone (P2O), a functionalized pentacene derivative that forms a self-assembled monolayer on Ag(110), as confirmed by low-energy electron diffraction and scanning tunneling microscopy. Employing photoemission orbital tomography, we combine experimental photoelectron momentum maps with density-functional-theory simulations to elucidate the character of the frontier molecular orbitals. Our results provide direct experimental evidence that the functional group in P2O disrupts the conjugation of the parent pentacene backbone, causing the electronic structure of P2O to resemble two electronically decoupled naphthalene units. This interpretation is further supported by the observed increase in the band gap upon functionalization.

O 83.3 Thu 15:30 HSZ/0201

Stochastic spin-state transitions in an Fe(II) spin-crossover complex on Cu(111) — •Jasmeen Jasmeen[1], Sujoy Karan[1], Karl Ridier[2], Reecht Gaël[1], and Manuel Gruber[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen, 47057 Duisburg, Germany — [2]2LCC, CNRS and Université de Toulouse, UPS, INP, 31077 Toulouse, France

Spin-crossover molecules can be switched between a low- (S = 0) and a high-spin (S = 1) state using external stimuli. Although the switching properties of crystalline powder were shown to strongly depend on the molecules environment, a full microscopic description is lacking. The switching of individual molecules in contact with a surface, evidenced in recent years, open new routes to further understand the impact of the local environment in the switching properties.

Using scanning tunneling microscopy at 4.5 K, we investigated the [Fe(HB(1,2,4-triazolyl)3)2] complex in direct contact with Cu(111) surface, focusing on the dynamics of its spin-state switching and the factors controlling switching behavior. The switching is triggered by injecting current at voltages above 0.5 V and monitored by the induced change in conductance.

We observe a drastic change of the switching yield with the local molecular environment, showing a clear dependence on both the number and the spin-state of neighboring molecules. These observations suggest that intermolecular interactions influence the switching efficiency.

Funding from the CRC 1242 is gratefully acknowledged.

O 83.4 Thu 15:45 HSZ/0201

Coordination and Molecular Band Dispersion of a 2D Metal-Organic Network — •Martin Anstett[1], Lu Lyu[2], Jannis Lessmeister[1], Alexander Schmid[2], Ralf Hemm[1], Vitaliy Feyer[3], Yan Yan Grisan Qiu[3], Simone Mearini[3], Martin Aeschlimann[1], and Benjamin Stadtmüller[2] — [1]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, 67663 Kaiserslautern, Germany — [2]Experimentalphysik II, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [3]Peter Grünberg Institute (PGI-6), Jülich Research Centre, 52428 Jülich, Germany

Two-dimensional metal-organic porous networks (2D-MOPNs) provide a versatile platform exploring emergent electronic and magnetic phenomena at designed surface nanoarchitectures. Here, we prepare a cobalt-coordinated hexaaza-triphenylene-hexacarbonitrile (HATCN) network on Ag(111) to fingerprint the role of metal centers in mediating electronic behaviour. Scanning tunnelling microscopy (STM) reveals an ordered network structure. Photoelectron momentum microscopy identifies a distinct hybrid interface state arising from the Co-mediated coupling with the molecules. These results reveal the microscopic mechanism underlying the role of metal centers in tailoring the electronic structures of 2D-MOPN systems.

O 83.5 Thu 16:00 HSZ/0201

Phthalocyanine-based bipartite lattices: Towards a molecular Lieb lattice — •Tzu-Chao Hung[1], Luis M. Mateo[2], Leo Gross[3], Diego Peña[2], and Jascha Repp[1] — [1]University of Regensburg, Germany. — [2]Universidade de Santiago de Compostela, Spain. — [3]IBM Research Europe - Zurich, Switzerland.

The Lieb lattice is a text-book example of topology governing material properties: Its sublattice imbalance gives rise to extended degenerate states resulting in a flat band. Here, we realize several different covalently bonded phthalocyanine (Pc)-based Lieb-lattice prototypical structures by means of on-surface synthesis. Bond-resolved atomic force microscopy images reveal planar structures with extended π-conjugation. Differential conductance maps, combined with density-functional theory calculations and tight-binding models, confirm strong intersite electronic coupling and quantum states with symmetry-enforced nodes and symmetry-protected degeneracy. Structures of increasing complexity allow exploring the evolu-tion of these symmetry-derived features.

O 83.6 Thu 16:15 HSZ/0201

Correlation-driven d-band modifications promote chemical bonding at 3d-ferromagnetic surfaces — •David Janas[1], Andreas Windischbacher[2], Alessandro Sala[3], Manuel Gruber[4], Mehdi Bouatou[4], Vitaliy Feyer[5], Iulia Cojocariu[5], Andrea Droghetti[6], Peter Puschnig[1,2], Giovanni Zamborlini[1], and Mirko Cinchetti[1] — [1]TU Dortmund University — [2]Karl-Franzens-University Graz — [3]CNR-Istituto Officina dei Materiali (IOM), Trieste — [4]University of Duisburg-Essen — [5]Elettra Sincrotrone Trieste — [6]Ca' Foscari University of Venice

Many-body effects at adsorbate-metal interfaces play a crucial but often overlooked role in designing spintronic and electrocatalytic materials. We recently showed that a chemisorbed oxygen layer on ferromagnetic (FM) Fe enhances electron correlation, causing narrowing of the Fe d-bands near the Fermi level, and a reduced exchange splitting, with direct implications for surface reactivity [1]. Here, we study a pentacene monolayer on oxygen-passivated Fe using momentum-resolved photoemission, scanning tunneling microscopy/spectroscopy, and Hubbard-corrected density functional theory (DFT+U) guided by dynamical mean-field theory (DMFT). Non-standard U values reproduce unexpectedly strong molecule-substrate interactions on a nominally passivated surface, highlighting the decisive role of electron correlation at organic/FM interfaces [2].

[1] Janas, D.M., et al. Adv. Mater., 35, 2205698 (2023).
[2] Janas, D.M., et al. accepted in Small.

O 83.7 Thu 16:30 HSZ/0201

A quantum dot-functionalized scanning tunnelling microscope tip: Sensing through electron-vibron coupling — •Stefan Schulte[1,2,3], Emilio Scontrino[1,4], Taner Esat[1,3], F. Stefan Tautz[1,3,4], and Ruslan Temirov[1,2,3] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]II. Physikalisches Institut, Universität zu Köln, Germany — [3]Fundamentals of Future Information Technology, Jülich Aachen Research Alliance (JARA), Germany — [4]RWTH Aachen University, Germany

Scanning tunnelling microscope (STM) tips functionalized with a single-molecule quantum dot (QD) have been used for quantitative measurements of electrostatic surface potentials through a technique known as scanning quantum dot microscopy (SQDM) [1]. The functionalization of STM tips with large organic molecules has further enabled measurements of electrostatic and magnetic fields at the atomic scale [2, 3]. Here, we attach a naphthalene tetracarboxylic dianhydride (NTCDA) molecule, acting as a QD, to the tip of an STM and investigate charge transport through the resulting junction. In the resonant regime, the transport through the NTCDA QD exhibits signatures of electron-vibron coupling. We propose that this electron-vibron coupling can be leveraged to map surface polarizability with sub-nanometre resolution.

[1] C. Wagner *et al.*, Phys. Rev. Lett. **115**, 026101 (2015).
[2] B. Verlhac *et al.*, Science **366**, 623 (2019).
[3] T. Esat *et al.*, Nat. Nanotechnol. **19**, 1466 (2024).

O 83.8 Thu 16:45 HSZ/0201

Spatial Mapping of Vibronic Excitations in a Single Organometallic Complex — Xiangzhi Meng[1], Kai Uwe Clausen[2], Marie-Laure Bocquet[3], •Alexander Weismann[1], Niklas Ide[1], Felix Tuczek[2], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Institut für Anorganische Chemie, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [3]Laboratoire de Physique de l'École normale supérieure, ENS, Université PSL, CNRS, Sorbonne Université, Université Paris Cité, 75005 Paris, France

Vibronic excitations in single molecules at nanoscale interfaces are central to molecular electronics and are usually modeled with a double-barrier tunneling junction that assumes a homogeneous electric field and ignores atomic details of the contacts. Using STM measurements of a nonplanar organometallic complex on Ag(111), we obtain spatially resolved vibronic maps that reveal shifts in excitation energies caused by reordering of occupied molecular orbitals under the rapidly decaying tip potential. These shifts vary strongly with tip position. Combined with modeling, our results show that tip-induced, atomically varying electric fields can actively control molecular orbitals and must be considered in studies of nonplanar molecules.

O 83.9 Thu 17:00 HSZ/0201

Exciton Dynamics and Charge Transfer at Prototype Organic/Organic Interfaces Studied with LEEM and 2P-PEEM — Franz Niklas Knoop, •Klaus Stallberg, and Winfried Daum — Institute of Energy Research and Physical Technologies, TU Clausthal, Germany

Organic semiconductor (OSC) films deposited on weakly interacting substrates, such as natively oxidized silicon, often suffer from poor structural order. Using low-energy electron microscopy (LEEM), we show that para-sexiphenyl (*p*-6P) molecules on SiO_2 serve as a wetting layer, promoting the growth of microcrystalline phthalocyanine (Pc) thin films, which renders Pc/*p*-6P/SiO_2 a structurally well-defined model for an organic heterojunction. Using two-photon photoemission (2PPE), we study the exciton dynamics in both CuPc and F_{16}CuPc films on *p*-6P/SiO_2. For F_{16}CuPc/SiO_2, i.e., in absence of *p*-6P, the S_1 exciton is observed with a lifetime of 50 ps, indicating negligible influence of the substrate on the exciton dynamics. In contrast, for F_{16}CuPc/*p*-6P/SiO_2, the S_1 exciton is quenched. Moreover, laser-induced changes in electron reflectivity reveal a surface potential shift for F_{16}CuPc/*p*-6P/SiO_2, which points to the formation of surface dipoles upon optical excitation of F_{16}CuPc. Accordingly, we attribute the S_1 exciton quenching to formation of charge transfer (CT) excitons, which is compatible with the type II energy level alignment at the F_{16}CuPc / *p*-6P interface. In contrast, at the CuPc/*p*-6P type I heterojunction no charge transfer takes place. Accordingly, neither exciton quenching nor significant surface potential shifts are observed.

O 83.10 Thu 17:15 HSZ/0201

Magnetic Excitations in on-surface metallacrown complexes — •Robert Ranecki[1,2], Stefan Lach[2], Anne Lüpke[3], Angeliki Athanasopoulou[3], Eva Rentschler[3], and Christiane Ziegler[2] — [1]QNS, Seoul, Korea — [2]RPTU Kaiserslautern-Landau and OPTIMAS, Kaiserslautern, Germany — [3]Inst. of Inorganic and Analytical Chemistry, JGU Mainz

The implementation of quantum information processing demands achieving electrical control over spin-qubits that can be integrated into scalable architectures. Addressing this challenge, multi-spin-carrying molecules on surfaces offer a route to surface-integrable qubits: chemically diverse with tunable spin properties. However, the interaction with the supporting substrate can dramatically modify the electronic and magnetic properties of such complexes. Here, we present spin-flip inelastic tunneling spectroscopy studies of pentanuclear metallacrown complexes, CuCu4 and CuFe4, under adsorption onto Au(111) surface. By comparing the experimental results with perturbative electron transport model simulations[1], we extract quantitative values of the exchange coupling constants and determine the ground spin states of the metallacrown complexes[2]. These findings advance our understanding of the spin interactions in complex molecular systems adsorbed on surfaces, paving the way towards future quantum technologies.

[1] Ternes, M. New J. Phys. 17, 063016 [2] Ranecki, R. et al., J. Phys. Chem. C 127, 13186; Ranecki, R. et al., J. Phys. Chem. C 126, 15907

O 84: 2D Materials: Electronic structure, excitations, etc. III (joint session O/HL/TT)

Time: Thursday 15:00–17:45 Location: HSZ/0204

O 84.1 Thu 15:00 HSZ/0204

Linearized augmented plane waves for low-dimensional materials — •Andris Gulans, Ernests Jansons, and Janis Uzulis — University of Latvia, Riga, Latvia

We address the challenge of efficient yet highly precise density-functional theory calculations of low-dimensional materials and present a set of tools and algorithms specific to linearized augmented plane waves (LAPW) that is implemented in the electronic-structure code `exciting`. First, we discuss our iterative eigensolver compatible with local and hybrid functionals. It is an extension of Davidson*s algorithm and does not require explicit Hamiltonian construction while overcoming difficulties associated with high condition numbers. The second important ingredient is the adaptively compressed exchange that represents

the non-local (screened) Fock exchange via a low-rank approximation. This approach enables computational complexity as low as $O(N^3 \log N)$ floating-point operations (FLOPs) with N being the number of atoms. It is a novel feature in hybrid functional calculations using LAPW as the standard approaches require $O(N^4)$ FLOPs. Finally, we introduce a cylindrical cutoff for the Coulomb interaction for handling the $q = 0$ singularity.

O 84.2 Thu 15:15 HSZ/0204

Graphene-Enabled Mott–Metal Transition in Silicon Dangling Bonds — •Niclas Tilgner[1], Siheon Ryee[2], Zamin Mamiyev[1], Philip Schädlich[1], Christoph Tegenkamp[1], Tim O. Wehling[2], and Thomas Seyller[1] — [1]Institute of Physics, Chemnitz University of Technology, Germany — [2]I. Institute of Theoretical Physics, University of Hamburg, Germany

Controlling emergent electronic phases in materials with strong Coulomb interactions remains a central challenge in condensed matter physics. Adatom lattices on semiconducting surfaces provide prototypical platforms for exploring such correlated phenomena. Recent advances have facilitated the synthesis of 2D Mott insulators in proximity to graphene (N. Tilgner et al 2025 2D Mater. 12 045022). Here, we demonstrate that alkali adsorption on a graphene/Si/SiC(0001) heterostructure – where the Si layer hosts correlated dangling bonds – enables controlled charge transfer to the Mott insulator. Beyond a critical carrier concentration, we observe a sudden collapse of the Mott gap, indicating a transition to a correlated metallic phase. Our results point to a finite proximity coupling between the Mott layer and graphene, as recently suggested by a theoretical study (N. Witt et al 2025 arXiv:2503.03700), which gives rise to nonlocal dynamical screening beyond simple electrostatics and provides a natural pathway for the observed phase transition.

O 84.3 Thu 15:30 HSZ/0204

From self-consistent DFT+DMFT to the two-particle level: Magnetic phase diagram of X:SiC(111) — •Lukas Bongardt[1,2], Niklas Enderlein[3], Giorgio Sangiovanni[4], Philipp Hansmann[3,5], and Henri Menke[1] — [1]Max Planck Computing and Data Facility — [2]Technical University of Munich — [3]FAU Erlangen — [4]Universität Würzburg — [5]University of Iceland, Reykjavík

Recently we have proposed a novel and versatile platform to realize a two-band Hubbard model with massless Dirac fermions and flat bands hosting strong correlations by depositing three different species of transition-metal adatoms on semiconductor surfaces (arXiv:2410.17165). Using state-of-the-art DFT+DMFT calculations we investigated the spectral properties of X:3C-SiC(111) (X = Ti, V, Cr). Due to the presence of well-defined Dirac cones and flat bands, indicating the potential for realizing topological and correlated phases, we identify transition-metal adatoms on SiC as a possible platform for exploring the interplay of correlations, topology, and magnetism in two-dimensional materials.

In this work, we explore the magnetic phase diagram of these systems within DMFT by calculating the generalized two-particle vertex and using it to solve the Bethe-Salpeter equation for the generalized susceptibility. This gives us a fully orbital-, spin-, and most importantly momentum-dependent susceptibility which carries the information about the ordering wave vector and is experimentally accessible through various techniques.

O 84.4 Thu 15:45 HSZ/0204

Cr 3*d* Orbital Hybridization and Electronic Structure in the Layered Magnetic Semiconductor $CrPS_4$ — •Lasse Sternemann[1], David Maximilian Janas[1], Richard Leven[1], Eshan Banerjee[2], Jonah Elias Nitschke[1], Marco Marino[1], Leon Becker[3], Ahmet Can Ademoglu[1], Frithjof Anders[1], Stefan Tappertzhofen[3], and Mirko Cinchetti[1] — [1]TU Dortmund University, Department of Physics, 44227 Dortmund, Germany — [2]Department of Materials, Imperial College London, London, SW7 2AZ, United Kingdom — [3]TU Dortmund University, Department of Electrical Engineering and Information Technology, 44227 Dortmund, Germany

Despite its promising spintronic and magneto-optical characteristics, the electronic band structure of the van der Waals magnetic semiconductor $CrPS_4$ is still unknown. Here, we report angle-resolved photoemission spectroscopy measurements of its band structure in the para- and antiferromagnetic phase, complemented by DFT+U calculations. Theoretical results reveal dominating Cr 3*d* and S 3*p* contributions to the valence band and a ligand-to-metal charge-transfer band gap. Crystal field split Cr 3*d* orbitals display distinct hybridization regimes with S 3*p* orbitals: t_{2g} orbitals are only weakly affected by hybridization, while e_g states experience a 4 eV anti-bonding/bonding splitting with S-mixing relaxing dipole selection rules, otherwise darkening optical *d*-*d* transitions. These findings establish the ground state electronic and orbital structure of $CrPS_4$ and provide essential benchmarks for understanding its optical and magnetic responses.

O 84.5 Thu 16:00 HSZ/0204

Spectroscopic Investigation of the Ni Valence States in $NiTe_2$ — •Tassaphon Tirasutt[1], Sheng-Huai Chen[1], Alexander C. Komarek[1], Chun-Fu Chang[1], Yu-Chieh Ku[2], Po-Yu Cho[3], Chun Sum Brian Pang[4], Mizuki Furo[5], Naoki Ito[5], Ulrich Burkhardt[1], Simone G. Altendorf[1], Atsushi Hariki[5], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]National Yang Ming Chiao Tung University, Hsinchu, Taiwan — [3]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [4]The University of British Columbia, Vancouver, Canada — [5]Osaka Metropolitan University, Osaka, Japan

Nickel-based transition metal compounds exhibit a wide range of properties arising from the strongly correlated *d* electrons. In this study, we investigate $NiTe_2$, a layered transition-metal dichalcogenide with reported type-II Dirac semimetallic properties. While its topological nature has been the focus of interest, the fundamental question of the properties of the Ni ions in $NiTe_2$ has rarely been discussed. We address this issue using soft X-ray core-level and valence-band photoelectron spectroscopy, as well as Ni-$L_{2,3}$ absorption spectroscopy, combined with a theoretical approach using LDA+DMFT. Our findings provide insights into the Ni 3*d* occupation and degree of correlation of the Ni in a metallic ligand bath of the $NiTe_2$ system.

O 84.6 Thu 16:15 HSZ/0204

TMDC surfaces as scattering targets in spin-polarization detectors: A case study of MoS_2 — •Christoph Angrick[1], Annika Henriksen[1], Nicole Edossa[1], Andre Reimann[1], Moritz Ewert[2,3], Lars Buss[2,3], Jens Falta[3], Jan Ingo Flege[2,3], and Markus Donath[1] — [1]University of Münster, Germany — [2]Brandenburg University of Technology Cottbus-Senftenberg, Germany — [3]University of Bremen, Germany

Spin-polarization detectors are employed in photoemission experiments to reveal the spin texture of electronic states. One well-proven approach is based on the VLEED process, where the spin-dependent electron reflection from targets influenced by exchange and/or spin-orbit interaction is used. The suitability of a target must be investigated beforehand [1,2]. In this talk, a first impression of TMDC-based detectors is given [3]. The spin-dependent electron reflectivity of spin-orbit-influenced MoS_2 is measured over a wide range of incident energies and angles for the following samples: a single layer of MoS_2 on Au(111) and cleaved MoS_2 single-crystal surfaces. On the basis of the resulting maps for the electron reflectivity, Sherman function, and figure of merit, promising features of MoS_2 for use in spin-polarization detection are discussed.

[1] Thiede *et al.*, Phys. Rev. Applied **1**, 054003 (2014).
[2] Angrick *et al.*, J. Phys.: Condens. Matter **33**, 115001 (2020).
[3] Angrick *et al.*, Phys. Rev. B, accepted for publication (2025).

O 84.7 Thu 16:30 HSZ/0204

Efficient GW calculations for metals from an accurate ab initio polarizability: the case of doped MoS2 monolayer — •Giacomo Sesti[1], Pino D'Amico[1], Alberto Guandalini[2], Claudia Cardoso[1], Andrea Ferretti[1], and Daniele Varsano[1] — [1]CNR-NANO, Modena, Italy — [2]Università di Roma La Sapienza, Roma, Italy

Many-body perturbation theory in the GW approximation has proved very successful for the calculation of quasiparticle (QP) band structures of semiconductors. QP corrections are less significant in metals and are typically disregarded for the computational cost involved. Also, GW calculations of metals suffer of specific methodological challenges to properly treat the screening. This is typically solved under the addiction of a Drude term, that however is inadequate at low dimensionalities[1]. Furtherly, even for metals, QP corrections become more relevant at lower dimensionalites.

Here, we present GW calculations of QPs for doped MoS_2 monolayer showing excellent agreement with experimental ARPES measurements[2]. Such an unprecedented agreement has been possible thanks to the W-av method, which combines a Monte Carlo integration with interpolation approaches. This technique originally developed for 2D semiconductors[3] is here extended to the metallic case.

1) Champagne et al. NanoLett. 23.10 (2023)
2) Liu et al. PRL. 122 (2019)
3) Guandalini et al., npj Computational Materials, 9 (2023)

O 84.8 Thu 16:45 HSZ/0204

Ultrafast Momentum Dependent Relaxation Dynamics in $TbTe_3$ — •Florian Denizer[1], Noah Meyer[2,3], Anisha Singh[3], Ian R. Fisher[3], Uwe Bovensiepen[1], Zhi-Xun Shen[2,3], and Patrick S. Kirchmann[2] — [1]Fakultät für Physik, Universität Duisburg-Essen — [2]Department of Physics, Applied Physics and Stanford Synchrotron Radiation Laboratory, Stanford University — [3]Geballe Laboratory for Advanced Materials, Departments of Physics and Applied Physics, Stanford University

Rare-earth tritellurides (RTe_3) form charge density waves (CDW) due to electronic instabilities at the Fermi-surface, because of an anisotropy of the crystal lattice between the two major in-plane crystal axes *a* and *c*. Unoccupied electronic states can be populated by ultrafast laser excitation. Electronic relaxation

and coherent vibrational modes including the amplitude mode have been investigated by time and angle resolved photoelectron spectroscopy (*tr*-ARPES). Among the manifold of laser-driven processes, the one that is responsible for the electronic instability has not yet been identified. With this objective in mind we perform a *tr*-ARPES experiment on $TbTe_3$ and investigate the momentum transfer along the a- and the c-axis as a function of excitation strength. At sufficiently low pump fluence below $F = 0.3$ mJ/cm^2 we identify (quasi-)elastic scattering in the vicinity of the Fermi surface. In the talk we will discuss isotropic defect-induced elastic scattering and directed quasi-elastic scattering determined by the nesting vector. Funding through the DFG within SFB 1242 and through the DOE is gratefully acknowledged.

O 84.9 Thu 17:00 HSZ/0204

Unconventional Topological Superconductivity in CrCl3/NbSe2 heterostructures — •Souvik Das[1], Benjamin Zhou[2,3], Anshuman Padhi[1], Jing-Rong Ji[1], Niclas Heinsdorf[2,3], Prajwal Rigvedi[1], Tianzhe Chen[1], Weibin Li[4], Pierluigi Gargiani[4], Manuel Valvidares[4], Marcel Franz[2,3], Banabir Pal[1], and Stuart S.P. Parkin[1] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Quantum Matter Institute, University of British Columbia, Vancouver, Canada — [3]Department of Physics and Astronomy, University of British Columbia, Vancouver, Canada — [4]ALBA Synchrotron Light Source, Barcelona, Spain

Topological p-wave superconductors can host non-Abelian particles useful for fault-tolerant quantum computing. Here we report experimental evidence of unconventional topological superconductivity in a heterostructure of monolayer, in-plane ferromagnetic CrCl3 islands on superconducting NbSe2. STM measurements show that, despite CrCl3 being ferromagnetic, the interfacial superconducting gap is more robust against out-of-plane magnetic fields than the s-wave gap of NbSe2, indicating unconventional pairing. We also find enhanced zero-energy states along CrCl3 island edges, consistent with the presence of edge modes. Theory suggests these features arise from an intrinsic helical p-wave state stabilized by interfacial Rashba spin-orbit coupling. This demonstrates a new route to create topological superconductivity via interface engineering.

O 84.10 Thu 17:15 HSZ/0204

Structural and Electronic Properties of CrSBr Nanoribbons: Insights from First-Principles Calculations — •Daniil Kruklinskii, Mahdi Ghorbani-Asl, and Arkady Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Experiments show that exfoliated CrSBr flakes naturally form nanoribbons along a specific crystallographic direction, and similar structures can be fabricated using an electron beam in the TEM as a cutting tool. Here, we employ density functional theory calculations to systematically investigate the stability as well as electronic and magnetic properties of CrSBr nanoribbons. Our results indicate that nanoribbons oriented along one of the two major crystallographic directions are the most stable under typical growth and exfoliation conditions and remain semiconducting, exhibiting pronounced electron-hole separation between the VBM and CBM. In contrast, nanoribbons in the perpendicular direction display a substantially reduced band gap due to strongly localized edge states. Both orientations retain strongly spin-polarized band-edge states near the Fermi level and show only a weak dependence of the band gap on ribbon width. Using *ab initio* molecular dynamics simulations, we further demonstrate that electron-beam irradiation with energies of at least 200 keV can facilitate the fabrication of nanoribbons directly from pristine monolayer CrSBr, favouring the formation of diagonal nanoribbons. These diagonal ribbons are metallic, in contrast to the monolayer, and host a high density of majority-spin edge states, giving rise to pseudo-half-metallic transport.

O 84.11 Thu 17:30 HSZ/0204

Band-selective coherent phonon-driven band renormalization in 1T-$MoTe_2$ — •Carl Jensen[1], Christopher Emeis[2], Stephan Jauernik[1], Petra Hein[1], Fabio Caruso[2], and Michael Bauer[1,3] — [1]nstitute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Institute of Theoretical Physics and Astrophysics, Kiel University, 24098 Kiel, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Kiel University, 24118 Kiel, Germany

Understanding the coupling between coherent phonons and the electronic system is crucial for controlling nonequilibrium properties in solids. Here, we investigate mode- and band-selective electron-phonon coupling in centrosymmetric 1T-$MoTe_2$ using time- and angle-resolved photoemission spectroscopy combined with frequency-domain analysis (FDARPES). Femtosecond near-infrared pulses excite coherent Ag-symmetric phonon modes at 2.34 THz, 3.34 THz, and 3.86 THz, which manifest as oscillatory modulations in photoemission intensity and binding energy across the valence bands. Pixel-wise Fourier analysis, based on a recently developed methodology [1], reveals pronounced band selectivity with distinct coupling strengths for different electronic states and phonon modes, enabling the evaluation of band-renormalization amplitudes in the few-meV range. Ab initio calculations using DFT/DFPT qualitatively reproduce the experimentally observed coupling patterns and relative trends, demonstrating the capability of combined experimental and theoretical approaches to resolve ultrafast electron-phonon interactions in quantum materials.

[1] N. Gauthier, H. Soifer, J.A. Sobota, H. Pfau, E. J. Sie, A. M. Lindenberg, Z.-X. Shen, P. S. Kirchmann, Rev. Sci. Instrum. 96 (2025)

O 85: Vacuum Science & Technology: Theory and Applications II

Time: Thursday 15:00–17:00 Location: HSZ/0401

Invited Talk O 85.1 Thu 15:00 HSZ/0401

From light to pressure: Laser-based quantum technologies for the realization of high-precision pressure and vaccum standards — •Tom Rubin — Physikalisch-Technische Bundesanstalt (PTB), Berlin

The new realization of the pascal in the range between 1 Pa and 100 kPa is achieved by means of photonic pressure measurement. This not only enables significantly lower measurement uncertainties, but also more robust and faster-operating systems that can cover the entire pressure range continuously and for different gases. Gas-density-based methods open up new perspectives: from precise calibrations at the highest metrological level to non-invasive applications in vacuum technology and the development of innovative pressure sensors for the mass market.

This presentation is about key findings and highlights from the EU projects *QuantumPascal* and *MQB-Pascal*. These include overcoming major challenges, such as the need for sub-mK-level gas temperature knowledge, the advantages of the GAMOR (Gas Modulation Refractometry) method, and the latest results from validation and comparison measurements.

O 85.2 Thu 15:30 HSZ/0401

Near Ambient Pressure ARPES for Operando Surface Studies at Synchrotron SOLEIL — •L. Dudy[1], E. Auffray[1,2], J.-J. Gallet[1,3], F. Bournel[1,3], M. Bouaziz[3], B. S. Mun[4], S. Jang[4], Y. Tsujikawa[5], H. Kondoh[5], S. Moser[6], V. Jovic[10], V. Mischke[7], P. Kessler[8], and S. Maehl[9] — [1]Synchrotron SOLEIL, France — [2]U Paris-Saclay, France — [3]Sorbonne U, France — [4]GIST, South Korea — [5]Keio U, Japan — [6]U Bochum, Germany — [7]TU Dortmund, Germany — [8]U Würzburg, Germany — [9]SPECS, Germany — [10]GNS Science, New Zealand

We present a near-ambient pressure angle-resolved photoemission spectroscopy (NAP-ARPES) setup for operando studies of electronic structure under gas exposure at Synchrotron SOLEIL. This development bridges the gap between conventional UHV ARPES and realistic surface environments, enabling momentum-resolved measurements during catalytic and energy-related processes at pressures up to several millibars. The approach is demonstrated using model systems, showing that band structure evolution can be tracked in real-time during adsorption and reaction. These results highlight the potential of NAP-ARPES for investigating dynamic surface phenomena. By extending ARPES into near-ambient conditions, this method opens new opportunities for studying functional materials under realistic environments for operando electronic structure analysis in surface science.

O 85.3 Thu 15:45 HSZ/0401

A new framework for analysing transport ARPES applied to the current induced insulator to metal transition in Ca_2RuO_4. — •Anders Sandermann Mortensen, Hippolyte Raymond Bourel, Katarina Ogliara Praest, Davide Curcio, and Philip Hofmann — Institute of Physics and Astronomy, Aarhus University

The advent of μm-resolution spatially resolved ARPES-measurements allows for in-operando measurements of modifications to the electronic band structure of electrical devices (transport-ARPES). However, this technique poses a new set of challenges, as local biasing of the samples results in systematic shifts of the measured energy, hindering direct comparison of ARPES spectra.

Here, we propose a novel solution to this problem: Realigning the spectra by minimizing the L1-norm between them. Combined with k-means clustering, this provides an effective framework for real-time analysis and characterisation of transport-ARPES measurements.

As a proof of concept, we apply our analysis scheme to transport-ARPES measurements of the current-induced insulator to metal transition in Ca_2RuO_4, and thus provide new, high statistics measurements of the changes to the electronic band structure during the current-induced insulator to metal transition.

O 85.4 Thu 16:00 HSZ/0401

Cross-correlation measurements of a Two-Color Infrared Free-Electron Laser — •Akash Chandra Behera, América Yareth Torres Boy, Sandy Gewinner, Marco De Pas, Gert von Helden, Martin Wolf, Wieland Schöllkopf, Gerard Meijer, and Alexander Paarmann — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Infrared-Free Electron Lasers (IR-FEL) uniquely provide high-power narrowband radiation for spectroscopic measurements, that is continuously tunable from the mid-IR to the terahertz spectral range.

The IR-FEL at the Fritz Haber Institute recently commissioned a two-color upgrade, enabling simultaneous lasing at two independently tunable wavelengths. This is realized by employing a high-frequency kicker cavity to feed alternating electron bunches into the two separate undulators. Within this scheme, a high intrinsic temporal synchronization between both FEL outputs is expected.

In our contribution, we present two-color optical cross correlation measurements proving this synchronization. By leveraging the independently tunable pulse durations in each FEL, we further explore the achievable time-resolution that can be expected when the two-color FEL is employed for future IR-IR pump-probe experiments

O 85.5 Thu 16:15 HSZ/0401

K-Means Clustering of Time-Resolved Diffraction: Dynamics of Laser-Excited Si(111)-(7x7) — •Jonas D. Fortmann[1,2], Alexander Neuhaus[1], Pascal Dreher[1,3], Birk Finke[1], Christian Brand[1], and Michael Horn-von Hoegen[1] — [1]Uni Duisburg-Essen, Duisburg, Germany — [2]MAX IV, Lund, Sweden — [3]Uni Würzburg, Würzburg, Germany

We present an unsupervised analysis workflow that leverages k-means clustering to extract characteristic dynamics from time-resolved diffraction data, using ultrafast reflective high energy electron diffraction (URHEED) measurements of laser-excited Si(111)-(7x7) as a case study. Delay-dependent intensity profiles of diffraction features are clustered by trajectory shape to reveal characteristic dynamics without prior model assumptions. When combined with a simple population model, relative integral-intensity changes of clusters yield lifetimes of coupled phonon systems and trace the excitation pathway to surface electronic states. The method is robust to practical limitations (e.g., camera light sensitivity), scales to large datasets, and is directly transferable to other diffraction modalities (ULEED, UTEM, and pump-probe X-ray diffraction), where clustering of intensity evolutions can provide an objective map of structural dynamics.

O 85.6 Thu 16:30 HSZ/0401

ESEM Automation - Agent-Oriented Autonomous Microscopy — •Maurits Vuijk[1], Johannes Zeininger[2], Karsten Reuter[1], Thomas Lunkenbein[3], and Christoph Scheurer[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]TU Wien — [3]Universität Bayreuth

Are the datasets captured in usual Environmental Scanning Electron Microscopy (ESEM) experiments truly representative? While focusing on a single view or feature, critical events may occur elsewhere on the accessible surface. In addition, effects such as beam damage and inhomogeneous gas concentration introduce further need for more representative surface sampling. Starting from an automation interface to the ESEM, we have built an agent-oriented framework that enables fully autonomous ESEM experiments. To achieve this, the actions normally carried out by the human operator are instead performed by various agents. To this end, a set of agents keep up image quality by controlling brightness and contrast, focus and astigmatism without interrupting the imaging flow. A set of computer vision agents analyze captured images on the fly for interesting features and activity. Using a dynamic priority queue system, high-resolution frames are automatically taken of identified active zones. Each overview image is processed and scored based on activity, feature presence, or other desired qualities. The queue system then assigns an acquisition frequency based on the score, giving priority to more active zones. This gives a full set of overview images and multiple smaller image sets of dynamically identified active areas.

O 85.7 Thu 16:45 HSZ/0401

Image Stacking: A Simple Method to Enhance SNOM Measurements — •Florian Mangold[1], Farid Aghashirinov[1], Enrico Baù[2], Julian Schwab[1], Bettina Frank[1], Andreas Tittl[2], and Harald Giessen[1] — [1]4th Physics Institute, Research Center SCoPE, and Integrated Quantum Science and Technology Center, University of Stuttgart, Germany — [2]Nano-Institute Munich, Department of Physics, Ludwig-Maximilians Universität München, Germany

Scanning near-field optical microscopy (SNOM) enables optical characterization with spatial resolution far beyond the diffraction limit, making it a powerful tool for studying nanoscale optical and material properties. However, achieving a high signal-to-noise ratio (SNR) in SNOM can be challenging and, depending on the experimental conditions, sometimes not feasible. We present a simple and equipment-free method to enhance SNOM performance by aligning and stacking multiple sequential measurements. This procedure effectively increases the SNR while avoiding drift-induced errors and system alterations. In addition, the stacking process suppresses outliers and isolated noise contributions, further improving data quality. We demonstrate that stacked SNOM measurements can surpass the quality of single measurements under comparable conditions. This straightforward method can be broadly applied to strengthen existing SNOM experiments and opens possibilities for measurements in challenging regimes, including low-signal materials, extended wavelength ranges, and higher-order demodulation schemes where conventional single-shot SNR would be insufficient.

O 86: Surface dynamics

Time: Thursday 15:00–17:45 Location: HSZ/0403

Invited Talk O 86.1 Thu 15:00 HSZ/0403

Ultrafast Dynamics at Surfaces with Machine Learning Surrogates — •Reinhard Maurer — University of Vienna, AT — University of Goettingen, DE — University of Warwick, UK

Ultrafast dynamics at surfaces (driven by light, electrons, or hyperthermal scattering) involve the concerted motion of electrons and atoms at comparable energy and time scales, giving rise to nonadiabatic effects. Excited electrons drive chemical conversions, induce phase transitions, and mediate energy transfer between adsorbates and surfaces. To reliably predict such effects with scalable, state-of-the-art nonadiabatic dynamics simulations requires the use of accurate and data-efficient high-dimensional machine learning (ML) surrogate models. This includes representations of energy landscapes, but also nonadiabatic couplings or excited-state properties that are required for nonadiabatic simulations. I will present recent strategies to construct high-dimensional ML surrogate models of electronic structure, including active learning and fine-tuning of foundation models that allow us to reduce the required electronic structure data to a few hundred data points per gas-surface dynamics model and even transfer learn across density functional approximations. Electronic properties such as electron-phonon coupling tensors or electronic Hamiltonians can be efficiently represented by encoding physical equivariance properties in the model. I will showcase the utility of the introduced models with recent dynamics applications on reactive molecular scattering and light-driven structural dynamics.

O 86.2 Thu 15:30 HSZ/0403

Ultrafast Structural Dynamics of Layered Material Surfaces — •Alp Akbiyik[1,2], Felix Kurtz[1,2], Hannes Böckmann[1,2], and Claus Ropers[1,2] — [1]Department of Ultrafast Dynamics, Max Planck Institute for Multidisciplinary Sciences, D-37077 Göttingen, Germany — [2]University of Göttingen, 4th Physical Institute, D-37077 Göttingen, Germany

Layered materials are promising candidates for studying and applying correlated phenomena, and their carrier dynamics have been extensively investigated, including through ultrafast pump-probe techniques. However, the structural evolution of their surface layers remains poorly accessible. Ultrafast low-energy electron diffraction (ULEED) leverages the surface sensitivity of low-energy electron pulses, with high spatial resolution and temporal resolution down to 1-2 ps. This allows us to monitor the momentum-dependent out-of-plane phonon populations across the Brillouin zone as well as changes in diffraction peak intensities [1,2]. Here, we contrast the phonon equilibration behaviour of transition metal dichalcogenides (TMDCs), such as WTe2, with graphite following electron-phonon coupling.

[1] G. Storeck et al., Structural Dynamics 7, 034304, 2020.
[2] F. Kurtz et al., Nat. Mater. 23, 890-897, 2024.

O 86.3 Thu 15:45 HSZ/0403

Nonadiabatic Energy Loss in Hyperthermal Gas-Surface Scattering: Going Beyond the Mean Field Approximation — •Ash Baldwin[1] and Reinhard J. Maurer[1,2] — [1]University of Vienna, Vienna, Austria — [2]University of Warwick, Coventry, United Kingdom

Nonadiabatic energy dissipation is known to play a crucial role in hyperthermal scattering at surfaces, leading to electron-hole pair excitation and highly inelastic scattering. For projectiles with unpaired spins, such as hydrogen atoms, hybridi-

sation with the metal surface results in strong non-adiabatic effects driven by a phase transition in its spin-polarisation. It is known that traditional mean-field descriptions of the resultant nonadiabatic dynamics using methods like MDEF and Ehrenfest dynamics break down in the presence of the transition, leading to divergent energy transfer rates and unphysical stopping powers at the location of the spin transition [Box et al. *J. Phys. Chem. Lett.* 15, 51 (2024); Lindenblatt et al. *Phys. Rev. Lett.* 97 (2006)].

Here, we model H/Cu(111) and H/Ag(111) scattering in the presence of on-site correlation in the adsorbate state using the Newns-Anderson Hamiltonian. We go beyond previous works by simulating the dynamics using stochastic trajectory surface hopping methods that capture the coupling between the nuclear and electronic degrees of freedom beyond the mean-field. By systematically classifying scattering regimes, we assess the applicability of mean-field and beyond mean-field methods for predicting nonadiabatic energy loss.

O 86.4 Thu 16:00 HSZ/0403

Manipulation of charge density wave order in 1H-TaS_2 to simulate broken lattice degeneracy of misfit layered chalcogenides — •Laura Pätzold[1], Sandra Sajan[2], Clara Pfister[1,3], Haojie Guo[2], Miguel M. Ugeda[2], and Tim O. Wehling[1,3] — [1]U Hamburg — [2]DIPC San Sebastian — [3]The Hamburg Centre for Ultrafast Imaging

Misfit layer compounds, a class of van der Waals heterostructures comprised of noncommensurate layers, are ideal platforms to explore the influence of broken lattice symmetries and incommensurability on collective electronic phases, such as charge density waves (CDWs). The simulation of these symmetry-broken ground states poses a computational challenge due to large numbers of inequivalent atoms. By employing an electron-lattice downfolding scheme [1] followed by molecular dynamics (MD) simulations, we obtain the (thermo-)dynamics of these systems with the accuracy of full first-principles calculations while reducing the computational cost by several orders of magnitude. Here, we explore CDW control parameters to analyze the influence of the PbS layer in the misfit layer compound $(PbS)_{1.13}TaS_2$, where a shift in CDW order accompanied by symmetry breaking is measured in the 1H-TaS_2 layer. Simulating charge doping, interlayer hybridization effects via external potentials and frustration effects via the supercell size, we show that only a combination of these effects reproduces the characteristics of the measured structure factor while being thermodynamically stable.

[1] A. Schobert et al., *SciPost Phys.* **16**, 046 (2024)

O 86.5 Thu 16:15 HSZ/0403

Control and thermal evolution of commensurate charge-density wave order in 1H-$NbSe_2$ — •Clara Pfister[1,2], Alexander Bäder[3,4], Laura Pätzold[1], Tobias Wichmann[3], Felix Lüpke[3,4], Mariana Rossi[5], and Tim O. Wehling[1,2] — [1]I. Institut für Theoretische Physik, Universität Hamburg — [2]The Hamburg Centre for Ultrafast Imaging — [3]Peter-Grünberg-Institut, Forschungszentrum Jülich — [4]II. Physikalisches Institut, Universität zu Köln — [5]MPI für Struktur und Dynamik der Materie, Hamburg

Charge-density waves (CDWs) are symmetry-broken ground states arising from electron-lattice interactions and offer a platform to study tunable ordered phases in quasi two-dimensional materials. Using *ab initio* calculations and a downfolding approach [1], we investigate how biaxial tensile strain and electron doping affect CDW order in 1H-$NbSe_2$. In both cases, a transition from the native 3×3 to a competing 2×2 CDW ground state is induced. The strain-induced 2×2 CDW is supported by experimental data of monolayer 1H-$NbSe_2$ flakes that are rotated with respect to the underlying bulk $NbSe_2$. By constructing phase diagrams, we are able to identify the strain- and doping-induced boundaries between the competing CDW ground states. Moreover, by performing molecular dynamics (MD) simulations, we find that strain-induced 2×2 order persists up to $T_{CDW} \approx 10$ K, whereas the doping-induced 2×2 CDW is thermally much less stable. Our MD results furthermore suggest that nuclear entropy is the driving mechanism in the melting process of the CDW.

[1] A. Schobert et al., *SciPost Phys.* **16**, 046 (2024)

O 86.6 Thu 16:30 HSZ/0403

Surface Resonant Raman Scattering of Ag(110) surfaces — Sandhya Chandola[1,2], •Norbert Esser[1], Mohamed Yassine Fatihi[3], and Simone Sanna[3] — [1]Institut für Festkörperphysik,TU Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Schwarzschildstr. 8, 12489 Berlin, Germany — [3]Institut für Theoretische Physik, Heinrich-Buff-Ring 16, 35392 Gießen, Germany

The phonon and electron scattering mechanism on Ag(110) surfaces is investigated using Surface Resonant Raman scattering (SRRS) and Reflectance Anisotropy Spectroscopy (RAS) in ultra-high vacuum (UHV). The surface electronic transition is clearly visible with RAS, with Raman spectra showing surface phonons near the resonant excitation. A low energy peak is also seen, which should be related to the Rayleigh mode at the Brillouin zone edge. This shows that the surface is rough, and that the intensity of this mode depends on the sample treatment. Consequently, RAS together with Raman spectroscopy allows optimization of surface reconstruction and control of surface morphology. By means of first-principles calculations within density functional theory, we demonstrate that the dominant Raman signature is coupled to an electronic transition between localized surface-states (calculated at 1.6 eV). The corresponding surface-localized phonon mode enhances the distance between the topmost surface layers. The combined experimental and theoretical approach to resonant surface Raman spectroscopy establishes a powerful tool for investigating surface vibrational dynamics and electron-phonon interactions.

O 86.7 Thu 16:45 HSZ/0403

Spatiotemporal control of Peierls heterostructures by valley-selective photoswitching — •Hannes Böckmann[1], Jan Gerrit Horstmann[3], Felix Kurtz[1], Manuel Buriks[4], Karun Gadge[4], Salvatore Manmana[4], Stefan Wippermann[5], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, Solids and Nanostructures, University of Göttingen, Germany — [3]Department of Materials, ETH Zurich, Zürich, Switzerland — [4]Institute for Theoretical Physics, University of Göttingen, Germany — [5]Faculty of Physics, Philipps University of Marburg, Germany

Phase competition and coexistence are hallmarks of strongly-correlated materials, promising tunable functionality on the nanoscale. Light allows for tilting the balance between distinct correlated states and phases with a prominent example given by the optical switching of an insulator to a metal. However, optical excitation generally lacks the specificity to select sub-wavelength domains. In this work, we employ valley-selective photodoping of correlated electronic states to drive the domain-specific quench of a textured Peierls insulator. Specifically, we exploit the anisotropic absorption of nanowire domains by tuning both the photon energy and the polarization to the transition matrix elements most strongly coupled to the structural transformation. We find that averting dissipation facilitates domain-specific carrier confinement, control over nanotextured phases, and a prolonged lifetime of the metastable metallic state.

O 86.8 Thu 17:00 HSZ/0403

Surface resonant Raman scattering from coinage metal surfaces — •Mohamed Yassine Fatihi[1], Sandhya Chandola[2,3], Norbert Esser[2,3], and Simone Sanna[1] — [1]Institut für Theoretische Physik and Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, 35392 Gießen, Germany — [2]Helmholtz Zentrum Berlin für Materialien und Energie GmbH, 12489 Berlin, Germany — [3]Institut für Festkörperphysik, TU Berlin, 10623 Berlin, Germany

The vibrational characterization of clean metal surfaces has remained largely inaccessible to optical spectroscopy, as Raman scattering from pristine metals is extremely weak and dominated by bulk phonon backgrounds. However, the first direct Raman observation of surface phonons on a Cu(110) single crystal has been recently reported[1]. We explain this Raman activity and predict it for the related Ag(110) surface from first principles, demonstrating by means of atomistic models how tuning the incident photon energy to the surface-state transition induces a striking resonant enhancement of the surface phonon signal. This mechanism selectively amplifies the surface response with respect to the bulk contribution. Our resonant surface phonon Raman approach establishes a powerful probe for investigating surface vibrational dynamics and electron-phonon interactions, creating new opportunities for real-time studies of metallic surfaces under diverse conditions, from ultra-high vacuum to catalytic and electrochemical environments

[1] Denk, M., et al. Phys. Rev. Lett. 128, 216101 (2022).

O 86.9 Thu 17:15 HSZ/0403

Manipulation of Optical Phonons by Thermal Expansion Mismatch in Bi/Si(111) Heterostructures — •Fabian Thiemann, Maja Penkl, and Michael Horn-von Hoegen — University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

We investigate how substrate-induced biaxial strain controls the temperature behaviour of the A_{1g} phonon frequency $\Omega(T)$ in epitaxial Bi(111) films on Si(111) in the time domain. Bismuth's anisotropic A7 structure, strong electron-phonon coupling and its Peierls' distortion make the out-of-plane c-axis vibrations highly sensitive to strain. Using *in situ* SPA-LEED and broadband femtosecond transient reflectivity on the same samples, we measured temperature-dependent lattice parameters and coherent-phonon frequencies. Strained Bi films on Si(111) exhibit a larger thermal redshift $\partial\Omega/\partial T$ compared to relaxed bulk or polycrystalline Bi. Applying an extended phonon-shift model reveals that the anharmonic multi-phonon term depends solely on the value of the c-axis lattice parameter. This identifies c-axis expansion as the key structural factor governing the A_{1g} phonon, enabling targeted strain-engineering of phonon properties in bismuth and related anisotropic materials.

O 86.10 Thu 17:30 HSZ/0403

Nested Sampling Simulations of Oxygen Induced Surface Reconstructions on Cu(100) — •Felix Riccius[1,2], Hendrik H. Heenen[1], Jutta Rogal[2], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG , Berlin — [2]Flatiron Institute, New York

Under operating conditions, catalysts can undergo structural, compositional, and morphological changes, which ultimately dictate their activity and stabil-

ity. However, extensive sampling of surface configurations at finite temperature and pressure is computationally expensive and non-trivial. To this end, nested sampling simulations can be used to explore the full configuration space, estimate the partition function, and directly access the desired thermodynamic ensemble averages. We here render such simulations tractable by using them in combination with a machine-learning interatomic potential, optimize the code to run efficiently on GPUs, and tailor system specific nested sampling moves. Applied to the early oxidation of Cu(100), the approach correctly captures clean surface configurations at various oxygen coverages and the relative stability of the O adsorption sites as a function of temperature. Moreover, nested sampling successfully predicts the experimentally observed and highly complex $(2\sqrt{2} \times \sqrt{2})$ R45°-O missing-row surface reconstruction and their defect states without any human bias.

O 87: Solid-liquid interfaces: Structure, spectroscopy

Time: Thursday 15:00–17:15 Location: TRE/PHYS

O 87.1 Thu 15:00 TRE/PHYS

Interfacial Enrichment and Reactivity of Organic Molecules in Ionic Liquids — •Alisson Ceccatto Santos[1], Luciano Sanchez Merlinsky[2,3], Luis M. Baraldo[2,3], Federico J. Williams[2,3], Florian Maier[1], and Hans-Peter Steinrück[1] — [1]Lehrstuhl für Physikalische Chemie 2, Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Departamento de Química Inorgánica, Analítica y Química Física, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires — [3]Instituto de Química Física de los Materiales, Medio Ambiente y Energía, CONICET- Universidad de Buenos Aires

Controlling the surface composition of metalloporphyrins in ionic liquids (ILs) is crucial for designing photoactive materials. Here, we investigate the interfacial behavior of zinc-didodecylporphyrin molecules (Zn-DDP) dissolved in the 1-butyl-3-methylimidazolium hexafluorophosphate [C4C1Im][PF6] IL using angle-resolved X-ray photoelectron spectroscopy (ARXPS). Upon mild heating, Zn-DDP undergoes spontaneous demetallation, evidenced by the appearance of aminic (-NH-) and iminic (=N-) nitrogen XPS signals. Our measurements reveal extremely high surface enrichment of porphyrins at the IL/vacuum interface, with the dodecyl chains oriented toward the vacuum. ARXP spectra reveal that the surface enrichment increases with increasing temperature. Our findings provide molecular-level insights to guide the design of photoactive interfaces in IL systems. Acknowledgements: Alexander von Humboldt Foundation for a Humboldt Research Fellowship for postdocs

O 87.2 Thu 15:15 TRE/PHYS

How is the hydrophobic force modified by an oscillation frequency in saline conditions? — •Chiara Wagner, Paul Stöcher, Laura Mears, and Markus Valtiner — Vienna University of Technology, Vienna, Austria

There have been many investigations over the years regarding the mechanism behind the hydrophobic force and over how long a range it can be felt [1]. We present a detailed set of AFM force measurements of hydrophobic SAM modified surfaces, with varying salt concentration and oscillation frequency (0-2kHz). We observe dynamic changes in the force curve characteristics with both salt concentration and oscillation frequency. The changes lead to a reduction of the average force with increasing applied frequency, while multiple distinct characteristic curves are present and enhanced by certain conditions. We also notice changes in the range of the force away from the surface. Altogether, the results we will present bring new insight into the mechanism of hydrophobic interactions.

[1] W. A. Ducker and D. Mastropietro, Current Opinion in Colloid & Interface Science, 2016, 22, 51*58.

O 87.3 Thu 15:30 TRE/PHYS

Interfacial non-Markovian friction determines non-linear spectral shifts at the water-graphene interface — •Johannes Schröter, Louis Lehmann, Shane Carlson, and Roland R. Netz — FU Berlin, Fachbereich Physik, Arnimallee 14 14195 Berlin

Understanding the behavior of aqueous interfaces is crucial for various applications. In particular, the graphene water interface plays a key role for energy storage and energy conversion, however, its properties remain poorly understood. Using DFT molecular dynamics simulations we show that the sum-frequency signal of non-hydrogen bonded OH bonds is significantly red-shifted at the water-graphene compared to the water-air interface, in agreement with recent experiments. The red shift is demonstrated to be caused by non-Markovian friction between the graphene surface and interfacial water, which offers a direct method to extract solid-water interfacial friction properties from non-linear spectroscopy.

O 87.4 Thu 15:45 TRE/PHYS

Structural Stability of NaCl and KCl Cleavage Surfaces in the BMIM-PF6 Ionic Liquid — •Ebru Cihan[1], Natalia Janiszewska[2], Kamil Awsiuk[2], Qingwei Gao[3], Rong An[4], Ronen Berkovich[5], and Enrico Gnecco[2] — [1]TU Dresden, Dresden, Germany — [2]Jagiellonian University, Krakow, Poland — [3]Shanghai University of Electric Power, Shanghai, China — [4]Nanjing University of Science and Technology, Nanjing, China — [5]Ben-Gurion University of the Negev, Beer-Sheva, Israel

An investigation was conducted into the evolution of freshly cleaved NaCl(100) and KCl(100) surfaces exposed to the ionic liquid (IL) 1-butyl-3-methylimidazolium hexafluorophosphate (BMIM-PF6). The surfaces were repeatedly scraped using AFM, resulting in contrasting responses from the two surfaces to the IL. In the case of NaCl, the cleavage step edges are slightly eroded, and the surface is progressively smoothed by the AFM tip. These changes are accompanied by a continuous increase in the friction force. In the case of KCl, a pronounced dissolution of the surface is evident immediately following contact with the IL. The surface is then smeared in the area scratched by the tip and even beyond. An increase in the friction force is also observed but only at the onset of the surface modification process. Crystallites (100-200 nm in size) are observed across the unscratched areas of KCl, but not of NaCl. This result was corroborated by MD simulations and Raman spectroscopy, which revealed that IL exhibits a stronger interaction with the KCl surface, ultimately forming a BMIM-PF6 adlayer. [1] E. Cihan et al., Langmuir 41, 13793 (2025)

O 87.5 Thu 16:00 TRE/PHYS

How Water Controls Ion Adsorption at Aqueous Interfaces via Entropic and Dielectric Interplay — •Florian Altmann[1], Matteo Olgiati[1], Moritz Zelenka[2], Joanna Dziadkowiec[3], Andreas Kretschmer[1], Alper T. Celebi[1], Laura L.E. Mears[1], Ellen H.G. Backus[2], and Markus Valtiner[1] — [1]Vienna University of Technology, Institute of Applied Physics, Wiedner Hauptstrasse 8-10, A-1040, Vienna, Austria — [2]University of Vienna, Faculty of Chemistry, Institute of Physical Chemistry, Währinger Straße 42, 1090 Vienna, Austria — [3]NJORD Centre, Department of Physics, University of Oslo, Oslo 0371, Norway

Ion-specific behavior at aqueous interfaces remains poorly understood. Using Li^+, Ca^{2+}, and Cs^+, we combine quantitative atomic force microscopy on muscovite mica with molecular dynamics simulations and sum-frequency generation spectroscopy to resolve interfacial thermodynamics at molecular resolution. Pair correlation functions link ion-water-surface organization to entropy and electrostatics. Small or highly charged ions compact interfacial water, creating entropic penalties and strong dielectric screening, whereas larger ions deplete interfacial water, lower screening, and promote overadsorption. This interplay between entropy and screening governs inner double-layer formation and provides a molecular framework for ion-specific adsorption in complex electrolytes.

O 87.6 Thu 16:15 TRE/PHYS

Accessing interfaces of ionic liquids in vacuum — •Florian Maier and Hans-Peter Steinrück — Lehrstuhl Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg

About one decade ago, the perspective "Surface science goes liquid" described possibilities of investigating surfaces and interfaces of vacuum-stable liquids with surface science tools under ultrahigh vacuum (UHV).[1]

Since then, new experimental concepts and setups have been developed considering the special requirements for handling ionic liquids (ILs) in vacuum in order to push the boundaries of surface science experiments further.

In this presentation, some of our experimental developments including key showcases will be presented demonstrating at which level molecular properties of IL interfaces can be accessed under ultra-clean and well-defined UHV conditions.

[1] H.-P. Steinrück, 2010, Surf. Sci. 604, 481-484
DOI: 10.1016/j.susc.2009.12.033.

O 87.7 Thu 16:30 TRE/PHYS

Beyond the Electric Dipole Approximation: Electric and Magnetic Multipole Contributions Reveal Biaxial Water Structure from SFG Spectra at the Air-Water Interface — •Louis Lehmann[1], Maximilian R. Becker[1], Lucas Tepper[1], Alexander P. Fellows[2], Álvaro Díaz Duque[2], Martin Thämer[2], Martin Wolf[2], and Roland R. Netz[1] — [1]Department of Physics, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Sum-frequency generation (SFG) analysis has been hindered by the lack of quantitative predictions for higher-order multipole contributions. Magnetic dipole and electric quadrupole terms, though determined by bulk properties, appear in all SFG spectra and obscure connections to interfacial structure. We present a simulation-based framework that predicts all multipole contributions and provides depth-resolved spectra for precise localization of features. Applied to the

air-water interface, it reproduces experimental spectra across polarization combinations in both bending and stretching regions. Higher-order multipoles are essential: in the bending band, electric and magnetic dipoles are comparable, while the quadrupole dominates; in the OH-stretch region, the quadrupole accounts for the 3600/cm shoulder. Isolating the true second-order electric-dipole susceptibility reveals pronounced biaxial ordering of interfacial water and enables reliable interfacial structure determination from SFG spectra.

O 87.8 Thu 16:45 TRE/PHYS

Heat transfer across nanometre-sized water meniscus — •Oscar Mateos[1], Ruben Lopez[2], Pablo Martinez[1,3], Guilherme Vilhena[1], Nicolas Agrait[2,4], and Juan Carlos Cuevas[3,4] — [1]Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), 28049 Madrid, Spain — [2]Departmento de Física de la Materia Condensada, Universidad Autónoma de Madrid, 28049 Madrid, Spain — [3]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, 28049 Madrid, Spain — [4]Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049 Madrid, Spain

Heat transfer in nanoscale gaps is of key relevance for a variety of technologies. Recent experiments have reported contradictory results shedding doubts about the mechanisms for heat exchange in nanometre-sized gaps. We aim at resolving this controversy by measuring the thermal conductance of gold atomic-sized contacts with a custom-designed scanning tunnelling microscope that incorporates a novel thermal probe, enabling the measurement of thermal and electrical conductance in different transport regimes. When the electrodes are separated by a nanometre-sized gap, we observe thermal signals which cannot be explained with standard heat transfer mechanisms. Through non-equilibrium molecular dynamic simulations, we elucidate that these anomalous signals are due to thermal conduction through water menisci that form between tip and sample under customary operation conditions.

O 87.9 Thu 17:00 TRE/PHYS

Charging dynamics of the electrical double-layer in nanometre sized channels — •Marco Schönig, Serge Lemay, and Marc Koper — Leiden University, Leiden, The Netherlands

Nanoporous electrodes play a crucial role in modern energy storage and conversion technologies. However, despite their ubiquitous usage, the impact of nanoscale geometrical confinement on their electrochemical properties remains poorly understood. This is particularly relevant when the pore dimensions become so confined that the double layers of opposing sides overlap. A key challenge in studying this phenomenon in a systematic manner is the necessary precise control of the experimental dimensions[1]. We aim to bridge this gap by utilizing modern nanofabrication techniques to fabricate model gold slit electrodes[2].

In this contribution, we present the charging behaviour of electrodes with 5 - 20 nm wide slits, under confined and unconfined conditions. We further explore the usage of ATR-IR spectroscopy to probe the electrolyte in the slit electrodes by using micro-grooved Si wafers as substrate[3].

References [1] J. Wordsworth et al. Angew. Chem. Int. Ed. 2022, 61, e202200755; [2] L. Rassaei et al. J. Phys. Chem. C 2012, 116, 10913; [3] T. A. Morhart et al. Anal. Chem. 2017, 89, 11818.

O 88: Catalysis and surface reactions III

Time: Thursday 15:00–17:45 Location: TRE/MATH

O 88.1 Thu 15:00 TRE/MATH

Trapping ionomer for efficient proton exchange membrane fuel cells — •Fanpeng Kong — Harbin Institute of Technology, Harbin, China

Both uniformity of ionomer distribution and adsorption dynamics of side-chain sulfonates are paramount in determining the performance of low Pt-loaded membrane electrode assembly (MEA), particularly at high current densities. However, the heterogeneity of Pt/C leads to strong sulfonate anion adsorption on Pt sites and deleterious ionomer aggregation on the carbon support. Here, we synthesize atomic dipole modulated Pt/C (SCDC-Pt) electrocatalysts for low Pt-loaded MEA. Remarkably,this catalyst delivers a superior peak power density (1.4 W cm-2) and only a 15% of activity loss after 30 000 square-wave cycles. Operando characterization and computational analysis demonstrate that surface charged dipole facilitates homogenous ionomer distribution, while mitigating sulfonate poisoning of Pt. Electrochemical diagnostic technique establishes the low sulfonate coverage (~8%) and local O2 transport resistance (38.6 S m-1).This finding demonstrates the viability of rationally designed high-performance surface composition-homogenization low Pt-loaded MEA.

O 88.2 Thu 15:15 TRE/MATH

Molecular Beam Surface Scattering and PECD to Probe Chirality in Surface Reaction Products — Arved Dorst[1,2], Johannes Diedrich[1,2], Rasika Dissayanake[1,2], and •Tim Schäfer[1,2] — [1]Georg-August-University of Göttingen, Germany — [2]Max-Planck Institute for Multidisciplinary Sciences, Göttingen, Germany

The epoxidation of olefins on Ag/O systems is an important industrial heterogeneous catalytic process. However, the mechanistic details of the surface reaction remain controversial, and it has been highly challenging to reconcile findings obtained under realistic reaction conditions with the highly detailed but static studies performed under ultra-high vacuum (UHV).

An additional level of complexity and opportunity arises when using prochiral olefin molecules. Their epoxidation can yield chiral epoxide products, provided the reaction pathway can be directed toward one enantiomer. In our studies, we combine molecular-beam surface scattering with laser spectroscopy to probe this process. By detecting the photoelectron circular dichroism (PECD) of the reaction products, we are able to determine their absolute chirality.

Our overarching goal is to achieve an atomistic understanding of reaction dynamics on chiral surfaces, ultimately bridging the gap between UHV studies and catalytic behavior under operational conditions.

O 88.3 Thu 15:30 TRE/MATH

From Processes to Mechanisms: Machine-Learning Based Automated Lattice Mapping as Prerequisite to Microkinetic Modeling — •Aditya Kumar[1], Patricia Poths[1], King Chun Lai[2], Christoph Scheurer[1], Sebastian Matera[1], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Max Planck Computing and Data Facility, Garching

Finding the reaction mechanism of a surface reactive system from first principles is a tedious task requiring a lot of human effort and being affected by human bias. To address these points, we have developed the Automatic Process Explorer (APE), which generates a comprehensive library of elementary reaction steps [1]. With easily thousands of steps identified, their manual assembly into a reaction network as a prerequisite to subsequent microkinetic modeling becomes intractable. To this end, we develop an automated framework that infers an effective lattice onto which all APE-discovered elementary steps may be coarse-grained. In this, atomic configurations from APE are analyzed using density-based hierarchical clustering, creating a fine-to-coarse hierarchy of potential lattice sites. All processes are then mapped onto the lattice as discrete occupation changes and, exploiting symmetry, a network of unique elementary reactions on this lattice is generated. We demonstrate the approach for a large set of elementary processes within the initial oxidation of Pd(100) terrace edges, and discuss the feasibility of subsequent efficient lattice-based microkinetic simulations.

[1] K.C. Lai *et al.*, Phys. Rev. Lett. **134**, 096201 (2025).

O 88.4 Thu 15:45 TRE/MATH

Investigating the Promotion Mechanism of Lanthanum on Cobalt Model Catalysts for Ammonia Production — •Clara C. Aletsee, Lau H. Wandall, Emanuel Biletter, and Ib Chorkendorff — DTU, Copenhagen, Denmark

Developing catalysts for ammonia synthesis under milder conditions than the Haber-Bosch process has gained significant interest. Recent studies demonstrate that usually unreactive magnetic materials, such as cobalt, can be activated for NH_3 synthesis by adding lanthanum.(1,2) According to theoretical calculations, this is attributed to not only an electrostatic, but also a beneficial spin promotion effect.(3) Herein, we examine the role of the promoter form on the catalytic performance. For this, either metallic La or La_2O_3 was deposited on a stepped Co(10-115) single crystal surface via e-beam evaporation. Additionally, mass-selected Co nanoparticles were deposited on two different magnetron-sputtered film supports: LaN and La_2O_3. All catalysts were characterized by X-ray photoelectron spectroscopy and low-energy ion scattering before and after reaction, and their activity was measured between 350-500°C at 1 bar in a UHV-compatible cell.(4) We show that Co/La_2O_3 exhibits the same activity as the LaN supported catalyst system at 350°C, but the stability decreases at higher temperatures.

References: (1) K. Zhang et al., Science 383, 1357 (2024). (2) T. N. et al., Nature 583, 391 (2020). (3) A. Cao et al., Nat Commun. 13 (2022). (4) K. Zhang et al., Rev. Sci. Instrum. 94, 114102 (2023).

O 88.5 Thu 16:00 TRE/MATH

Bridging the Pressure and Materials Gaps in NO Adsorption on Ceria — •Lukas Bolz[1], Ali Essa[1], Zairan Yu[1], Alexei Nefedov[1], Julia Vecchietti[2], Adrian Bonivardi[3], Yuemin Wang[1], and Christof Wöll[1] — [1]Insitute of Functional Interfaces, KIT, Eggenstein-Leopoldshafen, Germany — [2]Instituto de Desarrollo Tecnológico para la Industria Química, UNL, Santa Fe, Argentina — [3]Facultad de Ingenieria, UBA, Buenos Aires, Argentina

Nitric oxide (NO) is well known to have adverse effects on human health and the environment. One effective approach to decrease its emission is the selective catalytic reduction of NO over metal oxide surfaces. Understanding the reaction mechanisms, by tracking the structural changes of the active sites and intermediates as a function of reaction atmosphere and temperature, is crucial. Here, we present results on UHV-IRRAS and FTIRS as well as in situ/operando DRIFTS studies at atmospheric pressures and elevated temperatures to investigate the interaction between NO and ceria (CeO_2). A reliable assignment of the IR bands observed in the complex DRIFTS spectra was achieved based on accurate references obtained for NO molecules adsorbed on single crystal surfaces and nanocrystalline powders, thereby bridging the material and pressure gap for oxidic catalysts. The combined results enabled the tracking of facet-dependent surface transformations, the adsorption and reaction of NO, and the formation of intermediates such as nitrous oxide (N_2O). This work was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - Project-ID 426888090 - SFB 1441, project B03 and A04.

O 88.6 Thu 16:15 TRE/MATH

Competing reaction pathways in decomposition of 2-propanol over V-doped Co3O4(111) model catalyst: a mechanistic study. — •Patrick Hubert[1], Jan Smyczek[1], Maximilian Galinski[1], Lina Marquardt[1], Justin Girschik[1], Philipp Fredersdorff[1], Paul Fröhlich[1], Bernd Hartke[1], Guntram Rauhut[2], and Swetlana Schauermann[1] — [1]Institute of Physical Chemistry, Christian-Albrechts-University Kiel, Max-Eyth-Str. 1, 24118 Kiel, Germany. — [2]Insitute of Theoretical Chemistry, University of Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart, Germany.

This study investigated catalytic decomposition of 2-propanol over Co_3O_4(111)/Au(111) and VO_x/Co_3O_4(111)/Au(111) model catalysts to unravel competing reaction pathways toward acetone or propene. Ultra-high vacuum (UHV) surface science techniques were employed, including scanning-tunneling microscopy (STM), molecular-beam methods, infrared reflection absorption spectroscopy (IRAS), and temperature-programmed desorption (TPD). The VO_x/Co_3O_4(111)/Au(111) surface exhibits structures with V^{3+}, V^{4+} adsorption sites and vanadyl groups (V=O). TPD measurements showed propene desorption at 480 K from 2-propanol adsorbed at 100 K on surfaces exceeding 0.6 ML VO_x coverage. At 180 K, 2-propanol dissociatively adsorbs on VO_x, consuming vanadyl groups during OH deprotonation, forming tilted 2-propoxy with surface-proximal methyl groups. At 400 K, a second intermediate forms via C-O bond scission and methyl deprotonation. IR spectra suggest this intermediate is a surface-bound propene-derived species.

O 88.7 Thu 16:30 TRE/MATH

Beyond U-Ce charge transfer: stabilization of Ce^{3+} states in epitaxial $Ce_{1-x}U_xO_2$ films grown on Ru(0001) — •Carlos Morales[1], Rudi Tschammer[1], Thomas Gouder[2], Hicham Idriss[3], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, Brandenburg University of Technology, Cottbus, Germany — [2]European Commission, Joint Research Centre (JRC), Karlsruhe, Germany — [3]Institute of Functional Interfaces (IFG), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Cerium oxide (CeO_2) stands out among reducible metal oxides for its stability and activity. Yet, promoting Ce^{3+} active states requires high energy. The conversion of Ce^{4+} to Ce^{3+} at lower temperatures for the thermochemical splitting of H_2O or CO_2 can be enhanced by doping ceria with other elements. Particularly, ceria mixing with uranium has been proven successful: substituting a fraction of Ce^{4+} by U^{4+} results in a charge transfer that promotes the formation of Ce^{3+} and U^{5+} states. We have explored the redox properties of 8 nm thick epitaxial (111)-oriented $Ce_{1-x}U_xO_2$ on Ru(0001). In line with previous studies focused on polycrystalline powders, the as-grown films exhibit a high Ce^{4+} to Ce^{3+} conversion, with a maximum reduction corresponding to approximately 20 % of U content. However, the concentration of Ce^{3+} states and oxygen is higher than predicted by density function theory (DFT) calculations for various U contents and spatial ordering. The observed behaviour could be likely related to the lattice distortion caused by the significant difference in the ionic radii of Ce^{3+} and U^{5+}. This effect has not been considered before in $Ce_{1-x}U_xO_2$ mixed oxides.

O 88.8 Thu 16:45 TRE/MATH

Product Selectivity in Fischer-Tropsch Synthesis — •Benjamin Rasmus Grimm, Luis Antonio Cipriano Marcos, Oliver Christensen, and Jens Kehlet Nørskov — DTU Physics, Kongens Lyngby, Denmark

The product selectivity and activity of Fischer-Tropsch synthesis (FTS) is important for producing synthetic fuels and chemicals from natural gas, coal, or biomass. Some catalysts generate mainly undesired methane, whereas others show higher selectivity toward longer hydrocarbons. In this study, density functional theory (DFT) is employed to calculate the activity- and selectivity-determining reaction steps and energy barriers of FTS on cobalt-based catalysts. Reaction rates and product selectivities are then evaluated using a microkinetic model that incorporates the rate- and selectivity-determining steps of the FTS mechanism. To describe the catalyst as realistically as possible, adsorbate coverage and migration effects under experimental conditions are taken into account. Finally, strategies to improve reaction rates and selectivity are discussed.

O 88.9 Thu 17:00 TRE/MATH

Low-Temperature CO2 Methanation over Ni/Ce-Sm Oxide Catalysts — •Rachow Fabian, Sichen Liu, Evgenia Charlafti, Raquel Sánchez-Barquilla, and Jan Ingo Flege — Brandenburg University of Technology, Cottbus-Senftenberg, Germany

Nickel catalysts on doped ceria are attractive for CO_2 methanation due to their redox flexibility and potential for improved efficiency and stability. In this work, we investigate Ni supported on mixed Ce–Sm oxides with Ce:Sm ratios of 3:1, 2:1, and 1:1. The catalysts are tested as powders in a fixed-bed flow reactor between 250 and 400°C and benchmarked against a conventional Ni/Al_2O_3 catalyst. Among the compositions, the Ce:Sm ratio of 2:1 shows the highest CO_2 conversion, with a pronounced enhancement in low-temperature activity compared to Ni/Al_2O_3. To relate performance to material properties, we combine X-ray diffraction (XRD), temperature-programmed reactivity (H_2-TPR), Raman spectroscopy, high-resolution transmission electron microscopy (HRTEM/EDX), as well as in-situ X-ray absorption near-edge spectroscopy (XANES) under reaction conditions, elucidating how Sm incorporation and Ce:Sm ratio influence the structural and redox characteristics of the oxide support, oxygen vacancy formation, and Ni dispersion, which together govern catalytic activity and stability. To assess practical applicability and scale-up, the optimized Ni/Ce–Sm (2:1) oxide formulation is deposited on Al_2O_3 spheres and evaluated under conditions representative of packed-bed operation with a limited amount of active material, revealing high conversion and stable, efficient operation in low-temperature CO_2 methanation.

O 88.10 Thu 17:15 TRE/MATH

Heteroepitaxial growth of Sm_2O_3 nanoislands on Cu(111) — •Björn Riedel[1], Raquel Sánchez-Barquilla[1], Lars Buss[1], Iulia Cojocariu[2], Tevfik Onur Mentes[2], Andrea Locatelli[2], and Jan Ingo Flege[1] — [1]Brandenburg University of Technology, Cottbus, Germany — [2]Elettra-Sincrotrone Trieste, Basovizza, Italy

Doping of CeO_2 with samarium can significantly influence its redox behavior by promoting the formation and stabilization of reduced Ce^{3+} species. Yet, studies of well-defined samaria model systems grown on single-crystal surfaces are scarce, leading to a lack of combined structural and spectroscopic studies and, hence, a gap in understanding the relationship between samaria's structure and its chemical behavior. We have investigated hexagonal and monoclinic Sm_2O_3 nanoislands grown on Cu(111) using a multi-method approach with high structural and chemical sensitivity, employing low-energy electron microscopy (LEEM), micro-spot diffraction (μLEED) and intensity-voltage LEEM in combination with X-ray absorption spectroscopy photoemission electron microscopy (XAS-PEEM). To study the influence of different structures and phases on the chemical behavior of Sm_2O_3 islands, we have examined their redox properties under reducing (H_2) and oxidizing (O_2) conditions. The results indicate a highly dynamic system that can be readily adjusted by varying the conditions during deposition, such as growth temperature and oxygen partial pressure.

O 88.11 Thu 17:30 TRE/MATH

Surface Modifications in Complex Mixed Oxide Activation for the Selective Oxidation of Hydrocarbons — •Kyeonghyeon Nam[1], L. Masliuk[1], T. Jones[1], Y. Song[1], A. Trunschke[1], R. Schlögl[1], T. Lunkenbein[1,2], K. Reuter[1], and C. Scheuer[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Universität Bayreuth

Calcination (thermal activation) is crucial for metal-oxide catalysts, enhancing activity and durability by preparing surface morphology and active sites. However, thermal treatment also induces dynamic surface changes, such as defect formation, reconstruction, and grain reorientation, complicating the continuous monitoring of a catalyst's surface. Here, identical-location STEM imaging of a ternary M1 $(Mo,V)O_x$ catalyst reveals that the (hk0) surface undergoes pronounced modification under calcination and oxidative dehydrogenation (ODH) conditions. The surface evolution is modeled using machine learning force fields. Molecular dynamics (MD) simulations reproduce the reconstruction of extended M1 regions from MoO_2-like motifs, as well as mass transport within the pentagonal motif that further activates the catalyst. Experimentally observed catalytic activity changes can be assigned to the presence of highly charged surface metal centers via DFTB Mulliken charge analysis. These surface transformations strongly influence the catalytic properties of ternary M1 catalysts, suggesting potential applications in improving catalytic performance through controlled surface modifications.

O 89: Spins on surfaces at the atomic scale II

Time: Thursday 15:00–18:00 Location: WILL/A317

O 89.1 Thu 15:00 WILL/A317

Magnetization Curves of Antiferromagnetic Spin Chains: Probing the Quantum to Classical Crossover — •Henrik Lichtl[1,2], Lukas Veldman[1,2], Nicolaj Betz[1,2], Johannes Schust[1], Laëtitia Farinacci[1,3], Fernando Delgado[4], Susanne Baumann[1], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies. — [2]Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart. — [3]Carl-Zeiss- Stiftung Center for Quantum Photonics Jena - Stuttgart - Ulm. — [4]Instituto de Estudios Avanzados IUDEA, Departamento de Física, Universidad de La Laguna.

As the size of a magnetic structure increases it undergoes a transition from a quantum system to a classical magnet, yet the evolution of the magnetization behavior at this crossover is largely unexplored. Here we introduce an approach to record high-speed magnetization curves in a scanning tunneling microscope (STM), reaching magnetic field sweep rates of up to 40kT/s. We analyze the statistics of the transitions between the two antiferromagnetic ground states of antiferromagnetic Fe spin chains on a Cu2N surface, which allows us to distinguish between quantum and classical regimes in their magnetization curves. Quantum signatures diminish rapidly with size of the chain, where chains longer than five atoms already show characteristics of classical nanoscale magnets. Accessing such high-speed magnetization curves at the atomic scale brings concepts originally developed for bulk materials into the STM, offering insight into how quantum spins interact with their environment during the quantum-to-classical transition.

O 89.2 Thu 15:15 WILL/A317

Optimizing On-Surface Quantum Spins for Quantum Information Processing — •Denis Jankovic[1,2], Hoang-Anh Le[1,2], Saba Taherpour[1,3], and Christoph Wolf[1,2] — [1]Center for Quantum Nanoscience, Institute for Basic Science, Seoul, Republic of Korea — [2]Ewha Womans University, Seoul, Republic of Korea — [3]Departement of Physics, Ewha Womans University, Seoul, Republic of Korea

The bottom-up engineering of quantum-coherent spins on surfaces with STM enables atomically precise quantum logic in on-surface qubits, and atomic-scale multi-qubit devices.

We use optimal control on an open-system model of exchange-coupled surface spins to counter decoherence, static coupling, and imperfect initialization, identifying high-fidelity gates compatible with current ESR-STM constraints.

Finally, building on advances in electrically driven nuclear spins, we will outline ongoing experiments using lanthanides on surfaces, where ESR-STM manipulates hyperfine-coupled nuclear-spin manifolds as on-surface qudits.

O 89.3 Thu 15:30 WILL/A317

Spin Lifetime Engineering using Superconducting Surfaces — •Máté Stark, Luise Renz, Jonas Arnold, Johannes Schwenk, Christoph Sürgers, Wolfgang Wernsdorfer, and Philip Willke — Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany

Extending the spin lifetime (T_1) and decoherence time (T_2) of atomic and molecular spins is central to realizing quantum-coherent spin systems on surfaces studied by scanning tunneling microscopy (STM). For instance, previous studies have demonstrated that T_1 can be extended to nanoseconds for Fe-OEP-Cl on superconducting Pb(111) to milliseconds for Fe on MgO/Ag(001) by exploiting superconducting protection or electronic decoupling, respectively [1,2].

Building on these concepts, we aim here to combine protection by a superconducting gap and insulating decoupling layers to explore and control spin lifetimes of single FePc spins. By switching from the normal-conducting into the superconducting state we discuss how superconductivity as well as decoupling from the substrate and tip govern the lifetime and dynamics of molecular spin excitations. We show first results using all electric pump-probe spectroscopy, which are performed in a home-built dilution refrigerator scanning tunneling microscope operating at 50 mK.

[1] Nat. Phys. 9, 765 (2013)
[2] Nat. Phys. 13, 403 (2017)

O 89.4 Thu 15:45 WILL/A317

Bottom-up realization of band structure using arrays of individual Cs atoms on InSb(110) — •Niek M.M. Aarts, Kira Junghans, Roel Burgwal, Daniel Wegner, and Alexander A. Khajetoorians — Institute for Molecules and Materials, Radboud Universiteit, Nijmegen, Netherlands

The combination of atomic manipulation and scanning tunneling spectroscopy has become a powerful platform for quantum simulation of electronic structure. The approach is based on the atomically precise placement of atoms and the flexibility to realize structures with a variety of shapes and symmetry. Inherent to this approach is role of finite size effects in the tailored electronic structure. This plays an integral role in understanding the influence of various interactions, like spin-orbit interactions, or electron-electron interactions, on any potential quantum phase of matter to be simulated.

Here, we study the evolution of the electronic structure as a function of lattice size, using the recently discovered quantum simulator platform of Cs on InSb(110). Using STM, we start by studying structures that exhibit atomic like states and expand these structures into the molecular limit. We study the changes in the localized states and the symmetry of the responsible wavefunctions. We then quantify the increase of states as the number of sites in the system increases, and band structure emerges. We also discuss the role of the size of the artificial atomic sites. This extension of the Cs/InSb(110) quantum simulator to larger systems enables the study of artificial band structure in the presence of strong SOC.

O 89.5 Thu 16:00 WILL/A317

Crystal field manipulation of magnetic atoms on an insulating surface — •Julian Zeitler[1], Johannes Schust[1], Nicolaj Betz[1,2], Lara Mezger[1], Lukas Veldman[1], Laëtitia Farinacci[1,3], Fernando Delgado[4], Philip Willke[5], Sebastian Loth[1,2], and Susanne Baumann[1] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies. — [2]Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart. — [3]Carl-Zeiss-Stiftung Center for Quantum Photonics Jena - Stuttgart - Ulm. — [4]Instituto de Estudios Avanzados IUDEA, Departamento de Física, Universidad de La Laguna. — [5]Karlsruhe Institute of Technology, Physikalisches Institut.

The magnetic behavior of ions in solid-state materials is predominantly driven by their immediate atomic-scale environment. The specific arrangement of surrounding charges creates a crystal field (CF), which alters and mixes the electronic states. For magnetic atoms on insulating thin films, this CF is strongly influenced by the atom's adsorption site on the underlying lattice. Using combined scanning tunneling microscopy (STM) and atomic force microscopy (AFM), we investigate the CF influence on magnetic atoms on thin-film MgO and use tip-atom forces to precisely reposition the atoms within their binding sites, thereby tuning the CF. We quantify changes of the local binding geometry by combining our measurements with multiplet calculations. Our measurements pave the way for harnessing magneto-elastic effects in individual atoms either by manipulating their magnetic properties via electric fields or local forces, such as mechanical strain.

O 89.6 Thu 16:15 WILL/A317

Topological End States of Chiral Graphene Nanoribbons on Proximitized Superconducting Au (111) — •Trisha Sai[1], Frederik Bauer[1], Stefano Trivini[1], and Jose Ignacio Pascual[1,2] — [1]CIC nanoGUNE-BRTA, 20018 Donostia-San Sebastián, Spain — [2]Ikerbasque, Basque Foundation for Science, 48013 Bilbao, Spain

Graphene nano-structures may host localized magnetic moments characterized by their geometry, heteroatom substitution, topological frustration, or bulk-boundary correspondence. However, observation of their open-shell configuration via on-surface synthesis can be inhibited due to charge transfer. This is in the case of (3, 2, 8) chiral graphene nanoribbons (chGNRs) synthesized on Au(111), whose symmetry-protected topological end states (SPTES) are quenched due to electron depopulation. In this work, we synthesize (3, 2, 8) chGNRs on thin films of Au (111) grown on a superconducting Nb (110) single crystal. Through controlled deposition of monolayers of Au, we observe a modulation in the surface state of Au (111), thereby a reduction in the work function of the resulting platform. Moreover, the substrate is also complemented with proximity induced superconductivity. Low-Temperature scanning tunneling spectroscopic (STS) measurements reveal that the SPTES of (3, 2, 8) chGNRs are retained in a mixed-valence regime where their spectral weight is distributed between an in gap Yu-Shiba-Rusinov (YSR) state and an orbital state close to Fermi energy. In case of a depopulated terminus, the YSR states are weak and suppressed while the orbital state is more pronounced.

O 89.7 Thu 16:30 WILL/A317

Confinement-modulated spin-orbit coupling tuned with atomic-scale gating fields — •Hermann Osterhage, Julian H. Strik, Anna M. H. Krieg, Ivan Ado, Mikhail Titov, Daniel Wegner, and Alexander A. Khajetoorians — Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands

In 2D, inversion symmetry breaking combined with a sizeable potential gradient leads to the well-known Rashba spin-orbit coupling (SOC), locking the spin and momentum. Using potential gradients to induce SOC is not limited to the Rashba case, but may be extended to lower dimensional structures, such as quantum dots. However, tuning SOC in these limits is challenging: it requires potential gradients that are comparable to the size of the confined structure itself.

Here, we demonstrate a new type of SOC, akin to the Rashba effect, where large potential gradients are formed within an atomically patterned quantum

dot. Using low-temperature scanning tunnelling microscopy and spectroscopy we create quantum dots of various shapes and sizes by patterning individual Cs ions on the surface of InSb(110). We find that we can tune the confinement potential, as shown by the presence of multiple localized states. In addition, by probing the resultant multiplet structure, we identify zero-field splittings within a given quantum dot that are induced by the geometry of the potential. We also discuss the magnetic field dependence of this level structure and explain the findings based on the 8-band Kane model.
[1] E. Sierda et al, Science 380, 1048 (2023).

O 89.8 Thu 16:45 WILL/A317

Tuning the Kondo temperature of MoS_2 mirror twin boundaries on graphene — •Tfyeche Y. Tounsi[1], Kuber Vyas[1], Camiel van Efferen[1], Affan Safeer[1], Achim Rosch[2], Jeison Fischer[1], Thomas Michely[1], Theo A. Costi[3], and Wouter Jolie[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [3]Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany

In scanning tunneling spectroscopy, the dI/dV signatures of the Kondo effect in MoS_2 mirror twin boundaries (MTBs) are the zero-bias resonance peak, in addition to the impurity levels [1]. The experimental data give access to the Anderson model parameters; The splitting U of the non-degenerate states, the impurity orbital's position ϵ with respect to E_F, and the impurity level's bare width γ_0.

In this work, we compare the Kondo temperature T_K measured in MTBs of MoS_2 grown on three different substrates. In the case of MoS_2 / Graphene (Gr) / Ir (111), T_K was in the range [10^{-4} K, 10^{-10} K] [1]. By intercalating with a single layer of Eu under Gr, we have noticed a decrease of γ_0, leading to a drop in T_K. The third system, MoS_2 / Gr / Ir (110), T_K increased significantly to the range [1 K, 10 K]. This enabled us to study the Kondo effect at the boundary between the weakly screened magnetic state above T_K and the Kondo singlet state below T_K.

References: [1] C. van Efferen et al, Nat. Phys. 20, 82-87 (2024).

O 89.9 Thu 17:00 WILL/A317

Statistical analysis of electron-induced switching of a spin-crossover complex — •Jonas Fussangel[1], Björn Sothmann[1], Sven Johannsen[2], Sascha Ossinger[3], Felix Tuczek[3], Richard Berndt[3], Jürgen König[1], and Manuel Gruber[1] — [1]Fakultät für Physik and CENIDE, Universität Duisburg-Essen, 47048 Duisburg, Germany — [2]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [3]Institut für Anorganische Chemie, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Spin-crossover complexes switch between two spin states, but the microscopic pathway remains unclear. Using low-temperature STM, electron-induced switching of $[Fe(H_2B(pz)(pypz))_2]$ on Ag(111) has opened new perspectives for understanding the switching mechanisms. Current time traces show two levels matching the spin states. An analysis of waiting-time distribution yields switching rates whose voltage dependence is explained by a simple model where transient molecular charging triggers switching. Comparing experiment and theory provides previously inaccessible estimates of LUMO energies [1]. The approach offers new insights into the switching mechanism and predicts higher switching rates when the molecule is electronically decoupled from the substrate, e.g., by introducing an ultrathin insulating layer.

[1] J. Fußangel et al., *arXiv*: 2506.13373 (2025)

O 89.10 Thu 17:15 WILL/A317

Decoupling strategies for YPc_2 molecular spin qubit platforms on metal surfaces — Franklin H. Cho[1,2], Soyoung Oh[1,2,3], Dan Chi Nguyen[1,2], Jinjoo Lee[1,2], We-hyo Soe[1,2], Luciano Colazzo[1,2], Jisoo Yu[1,2], Pierre Josse[1,2], Caroline Hommel[1,2], Lukas Spree[1,2], Christoph Wolf[1,2], and •Fabio Donati[1,2] — [1]IBS Center for Quantum Nanoscience, South Korea — [2]Ewha Womans University, South Korea — [3]The Clarendon Laboratory, University of Oxford, The United Kingdom

Yttrium phthalocyanine double-decker (YPc_2) is an appealing building block for surface spin-qubit architectures due to its delocalized $S = 1/2$ radical and planar structure [1]. Here, we investigated the morphology, electronic structure, and spin properties of single- and multi-layer YPc_2 on Cu(111) single crystals and on zinc phthalocyanine (ZnPc) grown on Cu(111). Low temperature scanning tunneling microscopy reveals the molecular layer structure and the variation of its electronic configuration when directly adsorbed on Cu(111) versus on a ZnPc decoupling layer [2]. X-band electron spin resonance using our custom-built surface-sensitive spectrometer [3] shows that the YPc_2 radical is preserved on ZnPc but quenched upon direct contact with Cu(111). Density functional theory attributes this quenching to the hybridization of molecular orbitals with the substrate electrons. Our study highlights the necessity of suitable decoupling layers to preserve radical spins near metallic surfaces. [1] F. Branzoli et al., Phys. Rev. B 83, 174419 (2011). [2] S. Oh et al., Nanoscale 17, 22163 (2025). [3] F. H. Cho et al., Rev. Sci. Instrum. 95, 063904 (2024).

O 89.11 Thu 17:30 WILL/A317

Inelastic Zoo: Spin, Vibrational, and Orbital Excitations in Conductance Spectra — •Arnab Banerjee, Richard Berndt, and Alexander Weismann — Institut für Experimentelle und Angewandte Physik, CAU Kiel, Germany

First-principle predictions of excitation energies and cross sections in inelastic tunneling spectroscopy are challenging, making it difficult to assign experimental features to specific excitations. There is a need for a reliable identification of conductance features. We investigated the spin-1/2 molecule cobaltocene on superconducting Pb(110) and use Yu-Shiba-Rusinov states combined with a superconducting tip to detect a large number of sharp spectral features. From a peak shape analysis, we find the coexistence of spin, vibrational, and orbital excitations within a single conductance spectrum.

O 89.12 Thu 17:45 WILL/A317

Current-induced Electron Spin Polarization in Magnetic Molecules — •Paul Greule, Wantong Huang, Máté Stark, Kwan Ho Au-Yeung, Johannes Schwenk, Christoph Sürgers, Wolfgang Wernsdorfer, and Philip Willke — Physikalisches Institut (PHI), Karlsruhe Institute of Technology, Karlsruhe, Germany

Electron spins of single molecules offer a promising platform for quantum information processing. To harness such spins as functional qubits, efficient initialization is essential. Electron spin resonance combined with scanning tunnelling microscopy (ESR-STM) has emerged as a powerful technique to probe molecular spins at the atomic scale. Using this technique, it has been shown that a spin-polarized tunnelling current can polarize the nuclear spin of a single Cu atom [1]. In this talk, we show that this concept can be transferred to the electron spin of molecules: Using Fe-FePc complexes with an electron spin of S=1/2 [2], we build molecular dimers. Here, the first complex serves as a readout and pumping system, while the energy-level occupation of the second complex is probed and manipulated. The exchange interaction between them enables remote spin-pumping, where angular momentum is transferred. Controlling the spin-polarized tunnel current via the bias voltage allows us to tune the spin polarization of the second complex remotely. Our findings establish an all-electrical technique to initialize molecular spin qubits and provide insights for enhanced control schemes. [1] K. Yang et al., Nat Nano 2018, 13, 1120-1125 [2] W. Huang et al., Nat Commun 2025, 16, 5208

O 90: Members' Assembly of the Vacuum Science and Technology Divison (VA)

Time: Thursday 17:15–18:15 Location: HSZ/0401

All members of the Vacuum Science and Technology Division are invited to participate.

O 91: Members' Assembly

Time: Thursday 19:00–19:30 Location: HSZ/AUDI

All members of the Surface Science Division are invited to participate.

O 92: Post-Deadline Session

Time: Thursday 19:30–20:30 Location: HSZ/AUDI

Contributed Post-Deadline Talks

O 93: Electronic structure of surfaces: Spectroscopy, surface states III

Time: Friday 9:30–12:00 Location: HSZ/0201

O 93.1 Fri 9:30 HSZ/0201

Identifying Electronic Doorway States in Secondary Electron Emission — •Anna Niggas[1], Maosheng Hao[2], Peter Richter[3], Felix Blödorn[1], Florian Simperl[1], Alessandra Belissimo[4], Joachim Burgdörfer[2], Thomas Seyller[3], Wolfgang Werner[1], Florian Libisch[2], and Richard A Wilhelm[1] — [1]Institute of Applied Physics, TU Wien, Vienna, Austria — [2]Institute for Theoretical Physics, TU Wien, Vienna, Austria — [3]Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [4]Institute of Photonics, TU Wien, Vienna, Austria

Secondary electron emission following low-energy (<200 eV) electron impact is fundamental to particle-solid interactions but remains incompletely understood. While high-energy electrons are described by reflected primaries undergoing inelastic losses, the low-energy (<20 eV) region is often considered featureless. Coincidence spectroscopy has revealed hidden structures, notably the 3.3 eV X peak in graphite arising from plasmon excitation and interlayer-state hybridisation. Following that, we have measured low-energy secondary electrons from graphite and quasi-freestanding single- and bilayer graphene, enabling a controlled transition from bulk to two-dimensional systems. We observe layer-dependent features and, supported by density functional theory, attribute them to Feshbach-type resonances of quasi-bound above-vacuum states coupling to the continuum. The strong 3.3 eV resonance appears only in systems with five or more layers [1].

[1] A. Niggas et al., Phys. Rev. Lett. 135, 166401 (2025)

O 93.2 Fri 9:45 HSZ/0201

A novel approach to depth-resolved magnetic spectoscopy: grazing-incidence XMCD — •Umut Parlak[1], Katharina Wehrstein[1], Pia Maria Düring[1], Oliver Rehm[1], Endrit Kusari[1], David Capalbo[1], Andrei Gloskovskii[2], Christoph Schlueter[2], Lutz Baumgarten[3], and Martina Müller[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Deutsches Elektronen-Synchrotron, 22607 Hamburg, Germany — [3]Peter Grünberg Institut, PGI-6, Research Centre Jülich, 52425, Jülich, Germany

Magnetic depth profiling plays a key role in understanding inter- and intralayer magnetic coupling mechanisms in multilayer thin films. We employ a synchrotron-based photoelectron spectroscopy approach (P22 beamline, DESY) to measure x-ray magnetic circular dichroism with depth-resolution taking EuO thin films grown on heavy metal (HM) underlayers as prototype sample. The presence of HM underlayer enables the near-total reflection x-ray excitation, where the incident and reflected x-rays interfere at the grazing angles forming high-intensity nodal points. The depth-resolution is achieved by probing at angles between 0.2 and 1°, i.e., tuning the position of the nodal points. Simulations of the x-ray intensity profile at these low angles allow us to optimize the MBE-grown MgO/EuO/HM trilayer structure for accessing both the upper and lower interfaces. Our results reveal the distribution of Eu^{2+} and Eu^{3+} ions throughout the EuO layer, which form ferromagnetic and paramagnetic oxides, respectively. The valency profile of the Eu ions directly aligns with the magnetic asymmetry profile.

O 93.3 Fri 10:00 HSZ/0201

Experimental Verification of the d-band Center Model in Au/Pt Systems: A Low-Energy XPS Study — •Justyna Piwowar[1,2,3] and Adam Lewera[3] — [1]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS), Seoul 03760, Republic of Korea — [2]Ewha Womans University, Seoul 03760, Republic of Korea — [3]Faculty of Chemistry, University of Warsaw Pasteura 1 02-093 Warszawa

This work presents an experimental verification of the relationship between electronic structure and electrocatalytic properties in Pt-based materials, specifically critically evaluating the d-band center theory. Using Au-modified Pt as a model system, surface electronic properties were probed via X-ray Photoelectron Spectroscopy (XPS). We demonstrate that employing low-energy X-ray sources (Zr Mγ, 151 eV) provides superior surface sensitivity compared to standard sources (~1500 eV), allowing for the detection of subtle surface electronic shifts otherwise masked by bulk signals.

We observed a nonlinear evolution of electronic properties in Au/Pt thin films, specifically in core-level binding energies, which correlates with synergistic catalytic activity in formic acid oxidation. Detailed analysis of the valence band spectra reveals that significant modifications in the Density of States (DOS) near the Fermi level can occur even when the calculated shift in d-band center is negligible, due to spectral redistribution on both sides of the centroid. These findings indicate that the d-band center parameter alone may be insufficient to describe complex electronic structure modifications.

O 93.4 Fri 10:15 HSZ/0201

Spin Polarization of Photoelectrons Excited by Deep-UV Pulses with Orbital Angular Momentum — •Paul Valerian Möllers, Ruwen Quenter, and Helmut Zacharias — Center for Soft Nanoscience, Universität Münster

It is well known that circularly polarized light can excite longitudinally spin-polarized photoelectrons from centrosymmetric crystal surfaces [1]. The light carries an angular momentum of $\pm\hbar$, and the selection rules dictate that the photoexcitation occurs into final states with a specific total angular momentum. In the presence of spin–orbit interaction, states with different total angular momenta are energetically separated, and the excited electrons can exhibit a net spin imbalance. Light with helical wave fronts carries orbital angular momentum as a degree of freedom that is independent of its polarization and not limited to $\pm\hbar$ [2]. As the light always acts on the orbital electron angular momentum during photoexcitation, it appears plausible to assume that the optical orbital angular momentum could translate into a nonzero photoelectron spin polarization. This hypothesis has yet to be tested experimentally. We present preliminary results of spin-resolved photoemission measurements on Cu(111) and Au(111) surfaces that address this issue. [1] G. Borstel, M. Wöhlecke, Phys. Rev. B 26, 1148-1155 (1982) [2] S. S. R. Oemrawsingh et al., Appl. Opt. 43, 688-694 (2004)

O 93.5 Fri 10:30 HSZ/0201

Imaging stripe dynamics in superconducting nickelate — •Uladzislau Mikhailau[1], Luke C. Rhodes[1], Matthias Hepting[2], Masahiko Isobe[2], Pascal Puphal[2], and Peter Wahl[1,3] — [1]University of St Andrews, St Andrews, United Kingdom — [2]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [3]Physikalisches Institut, Universitat Bonn, Germany

In the Hubbard model, there is a competition between charge localization due to Coulomb repulsion and delocalization due to the energy reduction from electrons hopping between sites. When both tendencies are equally strong, a unique correlated stripe order can be stabilized [1]. Such a state is known to be realized in lightly doped high temperature superconducting cuprates and in nickelates.

Our STM investigation shows that commensurate stripe order forms in the metallic state of the recently discovered high-temperature superconductor $La_4Ni_3O_{10}$. Quasi-1D channels of delocalized charge appear as solitonic domain walls in charge density probed by STM. Interestingly, electrons tunnelling from the tip can induce local stripe fluctuations, pointing at the weak pinning of the order to the lattice.

Observation of stripe orders in normal states of high temperature cuprates and nickelates suggests shared correlated physics as a precursor to high-temperature superconductivity in both systems. Such experimental evidence is a valuable foundation for investigations into the mechanism of high-temperature superconductivity in both systems.

[1] J. Zaanen and O. Gunnarsson. Phys. Rev. B, 40(10):7391-7394 (1989).

O 93.6 Fri 10:45 HSZ/0201

Surface Rashba effect influence on bulk states: test case on Au(111) — •Laurent Nicolaï[1], Ján Minár[1], Christine Richter[2,3], Olivier Heckmann[2,3], Laxman Nagi Redi[2,3], Sourour Ayari[1], Aki Pulkkinen[1], Mauro Fanciulli[2,3], and Karol Hricovini[2,3] — [1]University of West-Bohemia in Pilsen, Czeck Republic — [2]CY Cergy Paris Université, France — [3]Université Paris-Saclay, CEA, France

Au(111) crystals are commonly used in the Photo-emission Spectroscopy field to calibrate instruments. When coming to spin-resolved ARPES, one uses the well-known surface states, spin-split due to the Rashba effect [1,2], as a reference. Au(111) being a centro-symmetric material, it is commonly assumed that bulk sates are spin degenerate. However, we here present measurements attesting a spin polarisation of bulk states within the valence band. The measurements are complemented with ab-initio calculations confirming the existence of bulk states' spin polarisation on a fundamental level.

[1] Yu A. Bychkov and E. I. Rashba, J. of Phys. C: Sol. St. Phys., 17:6039-6045, 1984 [2] S LaShell et al. , Phys. Rev. Lett. 77 3419, 1996

O 93.7 Fri 11:00 HSZ/0201

calcQPI - a tool to simulate quasiparticle interference — •Peter Wahl[1,2], Luke Rhodes[1], and Carolina de Almeida Marques[1] — [1]SUPA, School of Physics and Astronomy, University of St Andrews, United Kingdom — [2]Physikalisches Institute, Universität Bonn

Quasiparticle interference imaging (QPI) is a powerful tool to study the low energy electronic structure of quantum materials and one of a few methods that can provide phase-sensitive information about the superconducting order parameter of unconventional superconductors, but the interpretation of QPI often requires complex modelling. This talk introduces calcQPI[1,2] as a new tool for the realistic simulation of QPI measurements. CalcQPI allows for the calculation of QPI from tight-binding models for a wide range of quantum materials, including magnetic materials, topological insulators and unconventional super-

conductors. I will give an overview of its capabilities and a few examples of how it can be applied to real materials.

[1] P. Wahl, L.C. Rhodes, C.A. Marques, calcQPI: A versatile tool to simulate quasiparticle interference, SciPost Phys. Codebases 61 (2025). [2] P. Wahl, L.C. Rhodes, C.A. Marques, Codebase release 1.0 for calcQPI, SciPost Phys. Codebases 61-r1.0 (2025).

O 93.8 Fri 11:15 HSZ/0201

Defect-driven polarity compensation on weakly polar $BaTiO_3$ (001) and $SrTiO_3$ (001) surfaces. — •Darin Joseph[1], Llorenç Albons[4], Florian Ellinger[2], Michele Reticcioli[2,3], Martin Setvin[4], and Cesare Franchini[1,2] — [1]University of Bologna, Italy — [2]University of Vienna, Austria — [3]CNR-SPIN, L' Aquila, Italy — [4]Charles University, Prague , Czech Republic

$BaTiO_3$ (001) and $SrTiO_3$ (001), commonly classified as Tasker Type I and nonpolar, exhibit surface instability, as evidenced by A-site (Ba/Sr) adatoms and vacancies on cleaved surfaces observed in experiments. Density Functional Theory (DFT) calculations revealed the work function variation between the TiO_2 and AO terminations and an electric field in the vacuum of asymmetric slabs, which are typically associated with polar surfaces. Our study reveals that both perovskites exhibit weak polar stacking along the crystallographic axis, leading to surface charges on the pristine terminations and creating an unfavorable electrostatic environment. Our analysis shows that the experimentally observed A-site defects act as compensation mechanisms by counterbalancing these charges to restore charge equilibrium. Charge compensation occurs at 12.5% Sr adatom and 12% vacancy coverage for $SrTiO_3$ and at approximately 12-13% defect concentration for $BaTiO_3$. These theoretical values are consistent with the experimental defect concentrations.

O 93.9 Fri 11:30 HSZ/0201

3D Mapping of Photoelectron Diffraction Patterns at Very Low Energies — •O. Tkach[1], T.-P. Vo[2], D. Biswas[3], J. Liu[3], O. Fedchenko[1,4], T.-L. Lee[3], J. Minár[2], H.-J. Elmers[1], and G. Schönhense[1] — [1]Univ., Mainz — [2]Univ. of West Bohemia, Czech Republic — [3]Diamond Light Source, UK — [4]Goethe Univ. Frankfurt

The full-field recording architecture of momentum microscopes (MMs) efficiently captures the (E,k) valence band structure along with the corresponding dichroism and spin texture [1]. Here, we apply the same approach to photoelectron diffraction (PED) in the low-energy range. Capturing PED in a solid angle up to 2π, including the corresponding core-level CDAD [2] reveals a wealth of structure far beyond that of standard PED measurements. The experiments are compared with calculated three-dimensional (E,k_x,k_y) patterns obtained via one-step photoemission calculations using the PED implementation [3] within the SPRKKR package. Calculated results over a wide range of kinetic energies (106 – 1036 eV) for the Ge 3d core level reveal striking patterns that change rapidly with photon energy. The high-energy end provides insight into bulk (Kikuchi-) diffraction, while the lower end with its high surface sensitivity yields structural information about the surface. This is indicative of the transition from a localized core level to an itinerant, time reversed LEED photoemission final state. In general, these results bridge the gap between PED analysis and electronic structure investigations.

[1] Medjanik et al. Nat. Mater 16, 615 (2017)
[2] Tkach et al. Ultramic. 250, 113750 (2023)
[3] Vo et al. npj Comput. Mater.11, 159 (2025)

O 93.10 Fri 11:45 HSZ/0201

Shaping Surface States: The Art of Designing Quantum Corrals — •Nadine Egger, Simon B. Hollweger, and Oliver T. Hofmann — Institute of Solid State Physics, TU Graz, Austria

Quantum corrals enable precise control over electron behavior on surfaces and can be designed to carry out tasks such as atomic-scale logic operations. However, determining the optimal corral shape and the precise placement of the individual building blocks is a nontrivial task. To address this, we introduce a simulation-based framework that automatically designs corral geometries to achieve specific functionalities. The approach combines surface-state electron simulations with an optimization algorithm that identifies not only the number of atomic building blocks required but also their optimal arrangement on the surface. As a first application, the framework is applied to design corrals capable of performing basic logic operations, such as AND or NOT gates. Beyond these examples, this method offers a versatile path toward creating atomically precise nanostructures with customized functional properties, paving the way for future developments in quantum device engineering.

O 94: Oxides and insulators: Adsorption and reaction of small molecules

Time: Friday 9:30–12:30 Location: HSZ/0204

Invited Talk O 94.1 Fri 9:30 HSZ/0204

Surface Chemistry on Copper Oxides — •Dario Stacchiola — Brookhaven National Laboratory, Upton NY, 11720, USA

The chemical and electronic properties of copper combined with its large natural abundance lend this material to impact a wide range of technological applications, including heterogeneous catalysis. The reactivity of copper in its Cu1+ oxidation state makes this specific state relevant in various chemical reactions, but the facile redox properties of copper make the isolation of individual states for fundamental studies difficult. I will present our work on model systems including Cu2O/Cu(111) films, bulk Cu2O crystals and copper-based mixed-oxides used to study the interaction of Cu1+ with small molecules making use of in-situ surface science techniques. Advantages and disadvantages of each system are discussed and exemplified through case studies of chemical adsorption and reactivity studies

O 94.2 Fri 10:00 HSZ/0204

Calculating vibrational bands for formic acid on magnetite surfaces — •Gregor Vonbun-Feldbauer — Institute for Interface Physics and Engineering, TU Hamburg, Germany — Institute of Surface Science, Helmholtz-Zentrum hereon, Germany

Understanding the adsorption properties of organic molecules on oxide surfaces, such as their adsorption geometry, is crucial for optimising processes in various applications, ranging from heterogeneous catalysis to hybrid nanocomposites. In this study, the adsorption of formic acid on magnetite surfaces (001), (111) and (112) is examined using Density Functional Theory (DFT). The vibrational properties are then calculated and compared with experimental infrared spectroscopy data for single crystalline surfaces and nanoparticles. This enables adsorption geometries and modes to be identified.

O 94.3 Fri 10:15 HSZ/0204

Thermal CO_2 Activation and Carbonate Formation on Fe_2O_3(012) — •Johannes Filzmoser, Moritz Eder, Florian Kraushofer, Jiri Pavelec, and Gareth Parkinson — Vienna University of Technology, Austria

The adsorption of CO_2 on hematite α-Fe_2O_3(012) has been investigated in ultrahigh vacuum (UHV) using temperature-programmed desorption (TPD) and infrared reflection absorption spectroscopy (IRAS). CO_2 adsorption on this surface exhibits complex behavior, resulting in multiple desorption features in TPD. For coverages up to one molecule per unit cell (0.5 molecules per Fe^{2+} cation), two desorption features centered around 150 K and 220 K increase concurrently with increasing coverage. IRAS shows that this behavior originates from a thermally activated conversion of weakly bound, physisorbed CO_2 into surface carbonate (CO_3^{2-}) species at temperatures above 100 K, a process that directly competes with molecular desorption. By supplying CO_2 at temperatures just below the carbonate desorption temperature, higher carbonate coverages can be obtained. These findings contribute to our understanding of CO_2 activation on Fe_2O_3(012) and will be a prerequisite for surface reaction studies.

O 94.4 Fri 10:30 HSZ/0204

Redox dynamics of Co_3O_4(111) during H_2S adsorption and decomposition — Jonas Hauner[1], Tomáš Skála[2], Nataliya Tsud[2], Fernando Stavale[3], •Yaroslava Lykhach[1], and Jörg Libuda[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Charles University, Prague, Czech Republic — [3]Brazilian Center for Research in Physics, Rio de Janeiro, Brazil

The redox interactions between transition metal oxides and sulfur-containing compounds play a key role in catalytic processes and gas sensing technologies. We investigated the redox dynamics of Co_3O_4(111)/Ir(100) model catalysts in response to the adsorption and decomposition of hydrogen sulfide (H_2S) using synchrotron radiation photoelectron spectroscopy (SRPES). Upon adsorption, H_2S partially dissociates to form a variety of species including sulfites, sulfides, chemisorbed H_2S, hydroxyl and sulfhydryl groups. Subsequent annealing in ultrahigh vacuum induces desorption and conversion of adsorbed species to sulfates. These transformations are accompanied by temperature-dependent redox processes which can be monitored as a function of Co^{3+}/Co^{2+} ratio. The obtained insights into H_2S–Co_3O_4 redox interactions offers a foundation for the rational design of cobalt oxide catalysts and sensors for H_2S detection and abatement.

O 94.5 Fri 10:45 HSZ/0204

Characterization of CO_2 adsorption configurations on stoichiometric, reduced and hydroxylated In_2O_3 — •Sarah Tobisch[1], Andreas Ziegler[2], Sarah Horak[1], Marco Knapp[1], Michele Riva[1], Michael Schmid[1], Ulrike Diebold[1], Bernd Meyer[2], and Margareta Wagner[1] — [1]TU Wien, Vienna, Austria — [2]FAU-Erlangen-Nürnberg, Erlangen, Germany

CO_2 reduction to methanol is a promising pathway towards a more circular economy, converting CO_2 into valuable fuels and feedstock for the chemical industry. In_2O_3-based catalysts have gained lots of attention in recent years due to their high selectivity towards methanol synthesis. Since catalytic reactions typically take place at the interface, it is important to understand how CO_2 molecules interact and adsorb on the surface on an atomic level.

In this work, the adsorption of CO_2 molecules was studied on three different $In_2O_3(111)$ surfaces: stoichiometric, reduced, and hydroxylated. We present atomically resolved non-contact AFM images which allow for the identification of the adsorption sites of all individual molecules. The CO_2-saturated, stoichiometric $In_2O_3(111)$ shows long range order, albeit breaking the threefold symmetry of the surface. Missing contrast inversion in nc-AFM combined with XPS measurements result in the identification of physisorbed and carbonate species. DFT calculations confirm adsorption sites and orientation of the individual molecules. CO_2 shows similar motifs on the reduced surface but partly displaces the In adatoms. On the hydroxylated surface, the OH groups block adsorption of CO_2 and long-range order is not observed.

O 94.6 Fri 11:00 HSZ/0204

How chirality controls catalysis: Spin-dependent effects in the catalytic OER from first-principles — •Suryansh Suryansh[1], Rafael Gutiérrez[1], Arezoo Dianat[1], and Gianaurelio Cuniberti[1,2] — [1]Institute of Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, Dresden 01062, Germany — [2]Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062, Dresden, Germany

The evolution of a mixture of unpolarized electrons into an ensemble of spin-polarized electrons after passing through a chiral molecule such as DNA, proteins, or peptides is a well-established phenomenon attributed to the chiral-induced spin selectivity (CISS) effect. This effect has important implications for electrochemical water-splitting. Experiments have shown that chiral molecules enhance the oxygen evolution reaction (OER) by controlling the spin of electrons at the electrode surface when the electrode is coated with a monolayer of chiral molecules, a film of chiral polymer, or a chiral inorganic oxide. This enhancement is associated with facilitating the singlet-to-triplet spin transition of oxygen at the interface. However, the microscopic origin and physical mechanisms behind CISS-based water-splitting remain unclear. In this work, we investigate the electronic and magnetic properties of ferrimagnetic surfaces functionalized with chiral and achiral molecules using first-principles calculations. We compute the reaction energy barriers of the individual OER steps and analyze the spin-polarized electronic states near the Fermi level, providing theoretical insights into the mechanisms underlying spin-assisted water-splitting.

O 94.7 Fri 11:15 HSZ/0204

Tailoring the OER activity of Co_3O_4 surfaces by Mn and V-doping: insights from DFT+U calculations — •Palani Muthu Kumar and Rossitza Pentcheva — Department of Physics, University of Duisburg-Essen

The rational design of efficient electrocatalysts for sustainable energy conversion demands an atomistic understanding of how surface modifications influence the overall activity. Here we present a detailed DFT+U investigation of Mn- and V-doping on the oxygen evolution reaction (OER) activity at Co_3O_4 surfaces. Mn-doping at the surface octahedral sites on both A- and B-terminated $Co_3O_4(001)$, reduces the OER activity. Conversely, V-doping demonstrates termination-dependent behaviour: at the B-termination, V^{5+} in a surface octahedral site reduces the overpotential at Co_{oct} from 0.48 V to 0.43 V. At the A-termination, V^{4+} in a subsurface octahedral site leads to the lowest overpotential of 0.18 V at Co_{tet} reaction site, reversing the intrinsic activity trend where pristine Co_{tet} sites (0.74 V) are less active than Co_{oct2} (0.55 V) sites. For most studied cases, the deprotonation of *OH to *O is the potential-determining step. The enhanced catalytic activity of the V-doped A-termination originates from the modification of surface Co^{3+}(IS) to Co^{2+}, weakening the *OH binding energy and lowering the PDS by 0.56 eV. These findings show that selective doping effectively tunes electrocatalyst performance. The scope of the investigation is further extended to the $Co_3O_4(111)$ surface, thereby broadening the understanding of facet-dependent effects.

O 94.8 Fri 11:30 HSZ/0204

Towards Understanding the Photoreactivity of SrTiO3 through Studies in Ultra-High Vacuum — •Anna Lemperle, Philip Petzoldt, Martin Tschurl, and Ueli Heiz — Chair of Physical Chemistry, Technical University of Munich, Lichtenbergstr. 4, 85748 Garching, Germany

Strontium titanate is renowned for its photocatalytic water splitting capabilities. However, the catalytic mechanism remains elusive. A promising approach to obtain insights into structure-reactivity relations is to investigate well-defined single crystal model catalysts under ultra-high vacuum conditions. This contribution discusses first results on the thermal and photoreactivity of water and oxygen on the bare strontium titanate (100) surface. Experiments combining temperature programmed desorption and studies under illumination point to a high importance of the dynamic behaviour of bulk and surface oxygen for the reactivity of strontium titanate (100).

O 94.9 Fri 11:45 HSZ/0204

Methanol photodecomposition on TiO_2(110) under UV illumination studied with vibrational SFG spectroscopy in ambient conditions — •Milad Salarinasab[1], Julian Andreas Hochhaus[1], Anas Akhtar[2], Kristina Tschulik[2], Carsten Westphal[1], Zhe Wang[1], and Ahmed Ghalgaoui[1] — [1]Department of Physics, TU Dortmund University, Otto-Hahn-Str. 4a, Dortmund, 44227, Germany — [2]Analytical chemistry II, Ruhr-Universität Bochum, Universitätsstrasse 150, 44801 Bochum, Germany.

Methanol is widely used as a model system for photocatalysis on TiO_2 surfaces, but many earlier investigations were performed in UHV and therefore do not reflect real catalytic conditions. To address this gap, we studied methanol photodecomposition on TiO_2(110) under realistic ambient conditions using vibrational sum frequency generation (SFG) spectroscopy. By recording spectra in the C-H stretch region, we followed CH_3, CH_2, and methoxy species during UV illumination and monitored how these surface species evolve in real time.

The SFG signals show clear differences from the reaction pathways commonly described in vacuum studies. Most importantly, we identify a new photodecomposition route that becomes active only under realistic conditions combined with UV excitation. This finding provides new insight into methanol chemistry on TiO_2(110) and helps connect surface science studies with photocatalytic behavior in practical environments.

O 94.10 Fri 12:00 HSZ/0204

Bridging the Gap: Interpreting Photocatalysis Under Ambient Conditions Based on Findings from Surface Science — •Martin Tschurl, Philip Petzoldt, Lucia Mengel, Paula Neumann, Anna Lemperle, and Ueli Heiz — Chair of Physical Chemistry, Technical University of Munich, Lichtenbergstr. 4, 85748 Garching, Germany

The interpretation of heterogenous photocatalytic reactions is usually closely linked to electrochemistry. Based on a qualitative, exclusively thermodynamic picture, it normally focuses on the properties of photon-generated charge-carriers. However, some years ago in ultra-high vacuum (UHV) studies, we discovered that for the heavily studied Pt-titania system, a fundamentally different reaction mechanism governs the photocatalytic conversion of alcohols. This mechanism underscores the critical role of surface chemistry - an aspect often neglected in the interpretation of applied photocatalysts. In this presentation, we will interpret systems operating under ambient conditions based on insights gained from UHV experiments. This way, we also demonstrate merit of surface science studies for a comprehensive understanding of photocatalysis.

O 94.11 Fri 12:15 HSZ/0204

Molecular Dynamics Simulation of Impingment of Atomic Oxygen on Alumina and Silica Surfaces — Stephen Hocker, Hansjörg Lipp, Aahmed Kassem, Ricco Isele, Leonidas Simitsis, and •Johannes Roth — Institute for Functional Matter and Quantum Technologies (FMQ), University Stuttgart, Germany

Atomic oxygen (AO) impinging on satellite surfaces in very low earth orbit (VLEO) transfers momentum and energy, leading to material degradation and drag forces. To be able to counteract these effects, we investigate the impact mechanisms of AO on alumina (Al2O3) and silica (SiO2) surfaces. In this talk we give an overview of our activities: Using molecular dynamics (MD) simulations with classical force fields, we study material stability, angular distributions of reflected particles, and adsorption rates. Our findings indicate that bare Al2O3 does not degrade under AO impacts but accumulates oxygen due to adsorption processes. The angular distribution of reflected particles is highly dependent on the surface structure and the angle of incidence, with a higher ratio of specular reflection observed on smoother surfaces and at larger incidence angles. This is confirmed by the few experimental results available. We further present first results of the impingement of AO on SiO2 surfaces obtained with the same method. Here we study especially the influence of different interactions. The talk is completed with an outlook on the role of specific interactions in general.

O 95: 2D Materials: Stacking and heterostructures (joint session O/HL/TT)

Time: Friday 9:30–12:30 Location: HSZ/0401

O 95.1 Fri 9:30 HSZ/0401

A new fabrication method for metal intercalated epitaxial graphene devices — •Marc Bothe[1], Stefan Wundrack[1,2], Marcelo Jaime[1], Klaus Pierz[1], Frank Hohls[1], Rainer Stosch[1], Hans Werner Schumacher[1], Andrey Bakin[2], and Teresa Tschirner[1] — [1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany — [2]Institut für Halbleitertechnik, TU Braunschweig, Hans-Sommer-Str. 66, 38106 Braunschweig, Germany

Epitaxial graphene grown on silicon carbide is a promising platform to achieve metal intercalation. It enables the creation of two-dimensional metal layers that are encapsulated and protected by graphene. However, the use of metal intercalated graphene samples for lithographic device fabrication presents two critical challenges. First, solvents used in the lithography process lead to the deintercalation of the metal atoms. Second, the presence of lattice defects in the graphene - necessary for the intercalation process - compromises the structural and electronic integrity of the device. We present a novel fabrication method that solves these problems. In our approach, the graphene devices are first pre-structured using lithography and subsequently intercalated. This is made possible by a spatial separation on the sample between the device structures and the intercalation origin and by intercalation channels that can guide the intercalation front reliably to the devices. We demonstrate this method on gallium intercalated epitaxial graphene Hall bars that exhibit superconducting behaviour.

O 95.2 Fri 9:45 HSZ/0401

Anisotropic Strain Observation in Naturally Occurring Buckling on Twisted Bilayer Graphene: A Nano-Raman Study — •Gustavo Soares[1], Rafael R. Barreto[1], Rafael Nadas[1], Kenji Watanabe[2], Takashi Taniguchi[2], Leonardo C. Campos[1], Luiz G. Cancado[1], and Angelo Malachias[1] — [1]Physics Department, Federal University of Minas Gerais, Belo Horizonte, Minas Gerais, 31270-901, Brazil — [2]National Institute for Materials Science, Tsukuba, Ibaraki, 3050047, Japan

This work investigates naturally occurring buckling and its relation with anisotropic strain relaxation in twisted bilayer graphene (tBG). In the tBG system a twist angle is imposed to influence graphene structural and electronic properties. Such condition directly implies in the occurrence of biaxial in-plane strain, with usual observation of buckled/wrinkled localized regions where the tBG morphology is no longer planar. Using tip-enhanced Raman spectroscopy, we conducted high-resolution mapping to analyze variations in Raman bands associated with twist angle variation and strain effects. Our findings reveal that localized strain gradients, modulated by twist angle variations, induce deterministic buckling in graphene layers, evidencing distinct uniaxial and biaxial strain regions. Finite element modeling further supports these observations, showing that buckling can store elastic energy sufficient to overcome usual tBG-substrate adhesion forces.

O 95.3 Fri 10:00 HSZ/0401

Kirkendall Voids in Monolayer $Mo_xTa_yS_2$ Alloys on Au(111) — Kai Mehlich[1], Thais Chagas[1], Francis H. Davies[2,3], Alessia Bardazzi[1], Catherine Grover[1], Arkady V. Krasheninnikov[3], and •Carsten Busse[1] — [1]Department Physik, Universität Siegen, Walter-Flex-Straße 3, 57072 Siegen, Germany — [2]Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [3]Department of Physics and Astronomy, University of Exeter, Stocker Road, Exeter, EX4 4QL United Kingdom

During the growth of monolayer MoS_2-TaS_2 heterostructures, we observe the Kirkendall effect: Diffusing vacancies agglomerate in MoS_2, forming what are commonly termed Kirkendall voids - here manifesting as holes in the 2D layer. This phenomenon has not been previously reported in systems with reduced dimensionality.

We prepare the lateral heterostructures by reactive molecular beam epitaxy on chemically inert and weakly interacting Au(111). First, compact MoS_2 cores are grown. In a second step, TaS_2 is added in a sulfur-rich environment at elevated temperatures which promotes diffusion at the interface. The resulting heterostructures exhibit characteristic 2D Kirkendall holes surrounded by a $Mo_xTa_yS_2$ alloy region. These findings reveal defect-mediated processes in low-dimensional systems and open new avenues for designing 2D lateral heterostructures with intricate morphologies.

O 95.4 Fri 10:15 HSZ/0401

Designing 2D Non-van der Waals Heterostructures — •Anastasiia Nihei[1,2], Tom Barnowsky[1,2], and Rico Friedrich[1,2] — [1]TU Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf

Heterostructure interfaces created by stacking two-dimensional (2D) materials offer a pathway to realizing advanced electronic and magnetic functionalities at the nanoscale. In this work, we present a high-throughput screening of non-van der Waals (non-vdW) 2D heterostructures; including sandwich-like stacking. Non-van der Waals 2D materials can be obtained by both top-down exfoliation as well as bottom-up growth approaches of non-layered bulk crystals [1]. Our approach uses the AFLOW-Hetbuilder - a newly developed tool for stacking 2D systems based on the coincidence lattice algorithm [2-4].

We investigate interfacial binding effects across a wide range of heterobilayers [5] and sandwich-like systems, analyzing their structural, electronic, and magnetic characteristics such as hybrid interface bands and robust magnetic coupling. Furthermore, we compare the binding energetics of non-vdW and conventional vdW heterostructures. The tunable interfacial properties of non-vdW 2D heterostructures provide a versatile platform for advanced functionalities with potential applications in electronics, spintronics, and the energy sector [5].

[1] R. Friedrich *et al.*, Nano Lett. **22**, 989, (2022).
[2] D.S. Koda *et al.*, J. Phys. Chem. C **120**, 10895, (2016).
[3] https://zenodo.org/record/4721346 .
[4] S. Divilov *et al.*, High Entropy Alloys Mater. **3**, 178 (2025).
[5] A. Nihei, *et al.*, arXiv DOI: 10.48550/arXiv.2503.12209 (2025).

O 95.5 Fri 10:30 HSZ/0401

Second-Order Nonlinear Imaging for Probing 2D van der Waals Structures — •Tao Yang[1], Ben John[1], Kyoung P. Lee[2], Nasim Mirzajani[1], Martin Wolf[1], Xiaoqin Li[2], Martin Thaemer[1], Alexandar Paarmann[1], Niclas S. Mueller[3], and Alexander P. Fellows[1] — [1]Fritz Haber Institute, Berlin, Germany — [2]University of Texas at Austin, Austin, USA — [3]Freie Universitaet Berlin, Berlin, Germany

Twisted and stacked multi-layer architectures offer new opportunities for tailoring the electronic and optical properties of two-dimensional (2D) van der Waals materials. Reliable determination of crystal structure, stacking sequence, and twist angle is therefore crucial. Second-order nonlinear optical microscopy, including second-harmonic and sum-frequency generation (SHG and SFG, respectively), provides high sensitivity to crystal symmetry and orientation in non-centrosymmetric lattices. Recently, we employed heterodyne-detected vibrational SFG microscopy to probe the local structure of hexagonal Boron Nitride (hBN) monolayers with sub-micron resolution. By employing our developed azimuthal-scanning approach, we fully resolved the crystallographic structure and edge termination in monolayer flakes. Here, we extend these measurements to multi-layer hBN structures, using the same azimuthal-scanning approach in a newly developed SHG microscope to gain insight into their different stacking configurations. Our results highlight second-order nonlinear microscopy as a powerful tool for quantitative structural analysis in 2D materials and for future studies of moiré and twisted heterostructures.

O 95.6 Fri 10:45 HSZ/0401

Moiré-Driven Electronic Modulations in Weakly Coupled h-BN/Graphite — •Fábio J. R. Costa[1,2,7], Daniel Arribas[2], Thiago G. L. Brito[2], Tin S. Cheng[3], Jonathan Bradford[3], Amelia Thompson[3], Alex Saywell[3], Christopher J. Mellor[3], Peter H. Beton[3], Sergey V. Novikov[3], Juliette Plo[4], Bernard Gil[4], Guillaume Cassabois[4,5], Luiz F. Zagonel[1], Klaus Kuhnke[2], Klaus Kern[2,6], and Anna Rosławska[2] — [1]University of Campinas, Brazil — [2]Max-Planck-Institut für Festkörperforschung, Germany — [3]University of Nottingham, UK — [4]Laboratoire Charles Coulomb, France — [5]Institut Universitaire de France, France — [6]EPFL, Lausanne, Switzerland — [7]Current address: Université de Strasbourg, CNRS, IPCMS, Strasbourg, France

Van der Waals materials and their heterostructures offer exciting opportunities for next-generation nanophotonic and electronic technologies. Their electronic and optical properties can be modulated by moiré superlattices that emerge when mismatched layers are stacked together. Hexagonal boron nitride (h-BN) is a key platform in this context, yet the influence of moiré patterns on weakly interacting h-BN interfaces remains underexplored. Here[1], we use scanning tunneling microscopy to resolve large moiré superlattices in h-BN/graphite and uncover pronounced nanoscale modulations of the electronic landscape, despite their weak interlayer interactions. These findings position moiré engineering in h-BN as a powerful tool to tailor local functionalities in van der Waals heterostructures.

Ref.: 1. Fábio J. R. Costa *et al.* ACS Nano 2025 19 (40), 35528-35538

O 95.7 Fri 11:00 HSZ/0401

μ-ARPES study on the fine electronic structure of misfit layer compound (PbSe)1.16(TiSe2)2 — •haruki muramatsu[1], natsuki mitsuishi[2,3], teppei ueno[4], kenichi ozawa[5], kaya kobayashi[4,6], and kyoko ishizaka[1,2] — [1]Dept. of Appl. Phys. & QPEC, Univ. of Tokyo — [2]CEMS, RIKEN — [3]Grad. Sch. Sci., Nagoya Univ. — [4]Dept. of Physics, Okayama Univ. — [5]KEK-PF — [6]RIES, Hokkaido Univ.

Misfit layered compounds have been attracting significant attention due to their lattice mismatches and resultant two-dimensional electronic structures reminiscent of van der Waals heterostructures. One such compound, (PbSe)1.16(TiSe2)2, consists of alternating stacking of PbSe monolayers (NaCl-

type, four-fold symmetry) and TiSe2 bilayers (CdI2-type, three-fold symmetry). To elucidate its electronic structure, we performed μ-ARPES measurements by carefully distinguishing the cleavage surface terminations. In the presentation, we will discuss the novel electronic states reflecting the natural incommensurate heterostructure as well as charge density wave in the buried TiSe2 bilayer.

O 95.8 Fri 11:15 HSZ/0401

Twisted $NbSe_2$ heterostructures — •Alexander Bäder[1,2], Clara Pfister[3,4], Tobias Wichmann[1,5], Laura Pätzold[3,4], Tim O. Wehling[3,4], and Felix Lüpke[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich — [2]II. Physikalisches Institut, Universität zu Köln — [3]I. Institute of Theoretical Physics, U Hamburg — [4]The Hamburg Centre for Ultrafast Imaging — [5]Institut für Experimentalphysik IV A, RWTH Aachen

We fabricated monolayers (MLs) of the van der Waals material $NbSe_2$ that are rotated with respect to the underlying bulk $NbSe_2$ using our developed ultra-high vacuum (UHV) stacking technique. These heterostructures were characterized through the use of scanning tunneling microscopy and spectroscopy at a base temperature of 1.4 K. The MLs realize a variety of twist angles relative to the underlying bulk lattice, with the lowest observed twist angle being 10°. The MLs display the coexistence of charge density waves (CDW) and moiré effects: In the absence of strain, the MLs develop a 3×3 CDW, however the application of strain through interfacial disorder results in a 2×2 CDW state, supported by theoretical calculations. Compared to isolated MLs the superconducting order parameter is enhanced due to the proximity effect from the underlying bulk.

O 95.9 Fri 11:30 HSZ/0401

band structure and charge density wave in a natural van der Waals heterostructure 4Hb-TaSe2 — •fumihiko kimura[1], tomoki maeda[2], natsuki mitsuishi[3,4], kazuki okada[2], takuya nomoto[5], kenichi ozawa[6], masahiro naritsuka[3], tetsuo hanaguri[3], shunsuke kitou[7], yuiga nakamura[8], taka-hisa arima[3,7], takao sasagawa[2], and kyoko ishizaka[1,3] — [1]Quantum-Phase Electronics Center & Department of Applied Physics, The University of Tokyo — [2]Laboratory for Materials and Structures, Science Tokyo — [3]RIKEN CEMS — [4]Graduate School of Science, Nagoya University — [5]Department of Physics, Tokyo Metropolitan University — [6]Institute of Materials Structure Science, High energy Accelerator Research Organization (KEK) — [7]Department of Advanced Materials Science, The University of Tokyo — [8]Japan Synchrotron Radiation Research Institute (JASRI), SPring-8

4Hb-TaSe2 is a natural van der Waals heterostructure charge density wave (CDW) material consisting of alternative stacking of monolayer 1T-TaSe2 (Mott insulator with Star-of-David CDW) and monolayer 2H-TaSe2 (superconductor with 3 by 3 CDW). Although transport measurements have suggested the existence of multiple CDWs, the details of the CDW and electronic structures remain unclear. In this study, we directly observed the electronic structure of 4Hb-TaSe2 by micro-focused angle-resolved photoemission spectroscopy with careful selection of the surface terminations. We discuss the temperature dependent electronic structure with comparison to the CDW structures obtained by scanning tunneling microscopy and X-ray diffraction.

O 95.10 Fri 11:45 HSZ/0401

Coexisting charge density waves in twisted NbSe2 bilayers — •Christopher Tat Shun Cheung[1], Zachary A. H. Goodwin[2], Yixuan Han[3], Jiong Lu[3], Arash A. Mostofi[1], and Johannes Lischner[1] — [1]Departments of Physics and Materials and the Thomas Young Center for Theory and Simulation of Materials, Imperial College London, London SW7 2AZ, U.K. — [2]Institute for Functional Intelligent Materials, National University of Singapore, Singapore 117544, Singapore — [3]Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom

Twisted bilayers of semiconducting transition metal dichalcogenide (TMD) monolayers have been studied extensively. In contrast, twisted bilayers composed of metallic monolayers, such as NbSe2, remain less understood.

Monolayer NbSe2 can host different types of charge density waves (CDWs), in which the Nb atoms move away from their high-symmetry positions. In twisted bilayer NbSe2, identifying CDWs in relaxed structures is challenging because atomic relaxations occur both because of CDW formation and also because of the moiré pattern.

We have carried out large-scale first-principles calculations using density functional theory to study the moiré relaxations and CDWs in twisted bilayer NbSe2. We have developed methods for revealing the CDWs, and for locally classifying the type of CDW. We find that different types of CDWs coexist in the moiré unit cell due to the interactions with strain induced by moiré relaxations [1].

[1] Cheung et al, Nano Lett. 2024, 24, 12088-12094.

O 95.11 Fri 12:00 HSZ/0401

MicroARPES studies of contact doping of monolayer transition metal dichalcogenides by RuCl3 — •Thomas Nielsen[1], Edvard Solbrekken[1], Alfred J. H. Jones[1], Zhihao Zhiang[1], Chakradar Sahoo[1], Kenji Watanabe[2], Takashi Taniguchi[2], Jill A. Miwa[1], Søren Ulstrup[1], Christian Overby[1], and Christian V-B. Fokdal[1] — [1]Aarhus University, Denmark — [2]National Institute for Materials Science, Japan

Placing van der Waals materials into contact with α-$RuCl_3$ has recently emerged as a method of modulating their electronic structures. The proximity to α-$RuCl_3$ has been observed to produce strong hole doping in the van der Waals material, and this has been established as a method to create better electrical contacts in transistor devices based on monolayer transition metal dichalcogenides (TMDs). Here, we use the microARPES endstation at the ASTRID2 synchrotron light source at Aarhus University in Denmark to study the valence bands and core levels of semiconducting monolayer TMDs in proximity to α-$RuCl_3$. We observe a large valence-band shift of 0.7 – 0.8eV indicating strong hole doping. α-$RuCl_3$ is highly sensitive to the temperatures and chemicals typically used in the dry-transfer fabrication procedures of van der Waals heterostructures. How the degradation of α-$RuCl_3$ affects the proximity-induced doping of the TMD is discussed based on the ARPES measurements.

O 95.12 Fri 12:15 HSZ/0401

STEM Investigation of Entropy Forbidden Ordering in CVD Grown WSe_2-$MoSe_2$ Alloys — •Max Bergmann[1], Matvei Kislitsyn[1], Julian Picker[2], Jürgen Belz[1], Robin Günkel[1], Badrosadat Ojaghi Dogahe[1], Shamail Ahmed[1], Andrey Turchanin[2], and Kerstin Volz[1] — [1]mar.quest | Marburg Center for Quantum Materials and Sustainable Technologies, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Faculty of Chemistry and Earth Sciences, Friedrich-Schiller-Universität, 07743 Jena, Germany

2D transition metal dichalcogenides have gained significant interest due to their optoelectronic properties, which can be tailored by structural variation. However, controllable production, namely growth, of such tailored structures still remains a key challenge towards large-scale production. In this study, we show lateral heterostructures of 2D $MoSe_2$ and WSe_2, grown on a SiO_2 TEM grid by chemical vapor deposition, that at the interface show a highly ordered structure of W and Mo atoms at the TMD positions, as observed by scanning transmission electron microscopy. This is in contrast to *ab initio* calculations, which ascribe unordered alloys as the preferred configuration, since entropy is the main driving force compared to formation enthalpy. We link this unexpected phenomenon to the initial nucleation of the material on a clean $MoSe_2$ crystal edge, present before the alloy growth, together with special precursor chemistry. Furthermore, we show *ab initio* results in conjunction with the special quasirandom structure method on the bandstructure and optical properties of this structure.

O 96: Plasmonics and nanooptics: Fabrication, characterization and applications

Time: Friday 9:30–12:30 Location: HSZ/0403

O 96.1 Fri 9:30 HSZ/0403

How to fix silver for plasmonics ? — •Jonas Graf[1], Björn Ewald[1], Leo Siebigs[1], Cheng Zhang[2], Achyut Tiwari[3], Max Rödel[1], Sebastian Hammer[1], Vladimir Stepanenko[4], Frank Würthner[4], Bruno Gompf[3], Bert Hecht[2], and Jens Pflaum[1] — [1]Experimental Physics 6, Univ. Würzburg, 97074 Würzburg — [2]Experimental Physics 5, Univ. Würzburg, 97074 Würzburg — [3]1. Physikalisches Institut, Univ. Stuttgart, 70569 Stuttgart — [4]Institute for Organic Chemistry, Univ. Würzburg, 97074 Würzburg

Silver (Ag) is an ideal plasmonic material for applications in the visible regime, but its use is hindered by poor chemical stability and structural quality of thermally evaporated thin films and nanostructures. Here, we present a simple approach to overcome these limitations by alloying Ag thin films with small amounts of gold (Au) through thermal co-evaporation. We analyzed $Ag_{100-x}Au_x$ thin films with Au contents ranging from 5 to 20 at.% with respect to their surface and bulk crystal quality, optical properties and chemical stability. Remarkably, already $Ag_{95}Au_5$ thin films exhibit a drastically enhanced chemical stability and excellent plasmonic properties outperforming pure Ag. This is related to the high film quality achieved without metallic wetting layers, epitaxial substrates or template stripping. As a proof of concept, we fabricate $Ag_{95}Au_5$ plasmonic nanoantennas demonstrating excellent long-term durability over one month under ambient conditions. Our approach thus demonstrates a simple and effective strategy to overcome the general limitations of Ag in plasmonic applications. B. Ewald et al., ACS Photonics 2025, DOI: 10.1021/acsphotonics.5c01659

O 96.2 Fri 9:45 HSZ/0403

Topological quasiparticles in a bucket: water waves as an experimental platform for emulating optical nearfields — •Alexander Neuhaus, Pascal Dreher, Philipp Gessler, Michael Horn-von Hoegen, Karin Everschor-Sitte, and Frank Meyer zu Heringdorf — Faculty of Physics and Center for Nanointegration, Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47048 Duisburg, Germany

Optical near fields can host a variety of topological quasiparticles, including merons, skyrmions, skyrmion bags and optical vortices, but their nanometric spatial scales and femtosecond time dynamics make them difficult to access experimentally. Modern techniques, such as time resolved photoemission microscopy or nearfield scanning optical microscopy can image these field configurations, but they are both experimentally challenging. Here, we demonstrate a much simpler 3d printed experiment that can be used as a model system to emulate the behavior of optical nearfields with capillary-gravity water waves. Although water waves and surface polaritons are vastly different wave phenomena, the displacement vector field in the water can be described by surface wave equations that are similar to the equations used to describe surface polaritons. We reconstruct the displacement field of the water wave by fast checkerboard decomposition of videos of the water wave propagation. Water-wave experiments yield the same topological quasiparticles as observed in optical nearfields, yet they do so in seconds instead of hours of experimental time.

O 96.3 Fri 10:00 HSZ/0403

Layer-Resolved Optical Metrology of MoS_2 Using Surface Plasmon Resonance Imaging — •Priyanka Thawany[1,2], Hesam Amiri[1], Lina Jäckering[2], Andrei Vescan[3], Thomas Taubner[2], Sven Ingebrandt[1], and Vivek Pachauri[1] — [1]Institute of Materials in Electrical Engineering 1 (IWE1), RWTH Aachen University — [2]I. Institute of Physics (IA), RWTH Aachen University — [3]Compound Semiconductor Technology, RWTH Aachen University

Conventional techniques such as scanning probe microscopy, Raman spectroscopy [1], ellipsometry [2], and terahertz microscopy [3] provide crucial information on optical and electronic parameters of 2D materials. However, they remain limited in measurement speed and spatial coverage for large-area characterization. To address these limitations, we demonstrate the use of surface plasmon resonance imaging (SPRi) as a complementary wide-field technique for mapping few-layer MoS_2 stacks. Thickness-dependent shifts in the SPR resonance angle and corresponding reflectance contrast allow clear discrimination of atomic-layer regions, consistent with theoretical predictions for MoS_2 optical permittivity changes. SPRi therefore offers a rapid, scan-free approach for real-time metrology of few-layer MoS_2, and similar measurements on other 2D materials show the same suitability for rapid optical characterization.

[1] Malard et al., *Phys. Chem. Chem. Phys.* **23**, 23428 (2021).
[2] Amiri et al., *Nano Trends* **111**, 100130 (2025).
[3] Whelan et al., *Sci. Rep.* **14**, 3163 (2024).

O 96.4 Fri 10:15 HSZ/0403

Launching and confining In-Plane Hyperbolic Phonon Polaritons in α-MoO_3 with In_3SbTe_2 nanostructures — •Umberto Saldarelli[1], Lina Jäckering[1], Lukas Conrads[1], Matthias Wuttig[1], Pablo Alonso-González[2,3], and Thomas Taubner[1] — [1]I. Institute of Physics (IA), RWTH Aachen University — [2]Department of Physics, University of Oviedo — [3]Center of Research on Nanomaterials and Nanotechnology, CINN (CSIC-Universidad de Oviedo)

Alpha-phase molybdenum trioxide (α-MoO_3), a van der Waals material, supports in-plane hyperbolic phonon polaritons (HPPs) with high confinement, low losses, and extremely directional propagation [1]. Rapid prototyping of nanostructures for tailoring polaritons can be achieved with the plasmonic phase-change material In_3SbTe_2 (IST) [2], switchable between amorphous and crystalline phases via laser-induced heating. This has been already shown for programmable resonator structures within hBN [3]. Here we combine α-MoO_3 with IST. We use scattering-type scanning near-field optical microscopy (s-SNOM) to explore HPP launching by antennas of different orientations. Next, we optically program a circular launching structure to focus polaritons. Finally, adding a second focusing disk and reconfiguring the disk distance, we tailor field enhancement and confinement. Our results enable rapid design of reconfigurable structures and provide an all-optical material platform for controlling in-plane HPPs.

[1] Ma et al. *Nat.* **562**, 557-562, (2018)
[2] Conrads et al. *Opt. Mat. Expr.* **15**, 2664-2687, (2025)
[3] Jäckering et al. *Nano Lett.* **25**, 15809, (2025)

O 96.5 Fri 10:30 HSZ/0403

Nanoscale Optical Readout of Antiferromagnetic Order by Photocurrent Nanoscopy — •Dario Siebenkotten[1], Anna Schmid[2], Dinghe Dai[1], Joao Godinho[2], Sam Fairman[1], Arne Hoehl[1], Tomas Janda[2], Tomas Ostatnicky[3], Bernd Kästner[1], and Jörg Wunderlich[2] — [1]Physikalisch-Technische Bundesanstalt, Berlin, Germany — [2]Institute of Experimental and Applied Physics, University of Regensburg, Regensburg, Germany — [3]Charles University, Faculty of Mathematics and Physics, Prague, Czech Republic

Antiferromagnets are prime candidates for next-generation spintronic technologies as they allow for rapid switching and miniaturization compared to ferromagnets. However, readout of their magnetic state remains an open challenge, as their vanishing net magnetisation suppresses conventional magnetic readout schemes. Therefore, new mechanisms are required to measure the state of antiferromagnetic domains, which are often confined to the nanoscale. Here, we report on the experimental observation of a previously only theoretically predicted light-induced, Néel-order-dependent transverse photocurrent that we refer to as the optical nonlinear anomalous Hall effect. We demonstrate the effect by nanoscale imaging of the photocurrent generated in PT-symmetric CuMnAs cross-bar devices by mid-infrared near fields at the apex of a sharp metal tip. We exclude purely thermal mechanisms by showing that the photocurrent reverses sign when the Néel vector is rotated by 180° via current-induced switching of nanoscale antiferromagnetic domains of a few hundred nanometers in size, consistent with a time-reversal-odd nonlinear anomalous Hall photocurrent.

O 96.6 Fri 10:45 HSZ/0403

Plasmonic Effects in a honeycomb metasurface of Ag Nanotriangles and Nanoholes — •Paul-G. Nitsch[1], Paul Oleynik[1], Markus Ratzke[1], David Stolarek[2], Jon Schlipf[2], Oliver Skibitzki[2], Rudi Tschammer[3], Carlos Morales[3], Jan I. Flege[3], Christian Wenger[2], and Inga A. Fischer[1] — [1]Experimentalphysik und funktionale Materialien, BTU-CS, Cottbus, Germany — [2]IHP - Leibniz- Institut für innovative Mikroelektronik, Frankfurt (Oder), Germany — [3]Angewandte Physik und Halbleiterspektroskopie, BTU-CS, Cottbus, Germany

Coupled lattices of metal nanoparticle and nanohole arrays can support spectrally narrow plasmonic resonances with potential applications, e.g., in biosensing. In nanohole arrays, the interplay of surface plasmon polaritons at metal-dielectric interfaces and Rayleigh anomalies can lead to Fano resonances, whose spectral positions are well described by Bragg coupling conditions. For nanoparticle arrays with small interparticle distances, the coupling of neighboring particles via their overlapping evanescent fields leads to resonances, whose dispersion relation has been described by tight-binding models. Here, we investigate resonances in coupled nanoparticle and nanohole lattices both experimentally and in simulation. We show that a variation in angle of incidence can be used to tune mode coupling and present results on the detection of near-surface refractive index changes with high sensitivities and figures-of-merit in our samples.

O 96.7 Fri 11:00 HSZ/0403

Hybrid Gold–Vanadium-Dioxide Tunable Plasmonic Devices — Rostislav Řepa, Jiří Kabát, Jiří Liška, Peter Kepič, Michal Horák, Tomáš Šikola, and •Vlastimil Křápek — Brno University of Technology, Brno, Czechia

Vanadium dioxide (VO_2) exhibits a metal-insulator transition near room temperature, which can be exploited in tunable plasmonic devices with compelling functions. However, devices based solely on VO_2 suffer from a large optical absorption and low chemical stability of VO_2 [1].

We present a hybrid material platform that combines high-quality crystalline self-assembled VO_2 nanoparticles [2] with lithographically defined gold nanostructures in a lateral arrangement In this way, we benefit from both the tunability of VO_2 and the high conductivity of gold. The lateral arrangement minimizes the amount of VO_2 and thus contributes to the high quality of the devices.

We demonstrate two tunable plasmonic devices based on the above-mentioned material platform: (1) Electric-magnetic switches, in which either an electric or magnetic hot spot is formed, following a design from Ref. [3]. (2) Resonance-energy switches, in which the spectral profile of the scattering or absorption is controlled, with possible applications in selectively-enhanced photoluminescence.

[1] Krpenský et al., Nanoscale Adv. **6**, 3338–3346 (2024).
[2] Horák et al., arXiv:2408.11972.
[3] Křápek et al., Nanophotonics **9**, 623–632 (2020).

O 96.8 Fri 11:15 HSZ/0403

Phonon Polariton Materials Discovery from First Principles — Elena Gelzinyte[1], Giulia Carini[1], Niclas S. Mueller[1], Martin Wolf[1], Karsten Reuter[1], •Johannes T. Margraf[2], Alexander Paarmann[1], and Christian Carbogno[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Universität Bayreuth

Phonon Polaritons (PhPs), quasi-particles that arise from strong coupling between infrared photons and optical lattice vibrations, are promising in nanophotonic applications for highly directional and confined light propagation with low optical loss [1]. So far, PhP studies have been mostly focused on a few canonical materials, and the trends in the material space that influence the emergence and properties of PhPs remain largely unexplored. To consider the suitability of various polar crystals for the formation of PhPs, we compute the infrared permittivity functions [2] of 3,000 materials in the JARVIS-DFT database [3]. We then categorize these compounds by their normalized light-matter coupling strength and Reststrahlen band width, whereby we also decompose these in terms of individual phonon mode contributions. A broad range of materials emerges with comparable or better properties than those of typically studied PhP compounds. Using orthorhombic PbO, monoclinic TiO_2, and trigonal $CdCN_2$ as represen-

tative examples, we validate our approach and discuss the PhP property trends that allow to identify and design promising PhP candidates.
[1] E. Galiffi *et al.*, Nat. Rev. Mater. **9**, 9 (2024).
[2] X. Gonze and C. Lee, Phys. Rev. B **55**, 16 (1997).
[3] K. Choudhary *et al.*, npj Comput. Mater. **6**, 1 (2020).

O 96.9 Fri 11:30 HSZ/0403

Infrared beam-shaping via geometric phase metasurfaces with the plasmonic phase-change material In_3SbTe_2 — •Lukas Conrads, Florian Bontke, Matthias Wuttig, and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University

Conventional optical elements are bulky and limited to specific functionalities, contradicting the increasing demand of miniaturization and multifunctionalities. Optical metasurfaces enable tailoring light-matter interaction at will, especially important for the infrared spectral range which lacks commercially available beam-shaping elements. While the fabrication of those metasurfaces usually requires cumbersome lithography techniques, direct laser writing promises a simple and convenient alternative. Here, we exploit the non-volatile laser-induced insulator-to-metal transition of the plasmonic phase-change material In_3SbTe_2 (IST) [1,2] for optical programming of large-area metasurfaces for infrared beam-shaping. We tailor the geometric phase of metasurfaces with rotated crystalline IST rod antennas to achieve beam steering, lensing, and beams carrying orbital angular momenta. Finally, we investigate multi-functional and cascaded metasurfaces exploiting enlarged holography, and design a single metasurface creating two different holograms along the optical axis. Our approach facilitates fabrication of large-area metasurfaces within hours, enabling rapid-prototyping of customized infrared meta-optics for sensing, imaging and quantum information.[3] [1] Heßler et al. *Nat. Com.* **12**, 924 (2021) [2] Conrads et al. *Opt. Mat. Ex.* **15**, 2664-2687 (2025) [3] Conrads et al. *Nat. Com.* **16**, 3698 (2025)

O 96.10 Fri 11:45 HSZ/0403

Ab Initio Theory of Chemical Interface Damping of Surface Plasmons — •Jordan Edwards[1], Johannes Lischner[1], Andrei Stefancu[2], Wenxuan Tang[3], Ming Fu[3], Ross Schofield[3], Toby Millard[3], Rupert Oulton[3], Pilar Carro[4], Naomi Halas[5], Peter Nordlander[5], and Emiliano Cortes[2] — [1]Imperial College London, London, United Kingdom — [2]Ludwig-Maximilians-Universität (LMU), Munich, Germany — [3]Imperial College London, London, United Kingdom — [4]University of Laguna, La Laguna, Spain — [5]Rice University, Houston, United States

Metallic nanostructures support surface plasmons, collective electron oscillations that give rise to unique optical properties. Molecular adsorption can strongly modify plasmon behaviour; for example, experiments showing that functionalisation reduces their propagation length, a phenomenon is known as chemical interface damping (CID). However, the origin behind CID remains debated, with two proposed mechanisms being: (1) excitation of electron-hole pairs involving the adsorbate orbitals, and (2) electronic scattering by adsorbate-induced dipoles.

To investigate the physical origin of CID, we perform first-principles density-functional theory calculations for different molecules adsorbed on Au(111) surfaces. We calculate the density of states projected onto the adsorbate orbitals to analyse surface-plasmon decay channels associated with mechanism (1). We also use cluster models of the surface to investigate mechanism (2). These results are compared to experimental measurements, offering insights into the origin of CID.

O 96.11 Fri 12:00 HSZ/0403

Tailoring hyperbolic phonon polaritons in hexagonal boron nitride with the phase-change material In_3SbTe_2 — •Lina Jäckering, Aaron Moos, Lukas Conrads, Matthias Wuttig, and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University

Polaritons in van-der-Waals materials (vdWM)[1] promise high confinement and multiple tailoring options by resonators and launching structures which conventionally require cumbersome lithography techniques. Optical programming of phase-change materials (PCMs) offers fast and reconfigurable fabrication of these structures. As the plasmonic PCM In_3SbTe_2 (IST) can be switched between a dielectric and metallic phase, IST is promising for nanophotonics[2], especially for optical programming of metallic launching structures to tailor and confine polaritons in vdWM. Here, we combine the vdWM hexagonal boron nitride (hBN) with IST.[3] We optically program circular resonators for hBN's phonon polaritons into IST through the hBN flake. We investigate the polariton resonators with near-field optical microscopy. Demonstrating the reconfigurability, we decrease the resonator diameter to increase the confinement up to $\lambda/39$ and achieve a quality factor of 72. Finally, we fabricate a focusing structure for hBN's polaritons whose focal point we reconfigure. We promote IST as a versatile platform for rapid prototyping of polariton optics in various vdWM such as α-MoO_3, β-Ga_2O_3 and $MoOCl_2$. [1] Basov et al. Science **354**, 6309 (2025) [2] Conrads et al. Opt. Mater. Express **15**, 2664 (2025). [3] Jäckering et al. Nano Letters **25**, 15809 (2025).

O 96.12 Fri 12:15 HSZ/0403

Self-assembled dielectric network metamaterials based on vanadium oxide — •Marcello Pozzi[1], Jeremi Setz[1], Noel von Wattenwyl[1], Georg Haberfehlner[2], Arnold Müller[3], Ralph Spolenak[1], and Henning Galinski[1] — [1]Laboratory for Nanometallurgy, ETH Zürich, Switzerland — [2]FELMI-ZFE, TU Graz, Austria — [3]Laboratory of Ion Beam Physics, ETH Zürich, Switzerland

Among scalable optical nanomaterials, network metamaterials stand out because of their large-area compatibility, versatility and low footprint. These systems are created by self-assembly in a reaction-diffusion process called "chemical dealloying", resulting in complex network structures with broadband optical response driven by plasmonic mode equipartition [1]. Typical network metamaterials consist of noble metallic elements and show plasmonic behavior. Here we propose a material system that extends the design space of network metamaterials to dielectrics. Using magnetron co-sputtering of aluminum-vanadium followed by chemical dealloying, we fabricate network metamaterials based on vanadium oxide. Through the combination of Rutherford backscattering spectroscopy (RBS) and focused ion beam (FIB) tomography we analyze the dynamics of pattern formation, while the light-matter interaction is studied combining full-wave simulations and various spectroscopy techniques. Finally, we determine the degree of hyperuniformity of the dielectric networks by measuring the scaling behavior of the volume fraction variance of the systems.

[1] Adv. Optical Mater. 2023, 11, 2300568

O 97: Solid-liquid interfaces: Reactions and electrochemistry III

Time: Friday 9:30–12:30 Location: TRE/PHYS

Invited Talk O 97.1 Fri 9:30 TRE/PHYS

Questions of Selectivity in Electrocatalysis — •Vanessa J. Bukas — Fritz-Haber-Institut der MPG, Berlin

Heterogeneous electrocatalysis is at the heart of developing sustainable energy technologies. The rational design of suitable electrocatalysts, however, depends on a deeper understanding of the underlying reaction mechanisms. Product selectivity, in particular, remains poorly understood and cannot be rationalized by popular thermodynamic models that currently define the state-of-the-art in computational electrocatalysis. In this talk, I will address a number of possible scenarios as to why this may be while challenging prevalent mechanistic assumptions. Atomistic models, based mainly on density-functional theory, will explore microscopic reaction mechanisms to demonstrate effects due to the local field at the electrical double layer, the delicate kinetic competition between electrochemical and non-electrochemical reaction steps, as well as the key role of mesoscopic mass transport. The emerging insight adds to our fundamental understanding of electrocatalysis and supports ongoing efforts toward optimal process design.

O 97.2 Fri 10:00 TRE/PHYS

Mechanism of Fe(II) Chemisorption on Hematite(001) Revealed by Machine Learning Molecular Dynamics — •Kit Joll[1], Philipp Schienbein[1,2], Kevin Rosso[3], and Jochen Blumberger[1] — [1]Department of Physics and Astronomy and Thomas Young Centre, University College London, London WC1E 6BT, United Kingdom; — [2]Ruhr-Universität Bochum, 44780 Bochum, Germany; Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, 44780 Bochum, Germany — [3]Pacific Northwest National Laboratory, Richland, Washington 99354, United States;

Understanding ion adsorption at mineral-water interfaces is key to explaining geochemical processes such as redox cycling, dissolution, and crystal growth. However, probing these reactions experimentally at atomic resolution remains challenging. Here, we employ reactive neural network potential molecular dynamics (NNP-MD) with umbrella sampling and reactive flux transition state theory to simulate the chemisorption of aqueous Fe^{2+} on hematite(001) at density-functional theory (DFT) accuracy and nanosecond time scales. We identify a dissociative mechanism for Fe^{2+} water-ligand exchange and multiple stable surface complexes, nonadsorbed, physisorbed, monodentate, and tridentate chemisorbed species, along the adsorption pathway. The overall process is exergonic, in contrast to previous classical force-field predictions. These results

demonstrate how machine-learning potentials bridge the accuracy of ab-initio methods with the sampling efficiency of classical molecular dynamics, providing new atomistic insight into reactive processes at oxide-water interfaces.

O 97.3 Fri 10:15 TRE/PHYS

How to Best Achieve a Steady State: Comparison of Different Methods to Acquire Tafel Plots — •Maren-Kathrin Heubach and Gregory Jerkiewicz — Department of Chemistry, Queen's University, Kingston, Canada.

The performance of an electrocatalyst is typically characterized by Tafel plots, which show a natural logarithm of the current density of a reaction as a function of the overpotential. Hereby, the exchange current density and the Tafel slope can be determined, giving insights into the mechanism of the electrocatalytic reaction. Even though Tafel plots are widely used, there is a large variety in performing the measurements to create Tafel plots.

In this contribution, we will discuss and compare several approaches to achieve the closest approximation to the desired steady state. These approaches will be showcased with the benchmark system of a polycrystalline Pt sample in an aqueous sulphuric acid solution.

O 97.4 Fri 10:30 TRE/PHYS

Exploring the Surface Structure of Ni Anodes and the Role of pH for Alkaline Oxygen Evolution Using SERS — •Justus Leist, Annika Neufischer, Roman Jocher, Benjamin Schilling, Timo Jacob, and Albert Engstfeld — Ulm University, Institute of Electrochemistry, Ulm, Germany

Sustainable hydrogen can be generated by electrochemical water splitting, but the process is typically limited by the sluggish kinetics of the oxygen evolution reaction (OER) at the anode. To avoid reliance on noble-metal catalysts such as Ir and Ru, Ni-based catalysts have attracted considerable interest due to their abundance and efficiency. Under OER conditions, where the Ni anode surface is accepted to be NiOOH, Raman spectroscopy enables *in situ* monitoring of both the surface structure and possible OER intermediates. In this work, using Surface-enhanced Raman spectroscopy (SERS) combined with DFT, we challenge the assumed presence of NiOOH under OER conditions.[1]

To probe the atomic composition of the oxidized Ni anodes, isotope-labelled Raman experiments were performed, revealing the absence of hydrogen in the lattice. The presence of NiO*, rather than NiOOH, is further supported by DFT-calculated spectra. Additionally, we illustrate that a band previously attributed to an OO- species is more likely related to overtones. By varying the pH from alkaline to near-neutral conditions, we examine the impact of pH on the Raman spectra during the OER and discuss these changes in relation to the vibrational Stark effect and possible OER intermediates.

[1] J. Leist et al. *ChemRxiv* DOI: 10.26434/chemrxiv-2025-jb73p

O 97.5 Fri 10:45 TRE/PHYS

Optimizing oxygen vacancies through grain boundary engineering to enhance electrocatalytic nitrogen reduction — •Xiu Zhong[1], Fu Yang[2], and Yong Lei[1] — [1]Institut für Physik & IMN MacroNano (ZIK), Technische Universität Ilmenau, Ilmenau 98693, Germany — [2]School of Environmental and Chemical Engineering, Jiangsu University of Science and Technology, Zhenjiang, Jiangsu 212100, China

This study develops an efficient N2-reduction catalyst by in-situ anchoring ultrafine MoO2 nanograins on N-doped carbon fibers. Optimized thermal treatment generates abundant grain boundaries that increase oxygen-vacancy concentration, enhance electron transfer, and create highly active N2-trapping sites. The optimal MoO2/C700 catalyst delivers superior performance, achieving an NH3 yield of 173.7 μg h-1 mgcat -1 and a Faradaic efficiency of 27.6% at -0.7 V vs. RHE in 1 M KOH. In-situ XPS and DFT confirm the electronic-structure modulation and strong N2-oxygen-vacancy interaction, revealing electron transfer between adsorbed nitrogen and Mo(IV). Correlating activity with interfacial effects further clarifies the origin of enhancement. The catalyst also shows stable operation for 60 h, demonstrating the promise of grain-boundary engineering to boost oxygen vacancies for efficient and sustainable electrochemical ammonia synthesis.

O 97.6 Fri 11:00 TRE/PHYS

Investigating the Role of Nuclear Quantum Effects at Zinc Oxide-Water Interfaces with High-Dimensional Neural Network Potentials — •Jan Elsner[1,2] and Jörg Behler[1,2] — [1]Theoretische Chemie II, Ruhr-Universität Bochum, Germany — [2]Research Center Chemical Sciences and Sustainability, Research Alliance Ruhr, Germany

Zinc oxide is a promising material for sustainable hydrogen production via catalytic water splitting. The interface of ZnO with water exhibits complex dynamical behaviour, including water dissociation and recombination, as well as long-range proton transport. Previous studies [1] have elucidated these mechanisms using High-Dimensional Neural Network Potentials (HDNNPs), which enable simulations at the system sizes and timescales needed for statistically converged interfacial properties. However, the validity of the classical approximation for atomic nuclei in such systems, particularly for describing interfacial proton transfer (PT), remains poorly understood. Here, we employ a new efficient parallel implementation of path-integral molecular dynamics with HDNNPs [2] to investigate the role of nuclear quantum effects (NQEs) at the ZnO-water interface. We show that NQEs significantly lower free energy barriers for PT, and discuss the resulting implications for the interfacial dynamics of the system.

[1] Quaranta V., Hellström M., Behler J., J. Phys. Chem. Lett. 2017, 8, 1476-1483
[2] Shiga M., Elsner J., Behler J., Thomsen B., J. Chem. Phys. 2025, 163, 134119

O 97.7 Fri 11:15 TRE/PHYS

Linking Water Structure to Proton-Coupled Electron Transfer at Metal Interfaces — •Julius Lonnes[1,2], Nicolas G. Hörmann[1], and Karsten Reuter[1] — [1]Fritz-Haber-Institut der MPG — [2]Technische Universität München

Understanding the kinetics of interfacial electrochemical reactions is essential for optimizing technologies such as fuel cells and batteries. To this end, the interfacial water structure plays a key role in determining the effects of pH and electrolyte cations on reaction rates, yet the mechanistic link between water arrangement and reaction barriers remains unclear. By examining the acidic Volmer step on Pt(111) and tuning the hydrogen-bond network surrounding the proton, we uncover how interfacial solvation modulates electrochemical activation barriers. We find that proton stability at the metal-water interface strongly influences the barrier height, a relationship that can be rationalized with Hammond's postulate:[1] variation in electrochemical potential shifts the transition state position along the reaction coordinate, altering its sensitivity to local solvation structure. We establish that interfacial solvation is a decisive factor in determining electrochemical activation energies, advancing fundamental understanding of proton-coupled electron transfer at charged interfaces.

[1] G.S. Hammond, J. Am. Chem. Soc. **77**, 334 (1955).

O 97.8 Fri 11:30 TRE/PHYS

Understanding of degradation of catalyst/semiconductor interfaces — Sergej Levashov[1], Tim Rieth[1,2], Ian D. Sharp[1,2], and •Johanna Eichhorn[1] — [1]TUM School of Natural Sciences, TU Munich — [2]Walter Schottky Institute, TU Munich

The performance of photoelectrochemical (PEC) materials are governed by interfacial processes where atomic structure, electronic states, and chemical reactions meet. Local defects and dynamic surface transformations at the nanoscale can dominate charge transfer and often trigger degradation under operating conditions. Accessing such mechanisms requires in-situ/operando techniques that probe interfacial structure and dynamics with nanoscale resolution. We employ in situ scanning probe microscopy to study the interfacial stability of TiO2/Pt photocathodes by monitoring local surface transformations and detachment events during operation. Pt catalysts are deposited on conformal TiO2 coatings either by sputtering, yielding continuous films, or by atomic layer deposition (ALD), forming discrete nanoislands and enabling atom-efficient utilization of precious metals. Under PEC conditions, both architectures show comparable onset potentials and saturation current densities, yet chronoamperometry reveals an enhanced long-term stability for the nanostructured ALD-Pt electrodes. We attribute this contrasting behavior to different bubble formation and detachment dynamics at the catalyst-semiconductor interface. These nanoscale insights highlight the importance of interfacial and morphological engineering, as well as the necessity of controlling reaction processes, to achieve durable and efficient PEC material systems.

O 97.9 Fri 11:45 TRE/PHYS

An Analytical Description for Atomic Diffusion involved Peaks in Cyclic Voltammograms: the Reversible Place-Exchange on Pt(111) — Jon Bjarke Valbaek Mygind[1], Francesc Valls Mascaró[2], Gerard J. Verbiest[3], and •Marcel J. Rost[4] — [1]Catalan Institute of Nanoscience and Nanotechnology, Campus UAB, Barcelona, Spain — [2]Faculty of Physical Chemistry, University of Innsbruck, Innsbruck, Austria — [3]Department of Precision and Microsystems Engineering, Delft University, Delft, The Netherlands — [4]Huygens-Kamerlingh Onnes Laboratory, Leiden University, Leiden, The Netherlands

Cyclic voltammetry (CV) is one of the most powerful tools for the experimental investigation and characterization of electron transfer processes in electrochemistry. As the unique electrochemical fingerprint of a particular system is given by specific (current) peaks in the cyclic voltammogram, it is not surprising that great effort is done to understand, describe, and model these peaks. However, the underlying thermodynamic and kinetic processes make this a difficult task, especially when features in the fingerprint change with the applied CV sweep rate. Here we show, on the example of the reversible Place-Exchange peak, a precursor in the electrochemical oxidation of the Pt(111) surface, that a combination of a Frumkin isotherm followed by an Arrhenius (atomic) diffusion process delivers a rather good description. We present an analytical theory that fits all peaks of all CVs, measured with different sweep rates, with only six fit variables. These variables deliver hard quantitative thermodynamic values.

O 97.10 Fri 12:00 TRE/PHYS

Machine Learning the Energetics of Electrified Solid-Liquid Interfaces — •Nicolas Bergmann[1], Nicéphore Bonnet[2], Nicola Marzari[2], Karsten Reuter[1], and Nicolas G. Hörmann[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Theory and Simulation of Materials, EPFL, Lausanne

Machine learning interatomic potentials (MLIPs) accelerate many aspects of computational chemistry. However, MLIPs fail to describe the biases introduced at applied potential conditions for typical electrocatalytic systems, where effects of the inner double layer play a critical role [1]. Here, we present the "Response Analysis in z-ORientation" (RAZOR) model [2], which machine-learns the work function, the first-order energy change to bias charges q. RAZOR is stabilized by additionally learning the atomic force derivative to q, equivalent to Born effective charges. The approach extends MLIPs to the variable charge case, by adding bias-induced energy and force changes to traditional zero-bias MLIPs. This enables large-scale molecular dynamics simulations at finite bias. We demonstrate RAZOR's capabilities by investigating OH adsorption on Cu(100) and explicit Pt(111)-H_2O interfaces, faithfully recreating *ab initio* and experimental results.
[1] N. Bergmann *et al.*, J. Chem. Theory Comput. **19**, 8815 (2023).
[2] N. Bergmann *et al.*, Phys. Rev. Lett. **135**, 146201 (2025).

O 97.11 Fri 12:15 TRE/PHYS

Entropy-Enthalpy Relationships in Heterogeneous Electrocatalysis: A Case Study of the Hydrogen Evolution Reaction — •Andrew J. Wong, Barbara Sumić, Elias Diesen, Nicolas G. Hörmann, Hendrik H. Heenen, Karsten Reuter, and Vanessa J. Bukas — Fritz-Haber-Institut der MPG, Berlin

Temperature is a key parameter in industrial electrolyzers. And yet, the vast majority of mechanistic lab-scale studies ignores temperature variations by operating at room temperature. This is surprising since existing experimental evidence has shown that even modest heating can significantly affect the rate and selectivity of electrocatalytic reactions. Understanding the origin of such effects is crucial for advancing fundamental electrocatalysis and exploiting temperature as a control parameter. Here, we explore temperature effects on the hydrogen evolution reaction (HER) by developing a simple mean-field microkinetic model based on first-principles energetics. An Arrhenius analysis on the HER rates across different metal catalysts reveals distinct entropy-enthalpy correlations, reflected in the apparent activation enthalpy and entropy-dependent prefactor. Despite the simplicity of our model, these trends are in remarkable qualitative agreement with experiments. A degree of rate control analysis explains the kinetic fingerprints in terms of a change in the rate-determining step, inducing a shift in kinetic regime. We thus conclude that the enthalpy-entropy compensation effect is explained, at least to a first approximation, by the surface kinetics. Our work overall highlights the subtle interplay between temperature, applied potential, and catalyst reactivity.

O 98: Ultrafast electron dynamics at surface and interfaces IV

Time: Friday 9:30–12:15 Location: TRE/MATH

Invited Talk O 98.1 Fri 9:30 TRE/MATH

Electron-phonon interactions in the time domain: from non-equilibrium phonon dynamics to theoretical spectroscopy — •Fabio Caruso — University of Kiel, Germany

First-principles simulations of electron-phonon interactions (EPI) are key to clarifying the microscopic origin of the ultrafast electron and phonon dynamics revealed by pump-probe experiments in crystalline solids [1]. In this talk, I will discuss recent advances in ab-initio simulations of the EPI and their application to light-driven electron and lattice dynamics. Building on recent progress in many-body theory and software, predictive atomistic simulations of complex non-equilibrium phenomena have now become feasible. I will highlight, in particular, non-thermal phonon populations [2], coherent phonons [3], and ultrafast polaron formation as representative examples. This progress forms the basis for a strong synergy between ab-initio theory and experimental ultrafast science.
[1] F. Caruso et al., J. Phys. Mater. **9**, 012501 (2025).
[2] Y. Pan et al., ACS Nano **19**, 11381 (2025).
[3] C. Emeis et al., Phys. Rev. X **15**, 021039 (2025).

O 98.2 Fri 10:00 TRE/MATH

Coherent phonon control beyond amplitude saturation in a sliding ferroelectric — •Jan Gerrit Horstmann[1,2], Christoph Emeis[3], Andrin Caviezel[1], Quintin Meier[4], Nicolas Wyler[1], Thomas Lottermoser[1], Fabio Caruso[3], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zurich, Vladimir-Prelog-Weg 4, Zurich, 8093, Switzerland — [2]University of Würzburg, Institute of Physical and Theoretical Chemistry, Am Hubland, 97074 Würzburg, Germany — [3]Institute of Theoretical Physics and Astrophysics, Kiel University, Leibnizstraße 15, Kiel, 24118, Germany — [4]Institut Néel, C.N.R.S-Université Grenoble Alpes, BP 166, Grenoble, 38042, France

Intense optical excitation can drive quantum materials into regimes where the usual linear relation between photo-excited carriers and lattice-driving forces no longer applies. Using time-resolved second-harmonic generation, we observe that the interlayer sliding phonon governing sliding ferroelectricity in WTe_2 saturates and even decreases at high single-pulse fluence. Density functional theory traces this nonlinearity to band-specific electron-phonon coupling that produces competing lattice forces. By dividing the same total fluence into two well-timed pulses, we avoid populating counteracting electronic states and achieve significantly larger coherent phonon amplitudes. The resulting enhanced sliding motion reveals anharmonic phonon coupling far from equilibrium and shows that nonlinear limits in driven solids can be overcome through temporal shaping of the optical excitation.

O 98.3 Fri 10:15 TRE/MATH

Ultrafast x-ray sonography: A novel technique to spatially resolve phase heterogeneity on picosecond timescales — •Maximilian Mattern[1], Angel Rodriguez-Fernandez[2], Roman Shayduk[2], Wonhyuk Jo[2], Vojtech Uhlir[3], Jon Ander Arregi[3], Anders Madsen[2], Daniel Schick[1], and Jan-Etienne Pudell[2] — [1]Max-Born-Institut, Germany — [2]European XFEL, Germany — [3]CEITEC BUT, Czech Republic

Laser-induced heterogeneities play an important role for ultrafast dynamics especially of first-order phase transitions due to the phase co-existence during nucleation. However, their probing on picosecond time and nanometer length scales is challenging.

To address this challenge, we introduce ultrafast X-ray sonography. It combines well-established ultrafast hard-X-ray diffraction with a propagating strain pulse as a universal and non-invasive structural marker. The signatures of the strain pulse in the phase-specific lattice dynamics localizes the different phases in both space and time. This non-invasive pump-probe technique can follow the coherent growth and stochastic nucleation of structural domains on picosecond timescales with almost no requirements for sample preparation and is broadly applicable to a broad class of materials, provided that the coexisting phases exhibit distinguishable diffraction signatures. As a benchmark, we apply this approach to the antiferromagnetic-to-ferromagnetic magneto-structural phase transition in FeRh and identify the ferromagnetic phase to nucleate at the surface as columnar domains of approximately 30nm diameter.

O 98.4 Fri 10:30 TRE/MATH

Ultrafast energy flow among electrons and phonons in a Pb/Si nanoscale heterosystem — •Christian Brand[1], Mohammad Tajik[1], Tobias Witte[1], Laurenz Rettig[2], Birk Finke[1], Björn Sothmann[1], Uwe Bovensiepen[1], and Michael Horn-von Hoegen[1] — [1]Department of Physics, University of Duisburg-Essen, Germany — [2]Department of Physical Chemistry, Fritz Haber Institute, Germany

Microscopic excitations in condensed matter interact on ultrafast time scales. In this study, we employed time-resolved photoelectron spectroscopy and ultrafast electron diffraction to probe the spatially confined dynamics of electrons and phonons in ultrathin epitaxial Pb films on Si(111) subsequent to fs-laser excitation. Spatial confinement is crucial here, as without it, the energy flow into the unexcited bulk would obscure the transient dynamics and prevent targeted investigation. Electrons dissipate their excess energy within 400 fs, while lattice vibrations gradually build up over 3-8 ps. During this time gap, energy is transiently stored in high-frequency phonon modes, as captured by a three-temperature model. The transient electron temperature provides direct experimental access to the occupation of these phonons after equilibration at ≈ 3 ps. Subsequent excitation of low-frequency phonons and full lattice thermalization at ≈ 20 ps are governed by anharmonic phonon-phonon coupling within the Pb film.

O 98.5 Fri 10:45 TRE/MATH

Ultrafast manipulation of topological transport properties in Td-MoTe2 via coherent phonon excitation — •Huimin Wang[1], Matthew Day[2,3], Juan Aranzadi[1], James McIver[2,3], and Michael Sentef[1] — [1]Institute for Theoretical Physics and Bremen Center for Computational Materials Science, University of Bremen, Bremen, Germany — [2]Department of Physics, Columbia University, New York, NY, USA. — [3]Max Planck Institute for the Structure and Dynamics of Matter, CFEL, Hamburg, Germany

Ultrafast control of topological properties in quantum materials has emerged as a promising route toward dissipative-free and fast optoelectronic functionalities. In type-II Weyl semimetals such as Td-MoTe*, selective photoexcitation of coherent phonons offers an efficient non-thermal pathway to drive topological phase transitions by modifying lattice symmetry. Yet the microscopic origin of the laser-induced interlayer shear mode*central to this process*remains unclear, with both electron*phonon coupling (EPC) and strong phonon anharmonicity expected to contribute. Here, using real-time TDDFT combined with non-adiabatic molecular dynamics, we map out the excitation pathways of this

shear mode under varying photon energies, polarizations, and field strengths. We reveal cooperative EPC and phonon*phonon mechanisms that enable control of the phonon phase and amplitude. The resulting lattice dynamics induce shifts of Weyl node positions and associated nonlinear photocurrents, providing insight into observed ultrafast Hall responses.[1]Nature 565, 61*66 (2019). [2]Nat. Commun., vol. 12, p. 1885, 2021.[3]Phys. Rev. X, vol. 9, no. 2, p. 021036, 2019.

O 98.6 Fri 11:00 TRE/MATH

Competition of electron-electron and electron-phonon scattering in thermalization of laser-excited electrons — •Christopher Seibel, Tobias Held, Markus Uehlein, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, 67663 Kaiserslautern, Germany

When an ultrashort laser pulse irradiates a metal, electrons are excited to a state of strong nonequilibrium. According to the common picture, they thermalize subsequently towards a hot Fermi distribution on a femtosecond timescale and transfer energy to the still cold lattice on a picosecond timescale. Often these two processes are considered to be independet and driven by different interactions. Electron-electron scattering is considered responsible for the thermalization, whereas electron-phonon scattering is considered responsible for the energy transfer to the lattice. However, there are indications that these two processes influence each other and can act on similar timescales.

We use a kinetic description based on full Boltzmann collision integrals to trace the dynamics of the electron distribution during the thermalization after ultrashort laser excitation. We show that electron-electron and electron-phonon scattering have different effects on the distribution, which both lead to thermalization. Comparing various excitation fluences, we find that the thermalization times of the two processes exhibit an opposite fluence dependence and can become comparable for weak excitations.

O 98.7 Fri 11:15 TRE/MATH

Interfacial charge dynamics in hybrid plasmonic-excitonic nanostructures — •Tommaso Pincelli[1], Alessandro De Vita[1], Gian Marco Pierantozzi[2], Manuel Izquierdo[3], Pavel Trofimov[4], Trideep Kadwe[4], Hélène Seiler[4], Niclas S. Müller[4], Caterina Cocchi[5], Laurenz Rettig[6], Martin Wolf[6], Ralph Ernstorfer[1], and Giancarlo Panaccione[2] — [1]Technische Univ. Berlin — [2]IOM - CNR — [3]EuXFEL — [4]Freie Univ. Berlin — [5]Fredrich Schiller Univ. Jena — [6]Fritz Haber Inst. - MPG

Hybrid interfaces that merge plasmonic surfaces with 2D semiconductors are pivotal in energy materials research, allowing to tailor local fields and functionalize charge-transfer excitations. In this work, we exfoliate few-layer WSe_2 on a plasmonic lattice of nanostructured Au in UHV. Angle-resolved reflectivity reveals a rich photonic band structure matching finite-element calculations. Using time and angle resolved photoemission spectroscopy (trARPES), we observe an ultrafast quench of excitonic signatures and hints of rapid interfacial charge transfer. Angle-integrated trPES at higher photon energies allows access to the buried interface by tracking shallow core levels. Notably, the plasmonic lattice induces a pronounced slowing of Au 4f peak shifting dynamics compared with unpatterned Au, suggesting a bottleneck in the interfacial charge transfer. These results highlight the potential of hybrid interfaces as flexible platforms for engineering optoelectronic responses at ultrafast timescales. We acknowledge the Energy Materials community proposal collaboration, the teams of SXP@EuXFEL and HEXTOF@FLASH.

O 98.8 Fri 11:30 TRE/MATH

Non-equilibrium electron dynamics in antenna-reactor plasmonic photocatalysts — •Henry T. Snowden[1] and Reinhard J. Maurer[1,2] — [1]University of Warwick, UK — [2]University of Vienna, AT

Antenna-reactor nanoparticles are a promising form of plasmonic photocatalyst, combining strong light absorption and high catalytic activity. A key materials design question is the correct nanoparticle geometry with proposals ranging from core-shell structures to nanoalloys. Optimal photocatalysts combine strong light absorption, effective carrier transport, and long carrier lifetime. Here, we study the non-equilibrium electron dynamics after pulsed laser excitation using the Athermal Electron Model (AthEM), which explicitly considers thermal and non-thermal electrons in contact with a phonon bath, and a laser source term. Electron-electron scattering effects are considered at the level of the relaxation time approximation. We investigate how athermal electron-hole pair distributions evolve in different classes of promising materials according to the interplay of electron-electron and electron-phonon scattering. Based on our findings, we propose optimal materials compositions and photocatalyst geometries.

O 98.9 Fri 11:45 TRE/MATH

Influence of sulphur vacancies on ultrafast charge separation in WS2-graphene heterostructures — •Johannes Gradl[1], Niklas Hofmann[1], Leonard Weigl[1], Camilla Coletti[2], Raül Perea-Causín[3], Ermin Malic[4], and Isabella Gierz[1] — [1]University of Regensburg, Regensburg, Germany — [2]Istituto Italiano di Tecnologia, Pisa, Italy — [3]AlbaNova University Center, Stockholm, Sweden — [4]University of Marburg, Marburg, Germany

Ultrafast charge separation following photoexcitation, commonly observed in van der Waals heterostructures, is a key process for future optoelectronic devices that rely on the conversion of light into electricity. While electron and hole transfer rates are largely determined by band alignment and interlayer hybridization, recent experiments have revealed that defects critically affect the lifetime of the charge-separated state [1][2]. A microscopic understanding of defect-assisted charge transfer, however, remains elusive. We disentangle the role of sulphur vacancies on ultrafast charge separation and recombination in WS2-graphene heterostructures by (i) systematically increasing the defect density and (ii) switching the defect-assisted charge transfer channel on and off. Using time-resolved ARPES, we probe the resulting charge-transfer dynamics on ultrafast time scales directly in the band structure.

[1] Phys. Rev. Lett. 127, 276401, (2021)
[2] Sci. Adv. 7, eabd9061, (2021)

O 98.10 Fri 12:00 TRE/MATH

Formation and thermalization of non-equilibrium excitonic occupations — •Paul Werner[1], Wiebke Bennecke[1], Jan Philipp Bange[1], Giuseppe Meneghini[2], David Schmitt[1], Marco Merboldt[1], Anna Seiler[1], AbdulAziz AlMutairi[3], G. S. Matthijs Jansen[1], Junde Liu[1], Daniel Steil[1], Stephan Hofmann[3], R. Thomas Weitz[1], Ermin Malic[2], Stefan Mathias[1], and Marcel Reutzel[3] — [1]I. Physikalisches Institut, Georg-August Universität Göttingen, Germany — [2]Fachbereich Physik, Philipps-Universität Marburg, Germany — [3]Department of Engineering, University of Cambridge, United Kingdom

Upon optical excitation, bright excitons can scatter into lower energy, potentially dark, exciton states. In these formation and relaxation processes, non-equillibrium exciton populations play a major role, but remain largely elusive because they are inaccessible by most spectroscopic methods. In this work we provide direct access to the formation and thermalization of non-equilibrium exciton states in 2H-homobilayer MoS_2. Using time-resolved momentum microscopy and microscopic many-particle calculations, we reveal the fingerprint of non-equillibrium exciton distributions and quantify their formation and relaxation timescale [1].

[1] Werner *et al.*, arXiv:2505.06074 (2025).

O 99: Spins on surfaces at the atomic scale III

Time: Friday 9:30–12:30 Location: WILL/A317

O 99.1 Fri 9:30 WILL/A317

Measuring magnetic exchange forces of individual quantum spins — •Nicolaj Betz[1,2], Lukas M. Veldman[1,2], Milton Aguliar[3], Eric Lutz[3], Susanne Baumann[1], and Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies, Stuttgart, Germany. — [2]Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart, Stuttgart, Germany. — [3]University of Stuttgart, Institute for Theoretical Physics, Stuttgart, Germany

Dynamics of single atomic spins are governed by interactions with the spins immediate, i.e. atomic scale environment. In that, spin-polarized scanning tunnelling microscopy (STM) can give access to some of these interactions, e.g. those between coupled spins, and it can also be used to detect the dynamics in form of individual spin switches. Atomic force microscopy (AFM) on the other hand, gives access to atomic-scale forces, for example the magnetic exchange interaction [1,2]. Here, we show magnetic exchange force detection on a dynamically switching single Fe atom on MgO/Ag(100). We can tune this spin to undergo a ground state reversal as a function of exchange interaction with the tip. We find that the switching spin interacts strongly with the AFM cantilever. Thus, access to these forces provides a new avenue to study dynamically switching single atomic quantum spins revealing information about the interplay between an atom's interactions and the dynamics of the spin.

[1] N. Hauptmann et al., Nat. Com. 11, 1197 (2020).
[2] U. Kaiser et al. Nature 446, 522-52 (2007).

O 99.2 Fri 9:45 WILL/A317

Tip induced f-π interaction of $YbPc_2$ Molecules utilizing STM — •Jonas Arnold[1], Kwan Ho Au-Yeung[1], Wantong Huang[1], Eufemio Moreno Pineda[1], Christoph Sürgers[1], Wolfgang Wernsdorfer[1], Mario Ruben[2], and Philip Willke[1] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany

Individual molecules constitute excellent building blocks for quantum technologies thanks to their small size, reproducibility and the benefit of self assembly. A promising class are rare-earth bis-phthalocyanine complexes (1). In this work, we investigate $YbPc_2$ molecules using a mK- scanning tunneling microscope (STM) to identify potential indicators of a magnetic signature. In the gas phase, the $YbPc_2$ molecule is expected to exhibit a radical spin localized at its ligands, an f-shell electron spin S = 1/2 as well as a nuclear spin (I = 1/2 and 5/2) for certain isotopes. Thus, this system is a potential candidate for a spin cascade (1). We perform measurements on self-assembled multi-layer islands of $YbPc_2$ on Ag(001) and MgO/Ag(001). We find that the proximity of the STM tip changes the spin state of the molecule by tuning states close to the Fermi level (2). We identify the emerging spectral features close to zero bias as inelastic electron tunneling excitations that result from the combined f-π system. This mechanism can be found for the first, second and third molecular layer on Ag(001) as well as MgO/Ag(001).

(1) Wernsdorfer, W. et al., Adv. Mat., 2019, 31(26), 1806687.
(2) Liao, X. et al., Nat. Com., 2025, 16(1), p.6263.

O 99.3 Fri 10:00 WILL/A317

Quantifying the interplay between atomic-scale magnetism and Josephson transport atom-by-atom — •Zhengyuan Liu, Sebastian Scherb, Manuel Steinbrecher, Nadine Hauptmann, and Alexander Khajetoorians — IMM, Radboud University Nijmegen, the Netherlands

Josephson transport can locally be affected by the presence of magnetic moments in the junction. For example, it was shown that the individual magnetic impurity, and the Yu-Shiba-Rusinov (YSR) excitations they induce in the superconductor can be used to induce a superconducting diode effect [1]. Furthermore, an intrinsic phase shift of π in its ground state can exhibit when a ferromagnetic layer with certain thickness is introduced in the Josephson junction, known as the π-junction [2]. Here, we study the effect of individual and coupled magnetic atoms on the Josephson transport between a superconducting tip and superconducting surface, using scanning tunneling microscopy. We study the evolution of the YSR states going from an individual impurity to a magnetic nanostructure. We correlate this evolution to changes in the Josephson junction properties locally, by using spatially-dependent I-V spectroscopy. We also review the local diode effect induces in these structures. [1] Trahms, M et al. Nature 615, 628*633 (2023). [2]Ryazanov et al. Phys. Rev. Lett. 86, 2427 (2001)

O 99.4 Fri 10:15 WILL/A317

Exchange-field model for electron spin resonance scanning tunneling microscopy — •Christoph Wolf[1,2], Jose Reina-Galvez[3], Xue Zhang[4], Jan Martinek[5], and Nicolas Lorente[6] — [1]Center for Quantum Nanoscience, Institute for Basic Science (IBS), Seoul 03760, Republic of Korea — [2]Ewha Womans University, Seoul 03760, Republic of Korea — [3]Department of Physics, University of Konstanz, D-78457 Konstanz, Germany — [4]Institute of Molecular Physics, Polish Academy of Science, Smoluchowskiego 17, 60-179 Poznan, Poland — [5]Spin-X Institute, China University of Technology, Guangzhou, China — [6]Centro de Fisica de Materiales, CFM/MPC (CSIC-UPV/EHU), Spain

Since the first experimental demonstration of electron spin resonance in a scanning tunneling microscope the understanding of how spin transitions are driven by oscillating electric fields has gone through several evolutions. In this talk, I will show how an exchange-field model can explain the magnetoelectric coupling between the electric field and a spin impurity. This model is based on an Anderson impurity model and non-equilibrium transport using magnetic electrodes. When the hopping between a magnetic electrode and the impurity is modulated on resonance with the Zeeman splitting one obtains an effective magnetic field that can coherently drive the spin. The sign and magnitude of the exchange field depends on the applied DC bias which gives full control over the position of the resonance and potentially can be used for DC-based quantum-logic operations.

O 99.5 Fri 10:30 WILL/A317

Revealing spatial inhomogeneities in superconducting 2H-NbS_2 using magnetic sensor atoms — •Werner M.J. van Weerdenburg, Margarete Huisinga, Constantin Flommersfeld, Lisa M. Rütten, and Katharina J. Franke — FachbereichPhysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Transition metal dichalcogenides (TMDCs) are an interesting material class in which multiple quantum phases such as charge-density-wave (CDW) order, superconductivity and pair-density-wave order may coexist [1]. Within the family of superconducting TMDCs, 2H-NbS_2 stands out as the only material that does not develop a CDW phase, but this interpretation is challenged in the presence of defects, since the material is very close to a lattice instability [2,3].

Here, we present how magnetic adatoms on a superconducting TMDC substrate can be used to investigate spatial inhomogeneities of 2H-NbS_2. By manipulating an individual Fe atom between binding sites with the tip of a scanning tunneling microscope, we probe the Yu-Shiba-Rusinov (YSR) states and their response to surface variations with high energy resolution. The sensitivity of YSR states to the crystal field, density of states and disorder allows us to analyze the relation between the YSR energies and the properties of the substrate, and to find indications of local charge-density-wave nucleation around intrinsic defects.

[1] Liu et al., Science **372**, 1447-1452 (2021); [2] Heil et al., PRL **119**, 087003 (2017); [3] Wen et al., PRB **101**, 241404 (2020)

O 99.6 Fri 10:45 WILL/A317

Magnetic quantum corrals on a proximity-superconducting Rashba surface alloy — •Jinkyung Kim, Harim Jang, Jens Wiebe, and Roland Wiesendanger — Department of Physics, University of Hamburg, Hamburg, D-20355, Germany

Quantum corrals can confine and resonate surface-state electrons at discrete eigenenergies. When coupled to superconducting substrates, quantum corrals can be used to sculpture Yu-Shiba-Rusinov (YSR) in-gap states as well as spin-degenerate Andreev bound states, referred to as Machida-Shibata (MS) states, due to proximity-induced Cooper pairing [1,2]. Here, we investigated quantum corrals crafted from Fe atoms on a proximity-superconducting BiAg2/Ag/Nb(110) heterostructure. Multiple in-gap states emerge with similar numbers of antinodes as in the eigenmode closest to the Fermi energy. They show an almost perfect spatial antiphasing between the particle- and hole-like components, reminiscent of long-range YSR states of individual magnetic atoms [3]. By further studying how these in-gap states evolve with corral size and the 3d metal atom species, our work characterizes the interplay between YSR and MS states within the quantum corral. [1] L. Schneider et al., Nature 621, 60-65 (2023) [2] K. Ton That et al., Nat. Phys. (2025) https://doi.org/10.1038/s41567-025-03109-y [3] H. Jang et al., arXiv:2506.17414 (2025)

O 99.7 Fri 11:00 WILL/A317

Spin and Charge States of Open-Shell Nanographenes over Functional Substrates — •Francisco Romero-Lara, Trisha Sai, Katerina Vaxevani, Dongfei Wang, Jon Ortuzar, Leonard Edens, Stefano Trivini, Fabian Schulz, and Jose Ignacio Pascual — CIC nanoGUNE, 20018 San Sebastián, Spain

Atomically precise open-shell nanographenes are platforms hosting spin states, which can be manipulated by local probes and by tuning their local environment. Here, we present the fabrication of aza-triangulenes-based nanostructures over two novel substrates with potential control over their charge and spin state: a rare-earth-gold alloy monolayer and a superconducting surface. The aza-triangulene platforms can host several weakly interacting spin states and a doublet ground state sensitive to Jahn-Teller distortion. We use scanning tunnelling microscopy to resolve their Kondo and spin excitation spectrum. We also resolve the presence of Yu-Shiba-Rusinov (YSR) states inside the proximity gap on the superconducting surface. Owing to an inhomogeneous local contact potential difference, the nanographenes on rare-earth-gold alloy surfaces appear with varying charge states depending on their adsorption site, which is also translated into variations of the spin ground state. Over a superconducting substrate, sub-gap spectral maps reveal with high precision their YSR excitations. They are interpreted based on a model theory as reflecting, in some cases, Jahn-Teller distortions. Overall, our results highlight the potential of unconventional substrates for on-surface nanographene synthesis and for tailoring and probing their intrinsic spin states.

O 99.8 Fri 11:15 WILL/A317

Extracting mechanical work from quantum spin switching of a single atom — Nicolaj Betz[1,2], Lukas M. Veldman[1,2], Milton Aguilar[3], Eric Lutz[3], Susanne Baumann[1], and •Sebastian Loth[1,2] — [1]University of Stuttgart, Institute for Functional Matter and Quantum Technologies — [2]Center for Integrated Quantum Science and Technology (IQST), University of Stuttgart — [3]University of Stuttgart, Institute for Theoretical Physics

Stochastic dynamics are ubiquitous in atomic-scale systems, often arising from dissipative processes through which energy is lost to the environment. Harnessing such dynamics to perform work is at the heart of molecular motors and quantum heat engines. Here, we demonstrate that a single magnetic atom can function as an electric motor that converts spin excitations into mechanical oscillations of a macroscopic cantilever. We couple an Fe atom on MgO/Ag(100) via magnetic exchange interaction to the tip of a combined atomic force (AFM) and scanning tunneling microscope (STM) at milli-Kelvin temperatures. Current-induced inelastic electron tunneling induces cyclic spin switching, creating an alternating exchange force that transfers energy between the quantum spin and the AFM cantilever with a power output sufficient for free-running operation. This single-atom electric motor bridges the quantum-classical divide and provides a platform for studying energy transfer in hybrid quantum-classical systems.

O 99.9 Fri 11:30 WILL/A317

Tuning the magnetic excitation of a single atom by local gating — •Anna M. H. Krieg, Hermann Osterhage, Julian H. Strik, Niels P. E. van Mullekom, Ben Verlhac, and Alexander A. Khajetoorians — Institute for Molecules and Materials, Radboud University, Nijmegen, the Netherlands

The description of single-atom magnetism depends on the interplay of various degrees of freedom and the balance of different interactions. This includes the interplay between the orbital, spin and charge degrees of freedom, as well as the balance between spin-orbit coupling, hybridization, and different exchange interactions, such as Hund's and Kondo exchange. To date, the strategy to change the magnetic behavior of a single atom is to explore different atom/surface combinations. However, in this way, nearly all these parameters are fixed by the material system and when changing the material system, the entire set of parameters changes. Here, we tune the local electrostatic potential in order to modify the magnetic excitations and tunneling transport of individual Fe atoms. We start with Fe atoms on the surface of InSb(110), and characterize its magnetic excitations as a function of magnetic field. We then harness a newly developed quantum simulator platform, based on patterning Cs atoms on the surface of InSb. We show that by varying the local density of Cs on InSb, we can tune the magnetic excitation of an individual Fe atom. These results serve as a starting point to develop quantum simulation to study magnetic models in which the spin, charge, and orbital degree of freedom can be tuned.

O 99.10 Fri 11:45 WILL/A317

Spin dynamics of atomic defects in monolayer MoS_2 — •Johanna Matusche[1,2], Kwan Ho Au-Yeung[1,2], Wantong Huang[1,2], Paul Greule[1,2], Jonas Arnold[1,2], Lovis Hardeweg[1,2], Máté Stark[1,2], Luise Renz[1,2], Affan Safeer[3], Daniel Jansen[3], Jeison Fischer[3], Thomas Michely[3], Wolfgang Wernsdorfer[1,2], Christoph Sürgers[1,2], Johannes Schwenk[1,2], Wouter Jolie[3], and Philip Willke[1,2] — [1]Physikalisches Institut (PHI), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]Center for Integrated Quantum Science and Technology (IQST), Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]II. Physikalisches Institut, Universität zu Köln, Köln, Germany

Scanning tunneling microscopy (STM) combined with electron spin resonance (ESR) has enabled coherent control of single ad-atoms and single molecules on surfaces [1]. Additionally, recent studies have revealed that defects in monolayer MoS_2 exhibit well-defined spin signatures [2]. In this talk, we combine these two advances for individual point-like defect spins in monolayer MoS_2 on graphene/Ir(111): First, we focus on stochastic resonance spectroscopy (SRS) [3] to periodically drive rapid transitions between spin states. This allows to identify the main relaxation mechanisms and to determine the T_1 relaxation times. Second, pulsed ESR enables coherent control of the defect spins via Rabi and Ramsey sequences, which provides direct access to their T_2 coherence times.

[1] K. Yang et al., Science, 366, 509-512 (2019).
[2] S. Trishin et al., Phys. Rev. B, 108, 165414 (2023)
[3] N. Betz et al., arXiv:2412.12647 (2025).

O 99.11 Fri 12:00 WILL/A317

Following Spin Interactions into a Chemical Bond Formation — •Dmitriy Borodin[1], Merve Ercelik[1], Andres Pinar Sole[1], Shadi Fatayer[2], Harald Brune[3], Christoph Wolf[1], Franz J. Giessibl[4], Fabio Donati[1], and Andreas Heinrich[1] — [1]IBS Center for Quantum Nanoscience, Seoul, South Korea — [2]KAUST, Thuwal, Saudi Arabia — [3]EPFL, Lausanne, Switzerland — [4]University of Regensburg, Regensburg, Germany

Exchange interactions are essential for the formation of chemical bonds between atoms and dictate the electronic structure of molecules. In a condensed-matter system, a manifold of exchange mechanisms coexist, ultimately defining the local magnetic structure and phase stability. A particularly interesting interaction occurs between transition metal atoms and rare earth elements, where the nature of magnetic coupling in their alloys remains not fully understood. In this work, we use low-temperature scanning probe microscopy to follow the spin interactions between a tip and an adatom on a surface into a chemical bond. By controlling atom-tip separations on the picometer scale, we continuously tune interaction energies and observe spin pairing between the adatom and the magnetic tip, a situation that is reminiscent of covalent bond formation.

O 99.12 Fri 12:15 WILL/A317

Dark state formation in a zero-field split molecular triplet — •Maria Steiner and Andrea Donarini — Institute of Theoretical Physics, Regensburg University, Regensburg, Germany

In analogy to atomic physics [1], we propose a protocol to prepare and probe a dark state in a single molecule. To this end, we coherently manipulate with a multifrequency magnetic field a three-level system in the V-configuration. Thus, within a density-matrix formalism for open systems, we extend existing protocols developed to probe Rabi oscillations in ESR-AFM on pentacene [2]. The dissipative dynamics of the reduced density matrix are interpreted in terms of multipole expansion and visualized using three intertwined Bloch spheres. We consider a molecule with a zero-field splitting of the first excited triplet. This splitting typically arises from the spatial anisotropy of the frontier orbitals and the spin dipole-dipole interaction between the unpaired electrons. Pentacene is an archetypal example, which, in addition to these properties, also exhibits anisotropic decay to the ground state singlet [3] and thus enables experimental readout of the occupied state [2]. We consider both ideal scenarios and realistic parameterization for ESR-AFM on pentacene to model the expected dark state signature.

[1] Arimondo and Orriols, Lett. al Nuovo Cim. **17**, 333 (1976).
[2] Sellies et al., Nature **624**, 64 (2023).
[3] Peng et al., Science **373**, 452 (2021).

O 100: Closing Talk Steinrück

Time: Friday 13:15–14:00 Location: TRE/PHYS

Topical Talk O 100.1 Fri 13:15 TRE/PHYS

Ionic Liquid Surface Science — •Hans-Peter Steinrück — Friedrich-Alexander-Universität Erlangen-Nürnberg

Traditional surface science is often limited to solids, due to the high vapor pressure of conventional liquids or solvents. Quite recently, low-vapor-pressure liquids such as ionic liquids (ILs) or liquid metal alloys have received significant attention as they offer new concepts in catalysis. This contribution focuses on ILs, which are liquid salts with melting points below 100 °C, often even below room temperature. Since their physical and chemical properties can be tailored over a wide range, they represent a fascinating class of liquid materials with interesting applications. Two important concepts in catalysis are the Supported Ionic Liquid Phase (SILP) and Solid Catalyst with Ionic Liquid Layer (SCILL) concepts. In both, a high surface area solid substrate is covered with a thin IL film. In SILP, the film contains a homogeneously dissolved transition metal complex; in SCILL, the film modifies catalytically active surface sites at the catalyst. The interfaces of the IL are thus of critical importance. Due to their extremely low vapor pressure, ILs can be investigated in great detail under well-defined ultrahigh vacuum conditions using surface science methods like angle-resolved XPS, STM, AFM and molecular beam techniques. In this presentation, both the IL/vacuum and the IL/support interfaces are addressed. In the first example, the buoy concept will be introduced, that is, the tailored enrichment of metal complexes at the liquid/vacuum interface. The second example addresses the modification of the properties of single crystal surfaces by an ultrathin IL film.

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Overview of Invited Talks and Sessions

(Lecture hall GÖR/0226; Poster P4)

Invited Talks

SOE 2.1	Mon	9:30–10:00	GÖR/0226	**Memory and equilibrium in collective animal behaviour** — •Thierry Mora
SOE 5.1	Tue	9:30–10:00	GÖR/0226	**Network Science in Criminology: Insights from Empirical Case Studies** — •Masarah Paquet-Clouston
SOE 8.1	Wed	9:30–10:00	GÖR/0226	**Dynamics and Structure in Temporal Networks** — •Natasa Djurdjevac Conrad
SOE 14.1	Thu	9:30–10:00	GÖR/0226	**Generative AI and diffusion models: a statistical physics approach** — •Giulio Biroli
SOE 16.1	Thu	11:30–12:00	GÖR/0226	**Tipping in Strongly Perturbed Open Networks** — •Marc Timme, Georg Börner, Marisa Fischer, Julian Fleck, Seungjae Lee, Philip Marszal, Gwendolyn Quasebarth, Malte Schröder, Moritz Thümler
SOE 17.1	Fri	9:30–10:00	GÖR/0226	**What can we learn from neural quantum states?** — Brandon Barton, Juan Carrasquilla, Anna Dawid, Antoine Georges, Megan Schuyler Moss, Alev Orfi, Christopher Roth, Dries Sels, Anirvan Sengupta, •Agnes Valenti
SOE 17.6	Fri	11:15–11:45	GÖR/0226	**Creativity in generative AI** — •matthieu wyart

Young Scientist Award Session

SOE 7.1	Tue	14:00–14:30	GÖR/0226	**What's that noise? Why does it make a difference? And why am I thinking about it all the time?** — •Dirk Brockmann
SOE 7.2	Tue	14:45–15:30	GÖR/0226	**How things spread: Complexity and criticality of inhomogeneous spreading models** — •Laurent Hébert-Dufresne

Invited Talks of the joint SKM Dissertationspreis 2025 Symposium (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	HSZ/0002	**Stochastic-Calculus Approach to Non-equilibrium Statistical Physics** — •Cai Dieball
SYSD 1.2	Mon	10:00–10:30	HSZ/0002	**Nonuniform magnetic spin textures for sensing, storage and computing applications** — •Sabri Koraltan
SYSD 1.3	Mon	10:30–11:00	HSZ/0002	**Anomalous Quantum Oscillations beyond Onsager's Fermi Surface Paradigm** — •Valentin Leeb
SYSD 1.4	Mon	11:00–11:30	HSZ/0002	**Coherent Control Schemes for Semiconductor Quantum Systems** — •Eva Schöll
SYSD 1.5	Mon	11:30–12:00	HSZ/0002	**On stochastic thermodynamics under incomplete information: Thermodynamic inference from Markovian events** — •Jann van der Meer

Invited Talks of the joint Symposium "The Sustainability Challenge: A Decade of Transformation" (SYSC)

See SYSC for the full program of the symposium.

SYSC 1.1	Mon	15:00–15:30	HSZ/AUDI	**Open-Endedness and Community-Based Approaches to Sustainability Challenges** — •Hiroki Sayama
SYSC 1.2	Mon	15:30–16:00	HSZ/AUDI	**Education as a Social Tipping Element: Evidence from Climate and Physics Education Research** — •Thomas Schubatzky
SYSC 1.3	Mon	16:00–16:30	HSZ/AUDI	**Mechanistic and Material Perspectives on Enzymatic Hydrolysis of Semicrystalline Polyesters** — •Birte Höcker
SYSC 1.4	Mon	16:45–17:15	HSZ/AUDI	**Decarbonization Options for Industry** — •Uwe Riedel
SYSC 1.5	Mon	17:15–17:45	HSZ/AUDI	**Impacts of Cosmic Dust and Space Debris in the Terrestrial Atmosphere** — •John Plane

Invited Talks of the Symposium "Tipping Points in Social and Climate Systems" (SYTP)

See SYTP for the full program of the symposium.

SYTP 1.1	Thu	15:00–15:30	HSZ/AUDI	**Social Tipping in Heterogeneous and Polarized Populations** — •Sara Constantino, Sonke Ehret, Elke Weber, Sonja Vogt, Charles Efferson
SYTP 1.2	Thu	15:30–16:00	HSZ/AUDI	**Tipping points and regime shifts in coupled social-climate systems** — •Chris Bauch
SYTP 1.3	Thu	16:00–16:30	HSZ/AUDI	**How to tune Earth system models toward tipping?** — •Sebastian Bathiany, Niklas Boers
SYTP 1.4	Thu	16:45–17:15	HSZ/AUDI	**Algorithmic amplification and contextual sensitivity in political information exposure** — Iris Damião, Ana Vranic, Paulo Almeida, Lília Perfeito, •Joana Gonçalves de Sá
SYTP 1.5	Thu	17:15–17:45	HSZ/AUDI	**The complex interplay between democracy and platform power** — •Philipp Lorenz-Spreen

Sessions

SOE 1.1–1.2	Sun	16:00–18:15	HSZ/0004	**Tutorium: Physics of Behavior (joint session SOE/TUT/DY)**
SOE 2.1–2.10	Mon	9:30–12:45	GÖR/0226	**Focus Session: Physics of Behavior (joint session SOE/DY)**
SOE 3.1–3.4	Mon	9:30–10:30	MER/0002	**Sustainability: Challenges and Solutions (joint session UP/CPP/SOE)**
SOE 4.1–4.9	Mon	18:00–21:00	P4	**Poster Session**
SOE 5.1–5.3	Tue	9:30–10:30	GÖR/0226	**Network Science**
SOE 6.1–6.7	Tue	10:45–12:45	GÖR/0226	**Mobility, Traffic Dynamics, Urban and Regional Systems**
SOE 7.1–7.2	Tue	14:00–15:30	GÖR/0226	**Award Session: Young Scientist Award for Socio- and Econophysics (YSA)**
SOE 8.1–8.4	Wed	9:30–11:00	GÖR/0226	**Networks, From Topology to Dynamics I (joint session SOE/DY)**
SOE 9.1–9.5	Wed	11:30–12:45	GÖR/0226	**Economic Models**
SOE 10.1–10.3	Wed	15:00–15:45	GÖR/0226	**Networks, From Topology to Dynamics II (joint session SOE/DY)**
SOE 11.1–11.5	Wed	15:45–17:15	GÖR/0226	**Polarization**
SOE 12.1–12.3	Wed	17:15–18:00	GÖR/0226	**Statistical Physics of Politics**
SOE 13	Wed	18:00–19:30	GÖR/0226	**Members' Assembly**
SOE 14.1–14.6	Thu	9:30–11:15	GÖR/0226	**Focus Session: Physics of AI I (joint session SOE/DY)**
SOE 15.1–15.6	Thu	11:15–12:45	ZEU/0118	**Networks: From Topology to Dynamics III (joint session DY/SOE)**
SOE 16.1–16.4	Thu	11:30–12:45	GÖR/0226	**Tipping Points in Social and Climate Systems (accompanying session for SYTP)**
SOE 17.1–17.10	Fri	9:30–12:45	GÖR/0226	**Focus Session: Physics of AI II (joint session SOE/DY)**

Members' Assembly of the Physics of Socio-economic Systems Division

Wednesday 18:00–19:30 GÖR/0226

- SOE poster award
- Report
- Election
- All other business

Sessions

– Invited Talks, Prize Talks, Topical Talks, Tutorials, Contributed Talks, and Posters –

SOE 1: Tutorium: Physics of Behavior (joint session SOE/TUT/DY)

The emerging field of the physics of behavior seeks to quantitatively characterize complex behavior in biological agents under naturalistic conditions, using tools from dynamical systems theory and statistical physics. Even in simple organisms, behavioral richness demands new methods of measurement and analysis, as well as new theoretical frameworks. In the absence of a first-principles theory, data-driven approaches are essential, and the many interacting degrees of freedom call for descriptions capable of handling high-dimensional systems.

This tutorial introduces how concepts from dynamical systems theory and statistical physics can be applied to quantify behavior across biological scales and to develop simple yet predictive models. It is intended for physicists at all levels, beginning with graduate students, who are interested in computational approaches to modeling animal behavior. The tutorial is accompanied by an openly accessible code repository to support hands-on exploration of selected topics.

Time: Sunday 16:00–18:15 Location: HSZ/0004

Tutorial SOE 1.1 Sun 16:00 HSZ/0004

Physics of Behavior — •Greg Stephens — Vrije Universiteit Amsterdam, Amsterdam NL — OIST Graduate University, Tancha, JP

In these tutorials we view behavior as a complex dynamical system and we incorporate insights from dynamical systems theory and statistical physics to quantitatively capture what animals do. Of course, such theory was not historically developed to understand animal behavior, and there are particular challenges associated with the modeling of living systems. Of these, the most important is a lack of first-principles theory necessitating a data-driven approach.

In the first half of our session we will introduce two primary concepts. (1) Posture Space Analysis via Dimensionality Reduction. We explore posture space analysis by demonstrating how to decompose high-dimensional postural data into a few meaningful eigenpostures using Principal Component Analysis (PCA). The dataset used comes from C. elegans posture tracking. (2) Posture Space Dynamics via State Space Reconstruction. We review the concepts of state space and chaotic systems through a toy model. We then introduce a modern data-driven technique for state space reconstruction.

15 min. break

Tutorial SOE 1.2 Sun 17:15 HSZ/0004

Physics of Behavior — •Antonio Carlos Costa — Paris Brain Institute, Paris, France

Animal behavior is inherently nonlinear and multiscale, spanning millisecond movements to hour-long strategies. In the second half of our session, we will complement first-principles approaches with data-driven methods to identify multiscale dynamics in behavioral data.

We will present three key techniques: (1) state space reconstruction combined with transfer operators to extract long-timescale modes from partial observations, (2) coarse-grained modeling to infer slowly-varying behavioral dynamics and explain heavy-tailed statistics, and (3) a multiscale distance metric for reconstructing behavioral phenotypes from dynamic observations.

We will review the theoretical foundations of slow mode identification using transfer operators (illustrated with stochastic and chaotic toy models), and then demonstrate their applicability to real-world data, including posture dynamics in C. elegans and zebrafish.

SOE 2: Focus Session: Physics of Behavior (joint session SOE/DY)

Organizers: Greg Stephens (Vrije Univ. Amsterdam), Pawel Romanczuk (HU Berlin)

Physics has made important contributions to the remarkable progress in characterizing the molecules, cells, and circuits that generate natural behavior. Yet our understanding of behavior at the scale of the whole organism and in ecological and social contexts remains significantly less advanced. Even in simpler organisms, natural behavior is complex, requiring new tools for measurement (often through novel imaging), analysis, and theoretical insight. The emerging field of the physics of behavior addresses this gap by seeking to quantitatively characterize complex behavior in naturalistic settings. This focus session will highlight recent advances at the intersection of physics, neuroscience, biology, and social sciences with contributions from both theorists and experimentalists.

Time: Monday 9:30–12:45 Location: GÖR/0226

Invited Talk SOE 2.1 Mon 9:30 GÖR/0226

Memory and equilibrium in collective animal behaviour — •Thierry Mora — Ecole normale supérieure and CNRS, Paris, France

Some animal groups behave in a highly coordinated way, reminiscent of ordered phases in physics. However, animals are also heterogeneous, have memory, and operate out of equilibrium. I will present recent attempts at modeling the complex dynamics of social groups of mice interacting freely in a controlled environment. I will then assess how far from equilibrium collective behaviour might be, both in recordings of real bird flocks and in flocking models.

SOE 2.2 Mon 10:00 GÖR/0226

Spin-Waves without Spin-Waves: A Case for Soliton Propagation in Starling Flocks — •Andrea Cavagna — Institute for Complex Systems, Rome, Italy

Collective turns in starling flocks propagate linearly with negligible attenuation, indicating the existence of an underdamped sector in the dispersion relation. Beside granting linear propagation of the phase perturbations, the real part of the frequency should also yield a spin-wave form of the unperturbed correlation function. However, new high-resolution experiments on real flocks show that underdamped traveling waves coexist with an overdamped Lorentzian correlation. Theory and experiments are reconciled once we add to the dynamics a Fermi-Pasta-Ulam-Tsingou term.

SOE 2.3 Mon 10:15 GÖR/0226

Modelling filamentous fungal growth — •Pascal Klamser[1], Carlos Aguilar-Trigueros[2] und Dirk Brockmann[1] — [1]Technische Universität Dresden, Dresden, Germany — [2]University of Jyväskylä, Jyväskylä, Finland

The growth of a filament forming fungi is mesmerizing and a great example of an organism that forms a transport network and explores its environment for nutrients. While recent research shows how nutrients and other compounds are transported through the network, we will focus on a transport-agnostic model to explore the possible ways of how the tip of a filament can choose its growth direction. We assume a purely external communication via the diffusion of enzymes released by the filaments and can recreate a wide range of phenotypes. We compare it with experiments by estimating the hierarchical structure of the network from microscopic images.

15 min. break

SOE 2.4 Mon 10:45 GÖR/0226

Understanding how movement behaviors shape animal encounters and their ecological consequences — •Anudeep Surendran — Helmholtz-Zentrum Dresden-Rossendorf, Görlitz, Germany

Encounters between individuals underlie key ecological processes such as predation, mating, and disease transmission, making encounter rates a direct link between individual movement behavior and population-level outcomes. We investigate how two common features of animal movement-directional persistence and range residency-jointly shape encounter rates. Using the Ornstein Uhlenbeck with foraging (OUF) model, which integrates these two properties of animal movement, we derive exact analytical expressions for encounter rates and show that, for range-resident animals, the effect of persistence depends strongly on the degree of home-range overlap. Based on this theoretical result, we then introduce a new encounter-based metric that quantifies the spatial organization of home ranges at scales relevant to animal encounters. We finally apply this metric to movement data from lowland tapirs (Tapirus terrestris) in Brazils Pantanal region, and find a significant level of home-range spatial segregation that is consistent with the solitary behavior of this species.

SOE 2.5 Mon 11:00 GÖR/0226

Composite and combined games in evolutionary dynamics in finite populations — Henry Brooks, Suzannah Gebbett, and •Jens Christian Claussen — University of Birmingham, UK

Evolutionary game theory connects dynamics to strategy by assuming few behavioral strategies, modeling costs and benefits from interactions via a payoff matrices, then casting these into replicator equations (in infinite populations) resp. stochastic processes (in finite populations) which comprise a "physics of behaviour" model of the collective decision dynamics (which may include cyclic oscillations). We build on previous results (PRL 95, 238701 and PRL 100, 058104 and subsequent) and discuss combinations of 2- and 3 strategy games in the context of different replicator dynamics, and stochastic processes derived from agent interaction models. We demonstrate how the previous concepts of drift reversal - how an attracting fixed point resulting from a Hopf bifurcation loses stabilty below a critical population size, applies to the combined games.

SOE 2.6 Mon 11:15 GÖR/0226

A reversal in agent preference reveals partial segregation in the Schelling model — •Maksim Prusakov and Dirk Brockmann — Center Synergy of Systems, TUD Dresden University of Technology, Dresden, Germany

The Schelling model is one of the most famous and seminal models used to describe spatial segregation in social systems. We introduce a small modification to the basic rules of the model: instead of avoiding locations with too many neighbors of a different type, agents now seek places with a high proportion of same-type neighbors. Although this change may seem minor, it leads to qualitatively different behavior. For certain parameter values the system enters an unexpected and new partial-segregation phase, where macroscopically stable segregated clusters coexist with mixed, dynamically active regions.

We construct the phase diagram across tolerance and density values and characterize all macroscopic regimes of the model. The partial-segregation phase emerges robustly across different neighborhood sizes, lattice geometries, and numbers of agent types, which suggests that this behavior follows from the modified preference rule itself rather than from microscopic implementation details. To complement these results, we develop a theoretical framework that describes the stability conditions of the observed phases, with particular attention to the mechanisms that sustain partial segregation. Ultimately, our findings show that even a minor change in the type of local preference can generate fundamentally new collective behavior within Schelling-type models.

SOE 2.7 Mon 11:30 GÖR/0226

Emergence of power-laws and the uncertainty principle in human contact duration — •Jun Sun — GESIS - Leibniz Institute for the Social Sciences, Cologne, Germany

Consider the mechanism underlying human contact duration distributions as an aggregate effect of time-homogeneous processes, where the persistent probability of a contact (pairwise or higher-order) is drawn from a distribution but remains constant during its lifetime (Starnini et al., 2013). I propose a thermodynamic interpretation of the model, in which the persistent probability of a contact is mapped to a negative log-energy, identifying time as the inverse temperature, and the duration distribution as the partition function. I prove that under mild conditions, the contact duration distribution exhibits a power-law with potential cutoffs, a phenomenon commonly observed in empirical data. Such distributions are special in the thermodynamic framework as they have constant specific heat capacity, which corresponds to both the power-law exponent and the effective degrees of freedom. When contact agents act independently, the degrees of freedom equal the contact order. Behavioral correlation between agents reduces the effective degrees of freedom (therefore also the power-law exponent). Finally, I establish an uncertainty relation between time and persistent probability, revealing a fundamental limit within which contact durations can be characterized. Unlike the once-controversial notion of temperature fluctuation, the uncertainty of time in contact data is well-defined.

15 min. break

SOE 2.8 Mon 12:00 GÖR/0226

Wired differently: Individual-level Adaptive Belief Networks — •Peter Steiglechner, Victor Møller Poulsen, Mirta Galesic, and Henrik Olsson — Complexity Science Hub, Vienna, Austria

Our beliefs about political issues are not independent; they are embedded within interconnected belief systems. Models such as the Networks of Beliefs (NB) theory (Dalege et al, 2025) formalise how individuals adjust their beliefs to reduce dissonance, and study how this leads to polarisation or consensus. In these models, the relations between beliefs are static, and the same belief network structure is assumed across individuals. This overlooks that perceived dissonance and belief relations can differ across individuals. And such heterogeneity in belief system structures can affect how individuals respond to external pressures or interventions, such as economic shocks or political scandals. We extend NB theory by allowing belief networks to evolve over time, shifting the focus from dynamics of belief content to the co-evolution of content and structure. In simulations of the model, individuals start with identical belief networks, but their structures diverge, producing stable disagreement between individuals. External events, inducing temporary pressure on a single belief, triggers lasting belief changes in some individuals (compliant), but only temporary or no changes in others (resilient and resistant), regardless of the strength of the pressure. Our model offers an illustrative and endogenous explanation of such asymmetries in responses to external events without requiring traits such as stubbornness, motivated cognition or identity biases.

SOE 2.9 Mon 12:15 GÖR/0226

Critical Transitions of Reinforcement Learning Dynamics in Social Dilemmas — •Balakrishna Prabhu B N and Wolfram Barfuss — Center for Development Research(ZEF), University of Bonn, Germany

Understanding how cooperation emerges and persists among self-interested agents remains a crucial question in the human, animal, and machine behavioral sciences. Specifically, the aspect of the timescales required to reach a cooperative outcome has received little attention.

While the field of equilibrium game theory has addressed the possibility of cooperative outcomes, it offers little insight into how agents select and reach these equilibria, or the timescales required to do so. Evolutionary game theory and reinforcement learning have addressed some of these questions, but are yet to examine the temporal aspects of strategy adaptation and the critical transitions that occur with changes to basic payoff structures.

In this work, we develop a framework based on deterministic dynamics of reinforcement learning to study critical transitions between different social dilemma games. We find that boundaries involving the Chicken game exhibit strong criticality, whereas transitions involving the StagHunt game do not. We also explore convergence times and equilibrium selection and their variations across these boundaries for static and dynamic systems.

By uncovering the dynamic behavior between game transitions, our work lays the foundation for an integrated theory of coupled social-ecological tipping elements.

SOE 2.10 Mon 12:30 GÖR/0226

Statistical mechanics of connected graphs in Scrabble — •Olivier Witteveen and Marianne Bauer — Department of Bionanoscience, Kavli Institute of Nanoscience Delft, TU Delft, Van der Maasweg 9, 2629 HZ Delft, The Netherlands

The crossword-like patterns of tiles in Scrabble form connected graphs of occupied sites on a square lattice. We are interested in describing the ensemble of these Scrabble graphs and comparing them across different languages. To find the most structureless description of Scrabble graphs, we build a maximum-entropy probability distribution; using real tournament data, we adapt a pseudo-likelihood method to the case of connected graphs on a lattice. We find that a maximum-entropy distribution that includes means and pairwise correlations captures the data: it correctly predicts simultaneous square occupation, word-length statistics, and geometric features of the Scrabble graphs, as well as the hierarchy among square types. Finally, we explore how language affects the structure of the Scrabble graphs. We adapt a Scrabble bot to self-play and generate graphs using different lexica. We find that the graphs produced by the bot have lower entropy compared to human players, and that lexica with shorter words yield higher entropy graphs. Remarkably, the pairwise maximum-entropy distribution is almost sufficient to correctly assign Scrabble graphs to their corresponding lexica.

SOE 3: Sustainability: Challenges and Solutions (joint session UP/CPP/SOE)

Accompanying session to Symposium SYSC

Time: Monday 9:30–10:30 Location: MER/0002

SOE 3.1 Mon 9:30 MER/0002

Making a university climate neutral: First experiences from implementing a Climate Protection Strategy at the University of Greifswald — •Christoph G. Hoffmann, Tiemo Timmermann, and Christian von Savigny — University of Greifswald, Greifswald, Germany

With a resolution of its Academic Senate, the University of Greifswald has in 2021 set the goal to achieve climate neutrality by the end of the decade.

While the aim of achieving climate neutrality within a few years is expectedly ambitious, a university as a bigger research institution has also a unique combination of knowledge to achieve it. This has already led to synergies from which particularly the teaching in the environmental subjects can benefit due to "home-made" practical experiences. This makes the whole University a living lab, in which the opportunities but also challenges of necessary transformations can be explored in an assessable setting.

Therefore, also the environmental physics group aims at contributing to and benefiting from this process. While our group is originally focused on basic atmospheric research, we cover a broader range of environmental physics topics in teaching, which overlap with the needs of the transformation process.

In this talk, we will give a short overview of the Climate Protection strategy of the University of Greifswald before we show some examples from our own work regarding the energy consumption of buildings.

SOE 3.2 Mon 9:45 MER/0002

Life Cycle Assessment practices for PV technologies: systematic literature review — •Zeena Patel — Technische Universität Ilmenau

In response to the growing importance of sustainability in solar energy development, this study addresses critical gaps in the application of Life Cycle Assessment (LCA) to photovoltaic (PV) technologies. A systematic review of 48 recent LCA studies across first-, second-, and third-generation PV systems was conducted to evaluate current practices, identify methodological inconsistencies, and highlight emerging trends. Despite increasing research interest and technological diversification, substantial variability exists in the definition of functional units, system boundaries, and impact categories, which hinders comparability and reproducibility. The widespread reliance on secondary databases and the limited use of primary, site-specific data further constrains the accuracy of environmental impact assessments. Additionally, the underutilization of Life Cycle Costing (LCC) and inconsistent application of sensitivity analyses reveal significant gaps in comprehensive sustainability evaluation. To advance the field, this study proposes standardization of LCA methodologies, improved data transparency, and expansion of impact categories beyond global warming potential to include toxicity and resource depletion. These measures are essential for enhancing the robustness, reliability, and policy relevance of PV LCA studies, thereby supporting sustainable innovation and deployment in the solar energy sector.

SOE 3.3 Mon 10:00 MER/0002

Electrochemical Modeling of SOFCs with Emphasis on Microkinetic and Anode Overpotential — •Iram Gul[1], Gabriela Soffiati[2], and Thiago Lopes[3] — [1]Research Center for Greenhouse Gas Innovation, University of São Paulo (USP), 05508-030, São Paulo * SP, Brazil — [2]Institute of Physics (IFUSP), University of São Paulo, Universidade, R. do Matão, 1371 - Butantã, São Paulo - SP, 05508-090 — [3]Research Center for Greenhouse Gas Innovation, University of São Paulo (USP), 05508-030, São Paulo * SP, Brazil

This study investigates Solid Oxide Fuel Cells (SOFCs) using a CO/H fuel mixture, focusing on thermodynamics, mass transport, and electrochemical kinetics. Thermodynamic properties such as heat capacity, enthalpy, entropy, and Gibbs free energy were analyzed across 600-800°C using MATLAB simulations. The Dusty Gas Model (DGM) revealed key mass transport behaviors in the anode, while Density Functional Theory (DFT) using VASP provided insights into surface reaction mechanisms. A microkinetic model examined the impact of anode overpotential on reaction kinetics and cell performance. Results show that higher temperatures improve mass transport and reduce Ohmic losses but slightly decrease the thermodynamic driving force. This multi-scale model enhances our understanding of SOFC behavior and offers a basis for improving fuel cell efficiency and material performance.

SOE 3.4 Mon 10:15 MER/0002

Thermal stability of ceria-zirconia oxides(CeZrO4) nanoparticles using combustion synthesis for the CO oxidation and NOx reduction — •Hamza Mohamed — IMMM, UMRS 6283 CNRS, Le Mans Université, Bd O. Messiaen, 72085 Le Mans Cedex 09, France

The study presents a green synthesis approach for fabricating ceria-zirconia oxide nanoparticles (CeZrO4 NPs) using the solution combustion synthesis method. The synthesized CeZrO4 nanoparticles were characterized using various sophisticated instruments and methods to determine their detailed properties. The UV-Vis spectra showed a characteristic absorbance peak at 242 nm and a band gap (Eg) of 3.05 eV. Simultaneously, Fourier transform infrared spectra of CeZrO4 NPs displayed bands at 418 cm-1, 991 cm-1, 1382 cm-1, 1658 cm-1, 2306 cm-1, 3288 cm-1, and 3643 cm-1, which indicates the presence of phytochemicals that facilitate the reduction and stabilization of CeZrO4 NPs. The major peaks for cubic CeZrO4 NPs were obtained with a crystalline size of 9.6 nm by X-ray diffraction. The microscopic analyses revealed irregular, ovoid, and aggregated morphologies with sizes ranging from 3 to 10 nm. The XPS analysis revealed the existence of Ce3d, Zr3d, C1s, and O1s states with their corresponding atomic percentages. Therefore, this investigation focuses on synthesizing catalysts that demonstrate both thermal stability and high catalytic activity for the oxidation of CO and the reduction of NOx.

SOE 4: Poster Session

Time: Monday 18:00–21:00 Location: P4

SOE 4.1 Mon 18:00 P4

Artificial "Minimal" Intelligence in a Decentralized Mechanical System — •Alex Leffell and Manu Prakash — Stanford University, California, USA

Computation is not exclusive to neurons or transistors. Simple, aneural organisms like Placozoa exhibit complex behaviors, demonstrating that intelligence can arise from non-neuronal physical dynamics. We model these organisms as Phased Active Elastic Sheets (PhAES) – networks of coupled active oscillators that compute via the dynamics of their vibrational modes. This approach builds on established work in both physical learning and active solids and extends it to understand animal behavior. Using both in-silico and robophysical models, we show that this system can perform complex behaviors like gradient climbing without any implicit memory and purely mechanical communication between cells. This perspective offers a direct path towards a new class of computational materials that physically embody sensing, actuation, and learning. Such systems would bridge the gap between rigid, centrally-controlled robots and task-specific soft matter, fundamentally expanding our notions on the physical basis of intelligence.

SOE 4.2 Mon 18:00 P4

Validating diffusion-based dimensionality reduction of political regimes: conflict and child mortality benchmark — •Paula Pirker-Diaz[1], Radost Waszkiewicz[1], Matthew Wilson[2], and Karoline Wiesner[1] — [1]University of Potsdam — [2]University of South Carolina

Political regime indices such as the Electoral Democracy Index (EDI) are widely used for measurement and policy analysis, yet their additive aggregation rules can obscure nonlinear relationships among regime indicators. In earlier work, we showed that a subset of EDI components lies on a low-dimensional nonlinear manifold recovered with the Diffusion Map method [1]. Here we introduce a new one-dimensional regime index by fitting this manifold, identifying the latent dimension along which regime features co-vary most strongly while preserving their nonlinear structure. The resulting index parallels the EDI's characterization of democracies but produces a different ordering among autocracies. By varying the smoothness penalty, we identify the indicators whose contributions to the latent structure remain most stable, providing a robustness-based measure of their relevance. The new index improves the resolution of intra-regime conflict onset probability and child mortality relative to the EDI, with the largest gains among autocratic regimes that the manifold distinguishes more effectively. These findings reinforce that political regimes lie on a nonlinear low-dimensional manifold identified by diffusion methods, which capture social and political variation more effectively than linear aggregation rules. [1] Pirker-Diaz et al., RSOS (2025)

SOE 4.3 Mon 18:00 P4

Realizable Circuit Complexity: Embedding Computation in Space-Time — •Benjamin Prada and Ankur Mali — University of South Florida, Tampa, FL

Parallel computation is typically modeled as a process carried out by abstract machines that ignore the constraints of physical reality. Although the evolution of real-world systems may be mapped to these abstractions, reverse translation is almost always impossible; most computations cannot be simulated in real-time by any device obeying finite propagation speed, bounded volume, or finite entropy. To remedy this discongruity between computational and physical theory, we introduce a framework of *realizable circuits* $\mathbf{RC}_d$ that incorporates a d-dimensional spatial embedding directly into the computation model. The key is that information must cross geometric boundaries at a finite rate: fine-grained entropy flow through a $(d-1)$-dimensional boundary limits the number of independent bits that can be transformed or erased within a d-dimensional region. This yields physically motivated lower bounds on parallel depth and communication, connecting known theoretical and empirical results such as Landauer's principle and Rent's rule. Although the framework is general, we illustrate its usefulness by analyzing modern neural architectures (e.g., transformers and recurrent networks), whose parallel speedups are similarly constrained by entropy flux through bounded interfaces. The resulting theory offers a physics-aligned perspective on the fundamental limits of parallel computation, independent of any specific classical or quantum computing substrate.

SOE 4.4 Mon 18:00 P4

Dynamics of Behavioral Contagion in Human and Artificial Agent Collectives: A Drift-diffusion Simulation Study — •Maryam Karimian[1,2] and Pawel Romanczuk[1,2] — [1]Institute for Theoretical Biology, Department of Biology, Humboldt-Universität zu Berlin, 10115 Berlin, Germany — [2]Science of Intelligence, Research Cluster of Excellence, Berlin, Germany

Behavioral contagion, the spread of behavior within a group, is a central topic in cognitive and collective behavior research. Prior work has either relied on first-person perspective that overlook dynamic social structure or on idealized collective models that neglect individual decision processes. To bridge this gap, we use an extended drift-diffusion model to simulate virtual-reality (VR) experiments, integrating cognitive mechanisms with group-level dynamics. We model agents' decision-making processes, responding to uncertain environmental signals, and influencing one another through an increment drift-diffusion process. Decision states evolve based on accumulated environmental evidence and socially conveyed information. Social information is derived from visually grounded interaction networks capturing first-person sensory constraints shaped by distance and occlusion. These networks are implemented as weighted, directed graphs modulated by group size and density. Using controlled experimental data, we parameterize the model and generate testable predictions on decision dynamics across different environmental and social conditions, highlighting how visual network properties shape vision-mediated contagion and related cognitive processes such as selective attention.

SOE 4.5 Mon 18:00 P4

Optimal transport with constraints: from mirror descent to classical mechanics — •Abdullahi Ibrahim[1,2], Michael Muehlebach[2], Caterina De Bacco[2], and Dirk Brockmann[1] — [1]Center Synergy of Systems, Dresden University of Technology, Dresden, Germany — [2]Max Planck Institute for Intelligent Systems, Cyber Valley, Tuebingen 72076, Germany

Over the past decades, a variety of transportation systems have been successfully modelled using optimal transport (OT), from biological networks as leaf venation, to engineering networks as urban transportation. In this context, adaptation equations that describe how conductivities, flows and pressure potentials evolve interdependently to consolidate into an optimal network structure. This has been used extensively to study a variety of transportation scenarios, and it has been shown to explain with a high degree of similarity observed on real networks. However, current approaches based on adaptation equations suffer from not considering constraints (beyond standard ones like conservation of mass and positivity) as part of the general framework. As a result, networks output from these models can be unrealistic in practice. We address this flaw by proposing a general framework powerful enough to accommodate nonlinear and nonconvex constraints in OT problems. Our approach follows a physics-based perspective on including constraints by leveraging the principle of d'Alembert-Lagrange from classical mechanics. This leads to a sparse, local and linear approximation of the feasible set leading in many cases to closed-form updates.

SOE 4.6 Mon 18:00 P4

GPU-Parallel Load-Flow Solvers with Low-Rank Updates for Contingency Analysis and Topology Optimization — •Marc Hunkemöller[1,2], Nico Westerbeck[3], Lars Schewe[4], and Dirk Witthaut[1,2] — [1]Forschungszentrum Jülich, Institute of Climate and Energy Systems – Energy System Engineering (ICE-1), 52428 Jülich, Germany — [2]Institute for Theoretical Physics, University of Cologne, Köln, 50937, Germany — [3]University of Edinburgh, School of Mathematics, Peter Guthrie Tait Road, Edinburgh, EH9 3FD, UK — [4]Elia Group, Boulevard de l'Empereur 20, 1000 Brussels, Belgium

Power-flow simulations based on the Newton-Raphson method are key tools for transmission system operators. GPUs may accelerate these computations and thus enable fast contingency analysis and new applications such as transmission topology optimization, which are increasingly important for integrating large shares of renewable energy and reducing dependence on fossil fuels. However, parallelization on GPUs is challenging, as the treatment of different topologies does not align well with the "Single Instruction, Multiple Data" paradigm. We present a GPU-parallel AC load-flow solver designed to overcome the difficulties introduced by changing sparsity patterns in the Jacobian matrix when the network topology varies. Our approach uses low-rank updates to separate the Jacobian's dependence on the network structure from its dependence on the system state, allowing topology changes to be incorporated efficiently. In combination with iterative linear solvers, we explore different update orders and strategies to identify stable and fast solver configurations suitable for large sets of topology scenarios.

SOE 4.7 Mon 18:00 P4

Modeling Predator-Prey Encounters via Interacting Ornstein-Uhlenbeck Motions — •Zihao Liu and Ricardo Martinez-Garcia — Helmholtz-Zentrum Dresden-Rossendorf

Most population dynamics models assume well-mixed and independent individuals. However, many animals anchor their movement around key resources such as food, water, or shelter, a behavior well captured by Ornstein-Uhlenbeck home-range dynamics. Previous work has shown that incorporating home-range behavior already leads to substantial deviations in encounter rates from classical predictions. In this study, we further relax the assumption of independence by introducing an explicit attractive interaction from the predator to the prey. Using analytical approximations and individual-based simulations, we explore how this interaction reshapes the encounter landscape across different home-range sizes, spatial separations, force magnitudes, and interaction ranges. We also discuss how small changes in individual movement behavior may influence group-level dynamics, with possible implications for foraging efficiency, spatial clustering, and coexistence conditions.

SOE 4.8 Mon 18:00 P4

Inference of network structures from partial observations — •Matthias Klaus[1,2], David Dahmen[1], and Moritz Helias[1,2] — [1]Institute for Advanced Simulation (IAS-6), Jülich Research Centre, Jülich, Germany — [2]Department of Physics, Faculty 1, RWTH Aachen University, Aachen, Germany

Today's recording techniques for neural activity allow one to access finite time windows of a few hundred to thousands of neurons. Since they are embedded in strongly connected networks of 10^5 neurons, the recorded data will be considerably influenced by the structure of these unobserved parts. Theoretical descriptions of the problem often assume spatial and temporal homogeneity across the system, i.e. that structure and activity of the entire network, on a statistical level, are close to the recorded part.

Here we model this statistical homogeneity by the variances of connectivity and of a globally independent driving white noise. Estimates for these parameters exist from prior experiments. Consequently, we use a Bayesian approach to obtain a posterior for the local connectivity by conditioning on the locally recorded activity. The theory involves a marginalization over unobserved activity, which is exact for a linear network with Gaussian activity. This condition can be relaxed by reasonably assuming a large network and applying dynamic mean-field theory (Sompolinsky, Crisanti, Sommers 1988; Schuecker, Goedeke, Helias 2018). We find that reconstruction of local connectivity is possible if the influence from unobserved parts reduces to a colored noise whose statistics is estimated correctly.

SOE 4.9 Mon 18:00 P4

A Conceptual Model for Temperature dynamics in the Climate System — •Fatemeh Aghaei and Holger Kantz — Max Planck Institute for the Physics of Complex Systems

we propose a simple conceptual model for tipping of the Earth's atmospheric dynamics due to feefback loops from global mean temperature on the release of greenhouse gases by natural processes. The model shows that the strength of this feedback is a relevant parameter which determined the speed of climate change after passing through a tipping point, to be extracted from earth system models. Also, we show that by data analysis, it might be possible to reconstrict the functional form of the feedback process. We illustrate both by the analysis of model data.

SOE 5: Network Science

Time: Tuesday 9:30–10:30 Location: GÖR/0226

Invited Talk SOE 5.1 Tue 9:30 GÖR/0226

Network Science in Criminology: Insights from Empirical Case Studies — •Masarah Paquet-Clouston — University of Montreal, Montreal, Canada

Network science has become a central tool in criminology, offering powerful ways to model illicit relationships and hidden organizational structures. This presentation draws on three empirical case studies that apply network-based methods to real-world criminological problems: mapping how cybercrime forum users connect with specific topics, tracing money flows in illicit cryptocurrency transactions, and identifying links among corporate secrecy vehicles.

These examples highlight both the analytical potential of network-based approaches and the methodological challenges inherent to criminological data. I will conclude by identifying open research questions that advances in related fields, such as complexity science, could help address.

SOE 5.2 Tue 10:00 GÖR/0226

Collective decision making with biases - Role of network topology — Yunus Sevinchan[1], Petro Sarkanych[2], Archili Sakevarashvili[1], Yurij Holovatch[2,3], and •Pawel Romanczuk[1] — [1]Institute for Theoretical Biology, Dept. of Biology, Humboldt Universität zu Berlin — [2]Yukhnovskii Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, Lviv, Ukraine; 𝕃4 Collaboration and Doctoral College for the Statistical Physics of Complex Systems, Lviv-Leipzig-Lorraine-Coventry, Europe — [3]Complexity Science Hub, Vienna, Austria

The accuracy of collective decision-making in groups depends on a complex interplay of factors, including prior information, biases, social influence, group composition, and the structure of the interaction network. In this work, we study a spin-type model in which interactions are mediated through a social field generated by an agent's neighbors, allowing for heterogeneous individual preferences. Building on previous results [1], we examine how network topology affects consensus formation. We show that, unlike the Ising model, the social-field model exhibits fundamentally similar behavior on both scale-free and Erdős-Rényi networks, a result that can be attributed to weaker hub-hub interactions. Finally, we investigate the extent to which a strongly biased minority can dominate the collective decision, even in the presence of an oppositely biased majority.

[1] Sarkanych *et al*, Phys Biol 20 (2023); Sarkanych *et al*, Cond Matt Phys 27 (2024); Sevinchan *et al*, Phys Rev Res 7 (2025)

SOE 5.3 Tue 10:15 GÖR/0226

Operational time and criticality in physics co-authorship networks — •Pouria Mirelmi[1] and Haiko Lietz[2] — [1]Leiden University, Leiden, The Netherlands — [2]GESIS – Leibniz Institute for the Social Sciences, Cologne, Germany

Many real-world complex networks display either fractal or small-world structure, but rarely both. Prior work explains this incompatibility through static architectural constraints: fractality emerges from critical branching trees, whereas small-world structure requires supercritical expansion supported by long-range shortcuts. Here we show that this dichotomy is not merely structural but dynamical. Using more than a century of APS co-authorship data, we construct a sequence of network time slices by tuning aggregation to the percolation transition. Measuring a set of macro-level parameters – including percolation observables and small-world indicators – we find that all scale as power laws with the networks' distance from criticality. Networks remain fractal near criticality but acquire small-world shortcuts only when aggregated beyond the critical point. We further show that the critical time scale emerging from this aggregation procedure constitutes an operational time to which the system self-organizes: citation avalanches obey dynamical scaling theory only when defined in this intrinsic time. These results indicate that static analyses are insufficient whenever the evolutionary time scale of a network is empirically accessible. A dynamical scaling framework is required to correctly identify and characterize critical and supercritical network states.

SOE 6: Mobility, Traffic Dynamics, Urban and Regional Systems

Time: Tuesday 10:45–12:45 Location: GÖR/0226

SOE 6.1 Tue 10:45 GÖR/0226

Percolation on the "urban influence" field: analyzing Europe's urban fabric — •Renan Lucas Fagundes[1] and Diego Rybski[1,2] — [1]IOER, Dresden — [2]CSH, Vienna

We investigate the connectivity of urban settlements using the concept of level-set percolation (LSP). Therefore, we introduce a notion of urban influence, quantifying the impact of the presence of urban settlements in their surroundings. To be specific, we define a power-law field over the urban settlements in Europe in 2018. This field can be understood in a similar fashion as 2D Gaussian Random Field but with a power-law. We find a relationship between the level where the second largest cluster reaches a maximum – an indicator of the percolation transition – and the imposed field-exponent. The exponential slope of the relation correlates with the size of the country. We speculate that the critical behavior of the field is being driven by the spatial organization of the urban structure.

SOE 6.2 Tue 11:00 GÖR/0226

Global settlement percolation: estimating critical distances — •Diego Rybski — IOER Dresden

Cities and settlements can be understood as percolating systems. We apply spatial clsutering, where any two items belong to the same cluster if their Euclidean distance is smaller than a threshold. Varying this threshold, at a critical distance a transtion occurs where a giant cluster emerges – resembling a percolation transition. We systematically analyze high-resolution data on the global scale and estimate this critical distance for various spatial units. We find that the critical distance is complementary to other geographical indicators. Our estimates can be of use for down-stream research.

SOE 6.3 Tue 11:15 GÖR/0226

Scaling laws beyond cities — •Yiwei Yang[1,2], Benedikt Grammer[1], Rafael Prieto-Curiel[3], David Frantz[4], Helmut Haberl[1], and Dominik Wiedenhofer[1] — [1]BOKU University, Vienna, Austria — [2]MPG-DLU, Jena, Germany — [3]CSH, Vienna, Austria — [4]Trier University, Trier, Germany

Urban scaling laws reveal that larger cities tend to be more resource-efficient and innovative, but the standard framework has two well-known limitations: (1) the one-city-one-value approach assumes that the entire urban area is the only meaningful unit of analysis; (2) carefully delineated city boundaries artificially divide what is in fact a continuous human settlement system. These issues motivate examining scaling relationships within cities and across the rural-urban continuum. We hypothesize that fine-scale properties, in particular infrastructure-related attributes tied to fractal urban form, scale with population across the full fabric of human settlements. We test this using high-resolution gridded maps for the contiguous United States, analyzing how built-environment material stocks, service provisioning, and operational greenhouse gas emissions scale with population at the settlement-cell level. Through stepwise empirical tests, we not only demonstrate that scaling is present at fine spatial scales within human settlements, but also identify three important features of intra-settlement scaling. Our findings reframe the view that the city is the sole scale at which scaling laws arise, reveal pronounced intra-settlement heterogeneities, and offer practical implications for the analysis and planning of sustainable settlement development.

15 min. break

SOE 6.4 Tue 11:45 GÖR/0226

Higher-order interactions yield synergistic infrastructure backbones — •Christoph Steinacker[1], Henrik Wolf[2], Marc Timme[1], and Malte Schröder[1] — [1]Chair of Network Dynamics, Center for Advancing Electronics Dresden (cfaed) and Institute of Theoretical Physics, TUD Dresden University of Technology, 01062 Dresden, Germany — [2]AMOLF, Amsterdam, Netherlands

Infrastructure networks essentially underlie human mobility across all modes of transport. Higher-order interactions among different network elements impact network performance as they generically induce modified usage at every element across the network. Here, we consider such higher-order interactions to reveal and quantify the synergies between different link upgrades in transport networks. While network expansion strategies based on first-order, individual link importance result in scattered, disconnected networks, sets of pairs of mutually synergistic links automatically form connected backbones of infrastructure networks. We illustrate the approach with a perturbed utility route choice model for bicycle traffic on empirical urban street networks. Our results not only provide a novel theory of evaluating complex transport networks beyond individual link importance, they may also help to guide strategic network planning in practice.

SOE 6.5 Tue 12:00 GÖR/0226

Where2Share–Complex system predictions of ridepooling potential in Germany — Philip Marszal, Felix Jung, Marc Timme, and •Malte Schröder — Chair of Network Dynamics, Center for Advancing Electronics Dresden (cfaed) and Institute of Theoretical Physics, TUD Dresden University of Technology, 01062 Dresden, Germany

Complex system modeling often provides general insights about similar systems in vastly different settings by identifying the key mechanisms driving their dynamics. Here, we demonstrate how this perspective may help avoid many individual case studies and expensive pilot projects when planning on-demand ridepooling services that promise to reduce the number of cars on the road and cut back emissions by dynamically combining trips of multiple users in the same vehicle. By exploiting the transferability of complex system models of ridepooling based on a small number of cornerstone parameters, we built an open-data framework to estimate the potential reliability and efficiency of these services. We apply our framework to create a map of the ridepooling potential in Germany, quantifying key performance and operating parameters of ridepooling services across more than 400 vastly different service areas. Our framework is easily applicable to other regions and provides valuable insights about the influence of network topology, fleet size, and demand structure on the potential performance of ridepooling services. The results presented here may help focus the planning of ridepooling services by informing decision-making from the earliest point.

SOE 6.6 Tue 12:15 GÖR/0226

Self-organized co-existence of fixed and flexible pooling routes — •Nora Molkenthin, Karolin Stiller, and Alexander Schmaus — Potsdam Institute of Climate Impact Research (PIK)

Shared pooled mobility describes a diverse class of nonlinear, non-locally coupled transport models, which give rise to rich, yet currently not fully understood dynamics. In this system we have observed the spontaneous emergence of periodic trajectories in passenger-optimized as well as fleet-distance optimized ridepooling simulations at moderate to high request densities. Despite the uniformly distributed origin-destination pairs as driving input, we find partially periodic routes for some parameter and network choices, while at others, all routes remain unstructured. This dynamical symmetry breaking from unstructured to partially periodic trajectories occurs as the request load increases. These findings suggest a new class of chimera-like behaviour in real-world-inspired, spatially embedded, non-oscillatory systems. This finding has a natural interpretation as a regime of emergent co-existence between shared pooled mobility and line-based public transport, even without policy intervention.

SOE 6.7 Tue 12:30 GÖR/0226

Pulses, waves, and chaos in migration dynamics — Niraj Kushwaha[1], Woi Sok Oh[2], and •Edward Lee[1] — [1]Complexity Science Hub, Vienna, Austria — [2]University of Waterloo, Waterloo, Canada

Decisions to migrate depend on others' decisions. Dependence can produce both stable long-term trends and sudden transitions, which appear in data but could be the result of either exogenous drivers or of endogenous dynamics. We propose a simple migration model that accounts for social influence and individual heterogeneity in decisions to migrate. The minimal model displays hysteresis, waves, and chaotic-like regimes. This occurs in special locations of parameter space, suggesting that migration response to external conditions could be highly dependent on whether the system is poised near or far away from dynamical instability. Conditioning on this distance would be key to determining "causal drivers" of migration. In the context of displacement, for example, this would be relevant for oft-considered correlates like armed conflict and onset of natural disasters. We show how the model aligns with features of migration statistics including from internal displacement and maritime crossings.

SOE 7: Award Session: Young Scientist Award for Socio- and Econophysics (YSA)

Time: Tuesday 14:00–15:30 Location: GÖR/0226

Topical Talk SOE 7.1 Tue 14:00 GÖR/0226

What's that noise? Why does it make a difference? And why am I thinking about it all the time? — •Dirk Brockmann — Center Synergy of Systems, TU-Dresden, Dresden, Germany

Replication is one of the central processes in biological, ecological, evolutionary and, in more subtle ways, also social systems. Unsurprisingly, many dynamical systems designed to describe such phenomena implement replication in one form or another. Some are even labeled as such, for example the replicator equation, a keystone system whose many variants populate ecological and evolutionary modelling with admirable persistence. Despite their conceptual simplicity, replicator systems have a habit of producing surprises and sit at the center of long-standing controversies. One of these is an apparent paradox: the competitive exclusion principle, often a generic hallmark of replicator dynamics, seems fundamentally at odds with the remarkable diversity of species with very similar ecological functions observed in real ecosystems. Nature, it appears, did not read the textbook. Fluctuating environments and, more generally, noise have been proposed as a way out of this dilemma. Yet models that include noise tend to disagree with one another, leaving the puzzle very much alive. In this lecture, I will discuss how noise can affect replication in qualitatively different ways, why it matters which noise you add and how, how this may help us understand coexistence in ecosystems, and why thinking about all this may quietly reshape how we understand cooperation as a pervasive feature of the biosphere.

Presentation of the Award to the Awardee

Prize Talk SOE 7.2 Tue 14:45 GÖR/0226

How things spread: Complexity and criticality of inhomogeneous spreading models — •Laurent Hébert-Dufresne — University of Vermont, Burlington VT, USA — Santa Fe Institute, Santa Fe NM, USA

Models of how things spread often assume that transmission mechanisms are fixed over space and time. However, the transmission of infectious diseases can depend on local human behaviour or quality of the surrounding infrastructure. Likewise, social contagions like the spread of ideas, beliefs, and innovations depend on local norms or culture, and they can lose or gain in momentum as they spread. Diseases mutate and find subpopulations where they can thrive, just as ideas can get reinforced, beliefs strengthened, and products refined. We study the impacts of these mechanisms in spreading and cascade dynamics. Using different modelling tools, we find that complexity and criticality are the norm: Superlinear relationships between exposure and transmission can emerge from linear interactions and power-law distributions with anomalous scaling can be observed away from any critical point.

SOE 8: Networks, From Topology to Dynamics I (joint session SOE/DY)

Time: Wednesday 9:30–11:00 Location: GÖR/0226

Invited Talk SOE 8.1 Wed 9:30 GÖR/0226

Dynamics and Structure in Temporal Networks — •Natasa Djurdjevac Conrad — Zuse Institute Berlin, Germany

Temporal networks are a powerful tool for describing real-world systems in which interactions change over time, such as social contacts or transportation systems. Understanding how these networks evolve is crucial for uncovering the mechanisms that drive system behavior. From a dynamical systems perspective, clustering temporal networks and tracking the dynamics of clusters enables the identification of long-lived structures, metastable states and tipping points. In this talk, I will present recent work on temporal network analysis using random walk-based approaches, with a focus on network clustering and detecting structurally coherent time-periods. These methods provide a natural connection between network science and dynamical systems, relating to transfer operator frameworks and spectral theory. Through examples from synthetic models and real-world datasets, I will illustrate how these tools uncover key patterns and dynamic changes in complex networks.

SOE 8.2 Wed 10:00 GÖR/0226

From Quiescence to Synchrony: Noise-Shaped Dynamics in Coupled Neuronal Systems — •Max Contreras[1,2] and Philipp Hövel[2] — [1]Technische Universität Berlin, Germany — [2]Saarland University, Saarbrücken, Germany

Stochastic fluctuations are usually regarded as promoters of activity in excitable and oscillatory systems, giving rise to phenomena such as coherence resonance. Here, we show that the opposite can occur in the small-noise regime, where noise

can inhibit spiking activity in weakly coupled neuronal units. Using a ring of diffusively coupled, oscillatory FitzHugh-Nagumo neurons, we demonstrate how the interplay of noise and coupling strength generates different collective behaviors. We systematically classify the dynamical scenarios by an in-depth time-series analysis that combines multiple, complementary measures. As a result, we are able to automatically identify distinct dynamical clusters in parameter space: quiescent state, noisy synchronization, complete synchronization, and intermittent switching. The presented workflow can be universally applied in coupled oscillator networks and provides a unified framework to study collective dynamics.

15 min. break

SOE 8.3 Wed 10:30 GÖR/0226

Learning collective variables for time-evolving networks — •Sören Nagel, Nataša Djurdjevac Conrad, Stefanie Winkelmann, and Marvin Lücke — Zuse Institute Berlin

We address the challenge of model reduction for time-evolving networks by identifying collective variables for stochastic rewiring processes driven by opinion homophily. [Lücke et al., Phys. Rev. E 109, L022301 (2024); Djurdjevac Conrad et al., Chaos 34, 093116 (2024)].

Utilizing the *transition manifold framework*, we identify a simple consensus measure as a collective variable for an ergodic and a non-ergodic model, and learn the dynamics of the projected system. We show that the learned model reduction can be obtained from the corresponding graphon process in the case of large and not too sparse graphs with uniformly distributed opinions. Our data-driven approach successfully identifies the collective variables in more general cases, highlighting the possibility to study low-dimensional model reductions in systems that have not been understood theoretically.

SOE 8.4 Wed 10:45 GÖR/0226

Time-delayed dynamics in regular networks of Kuramoto oscillators with inertia — •Philipp Hövel[1], Esmaeil Mahdavi[2], Mina Zarei[2], and Farhad Shahbazi[3] — [1]Saarland University, Saarbrücken, Germany — [2]Institute for Advanced Studies in Basic Sciences, Zanjan, Iran — [3]Isfahan University of Technology, Isfahan, Iran

We investigate the complex interplay between inertia and time delay in regular rotor networks within the framework of the second-order Kuramoto model. By combining analytical and numerical methods, we demonstrate that intrinsic time delays – arising from finite information transmission speeds – induce multistability among fully synchronized phase-locked states. Unlike systems without inertia, the presence of inertia destabilizes these phase-locked states, reduces their basin of attraction, and gives rise to nonlinear phase-locked dynamics over specific inertia ranges. In addition, we show that time delays promote the emergence of turbulent chimera states, while inertia enhances their spatial extent. Notably, the combined influence of inertia and time delay produces dynamic patterns reminiscent of partial epileptic seizures. These findings provide new insights into synchronization phenomena by revealing how inertia and time delay fundamentally reshape the stability and dynamics of regular rotor networks, with broader implications for neuronal modeling and other complex systems.

SOE 9: Economic Models

Time: Wednesday 11:30–12:45 Location: GÖR/0226

SOE 9.1 Wed 11:30 GÖR/0226

Macroscopic Stochastic Model for Economic Cycle Dynamics — •Eckehard Schöll[1,2], Sören Nagel[2,3], and Jobst Heitzig[2] — [1]TU Berlin — [2]Potsdam Institute for Climate Impact Research — [3]Zuse Institute Berlin

We present a stochastic dynamic model which can explain economic cycles [1]. We show that the macroscopic description yields a complex dynamical landscape consisting of multiple stable fixed points, each corresponding to a split of the population into a large low and a small high income group. The stochastic fluctuations induce switching between the resulting metastable states, and excitation oscillations just below a deterministic bifurcation. The shocks are caused by the decisions of a few agents who have a disproportionate influence over the macroscopic state of the economy due to the unequal distribution of wealth among the population. The fluctuations have a long-term effect on the growth of economic output and lead to business cycle oscillations exhibiting coherence resonance, where the correlation time is controlled by the population size which is inversely proportional to the squared noise intensity.

[1] S. Nagel, J. Heitzig, and E. Schöll: Macroscopic stochastic model for economic cycle dynamics. Phys. Rev. Lett. 134, 047402 (2025).

SOE 9.2 Wed 11:45 GÖR/0226

Kinetic theory re-examination of the mean-field theory of Santa Fe financial market model — •Taiki Wakatsuki and Kiyoshi Kanazawa — Department of Physics, Graduate School of Science, Kyoto University, Kyoto 606-8502, Japan

Understanding and accurately modeling the statistical phenomena observed in real financial markets remains a central challenge in econophysics. In particular, the Santa Fe model, where order events occur according to a Poisson process, has been widely used as a verifiable financial market model. Simulation results of the Santa Fe model clearly demonstrate that it can explain the statistical laws of real markets to a certain extent. However, previous theoretical explanations of these statistical laws, which relied on dimensional analysis and mean-field theory, are neither unique nor fully sufficient. Therefore, this study will re-examine the mean-field theory of the Santa Fe model using kinetic theory. This presentation provides a theoretical analysis of the bid-ask spread and reports on its scaling.

SOE 9.3 Wed 12:00 GÖR/0226

Hallmarks of deception in asset-exchange models — •Kristian Blom[1], Dmitrii E. Makarov[2], and Aljaz Godec[3] — [1]Institute of Theoretical Physics, University of Münster — [2]Department of Chemistry, The University of Texas at Austin — [3]Mathematical bioPhysics group, MPI for Multidisciplinary Sciences

Asset-exchange models, such as the Bennati-Dregulescu-Yakovenko money game, have emerged in econophysics as simple models that capture generic features of wealth dynamics. In the BDY game, the wealth of a single player undergoes a one-dimensional random walk. Because the exchange probability of losing and gaining money are equal, one may surmise that this walk is unbiased, but this is not the case: the boundary condition that each player's wealth cannot be negative introduces a loss bias because of the possibility that an exchange partner has zero wealth. This results in an exponential steady-state distribution. Here, we extend the BDY game by introducing probabilistic cheaters that can misrepresent their financial status with a given probability. Cheaters deceive their exchange partners by claiming that they have no money, enabling them to evade potential losses. In a system consisting of honest players and cheaters, we show how cheating alters the transient dynamics as well as steady-state distributions of wealth. We identify a threshold probability for cheating beyond which cheaters accumulate more than half of the total money. Additionally, we show under which conditions cheating becomes beneficial and establish the existence of a critical cheating probability at which the wealth of cheaters undergoes a second-order discontinuity.

SOE 9.4 Wed 12:15 GÖR/0226

Identifying higher order cascading failures in supply chain networks of a national economy — •Jan Fialkowski[1,2], Stefan Thurner[1,2,4], and Shlomo Havlin[3] — [1]Complexity Science Hub, Vienna, Austria — [2]Institute of the Science of Complex Systems, CeDAS, Medical University Vienna, Vienna, Austria — [3]Department of Physics, Bar-Ilan University, Ramat-Gan 52900, Israel — [4]Santa Fe Institute, Santa Fe, USA

Cascading Failure scenarios are a central concern for the design of complex systems. In financial and economic systems these cascading failures give rise to the notion of systemic risk, where the failure of a single entity leads to large disruptions in the entire system. Exhaustively examining the failure of larger sets of elements is difficult due to computational constraints. Here we study the recently introduced notion of economic systemic risk in national supply chain networks of firm-firm interactions. We use an empirical dataset of the ecuadorian economy, consisting of almost 100.000 firms and more than three million buyer-supplier links. Using a modification of the "Random Chemistry" method we can identify small sets of firms, whose simultaneous failure leads to failure cascades that are larger than would be expected from their individual failure cascades.We compare the final cascade size of the small sets of firms with the sum of cascade sizes of the individual firm failures and find pairs that are up to 260 times more destructive than the individual firms themselves. We also provide a classification of the underlying mechanisms leading to this strong increase of the final cascade size.

SOE 9.5 Wed 12:30 GÖR/0226

Overcoming the Prestige Trap: Modelling the Transition to Community-Led Academic Publishing — •Valentin Lecheval[1,2], Clémence Bergerot[1,3], Valerii Chirkov[1,2], Giuseppe Maria Ferro[4], and Daniel Rubenstein[4] — [1]Department of Biology, Humboldt Universität zu Berlin, Berlin, Germany — [2]Science of Intelligence, Research Cluster of Excellence, Berlin, Germany — [3]Charité-Universitätsmedizin Berlin, Einstein Center for Neurosciences Berlin, Berlin, Germany — [4]Department of Ecology and Evolutionary Biology, Princeton University, Princeton, NJ, USA

The academic publishing industry is dominated by a few for-profit companies, resulting in the corporate capture of a substantial share of public funds that

could instead support academia. While alternative publishing models are not lacking–community-led publishers offering diamond open-access, or directing article processing charges towards academic services–they suffer from reduced attractivity compared to their for-profit counterparts, possibly due to first-mover advantages and path-dependent reputational dynamics. Here, we introduce a multi-scale agent-based model depicting the joint dynamics of research groups and journals. The parameters of research groups dictate their preference for journals, weighting various attributes, such as reputation or community services–attributes that can depict for-profit journals, society-based journals, open-access mega-journals or predatory journals. We simulate the model on a wide range of parameters to investigate the conditions leading community-led journals to overcome path-dependent barriers and dominate the publishing landscape.

SOE 10: Networks, From Topology to Dynamics II (joint session SOE/DY)

Time: Wednesday 15:00–15:45 Location: GÖR/0226

SOE 10.1 Wed 15:00 GÖR/0226

Combining machine-learning and dynamic network models for sepsis prediction — •Juri Backes[1,3], Artyom Tsanda[1,2], Tobias Knopp[1,2], Wolfgang Renz[3], and Eckehard Schöll[4] — [1]TU Hamburg — [2]UKE Hamburg — [3]HAW Hamburg — [4]TU Berlin

We enhance short-term sepsis predictions by integrating machine learning techniques like Auto-Encoders and Gated-Recurrent-Units with a dynamical 2-layer network model of adaptive phase oscillators [1] representing the interaction between parenchymal cells (functional organ cells) and the immune system via cytokines. The model trajectories determined by machine learning are used for detection and prediction of critical infection states and mortality. The model-based predictions are compared with those of purely data-based approaches in terms of predictive power and interpretability. To this end we project real high-dimensional medical patient data into the low-dimensional parameter space of the model.

[1] R. Berner, J. Sawicki, M. Thiele, T. Löser, and E. Schöll: Critical parameters in dynamic network modeling of sepsis. Front. Netw. Physiol. 2, 904480 (2022).

SOE 10.2 Wed 15:15 GÖR/0226

Forecasting emergency department visits in the reference hospital of the Balearic Islands: the role of tourist and weather data — •Paride Crisafulli, Tobias Galla, Raul Toral, and Claudio Mirasso — IFISC (UIB-CSIC), Palma de Mallorca, Spain

Accurate forecasting of patient arrivals at emergency departments (EDs) is vital for efficient resource allocation and high-quality patient care. Despite its significance and extensive prior research, certain conditions can significantly impact the accuracy of these estimates. This study investigates the relevance of tourism and weather data alongside traditional calendar and demographic variables in forecasting ED visits in the reference hospital in Palma de Mallorca, a city with significant seasonal population fluctuations due to tourism. Utilizing a machine learning approach, we develop a model that predicts ED visits based solely on exogenous variables. We test three different machine learning algorithms (random forests, support vector machines, and feed-forward neural networks) with four different input combinations, comparing their mean average percentage errors (MAPEs) and prediction horizons.

SOE 10.3 Wed 15:30 GÖR/0226

Beyond Averages: How Disease Severity and Social Structure Interact to Shape Pandemic Dynamics — •Fabio Sartori, Sophia Horn, Sven Banisch, and Michael Maes — Chair of Sociology and Computational Social Science, Karlsruhe Institute of Technology, Karlsruhe

Epidemiological models typically rely on population averages, overlooking behavioral polarization and social structure. We developed a compartmental framework examining how polarization and homophily shape outcomes across mask-wearing, testing, and vaccination interventions. Results reveal intervention-specific effects: polarization benefits masks but harms testing and vaccination. Homophily worsens outcomes for low-infectivity diseases by removing protective barriers, but improves outcomes for highly infectious diseases through protective bubbles. Calibrating with German survey data (n=1,612), homogeneous models showed large errors. Intervention effectiveness depends critically on social structure and pathogen characteristics, not just average compliance.

SOE 11: Polarization

Time: Wednesday 15:45–17:15 Location: GÖR/0226

SOE 11.1 Wed 15:45 GÖR/0226

Accurate mean-field predictions for cognitively grounded social influence dynamics with confirmation bias — •Sven Banisch — Karlsruhe Institute of Technology

Collective opinion formation in human groups is often modeled through cognitively rich agent-based dynamics, yet the resulting high-dimensional systems typically resist analytical treatment. Here we show that a class of cognitively grounded argument-exchange models with confirmation bias admits a low-dimensional and fully tractable mean-field representation. The key idea is to project pairwise agent rules onto an influence response function and then derive a two-compartment mean-field system whose Jacobian separates into a mean mode and a polarization mode. This yields a simple stability test that diagnoses the onset of symmetry breaking. We recover the consensus-to-polarization tipping point and identify a second threshold at which polarized equilibria become fully stable. Across all parameter regimes, the mean-field bifurcation structure accurately reproduces the behaviour of the full agent-based model. Our results provide a general mechanism-level framework for understanding how cognitive biases shape macroscopic opinion patterns, and demonstrate that high-dimensional social influence dynamics can exhibit simple and universal phase-space structure amenable to analytical classification.

SOE 11.2 Wed 16:00 GÖR/0226

Dynamics of ideologically polarized social media users — •Tristram Alexander and Jamie Tyler — University of Sydney, Australia

Social media users have been shown to exhibit different types of behaviour and preference on social media, depending on their ideological position on a left-right axis. This work investigates whether observed differences may be attributed to intrinsic differences in the users, or whether the differences emerge based on interactions in the social media environment.

The study is based on interactions between users on the Twitter/X platform. Users are classified on a left-right scale based on their retweet activity, and placed into categories based on their position on this scale. The reply activity between users is then examined to determine the rates of interaction between the different classes of user. The population of the users in each interaction class is then estimated, based on frequencies of interaction between the classes.

The study finds that users appear to have the same intrinsic behaviour, irrespective of ideological class, but that they behave differently due to the population imbalance between the classes on the platform. This leads right-leaning users to be more active then left-leaning users, which is posited as a reason for greater observed departure rates of right-leaning users from the platform. A model of this interaction behaviour is developed and mapped to the observations. The results of this work may inform the further development of opinion dynamics models.

15 min. break

SOE 11.3 Wed 16:30 GÖR/0226

Campaign-spending driven polarization transition in a double-random field model of elections — •Jan Korbel[1], Remah Dahdoul[1], and Stefan Thurner[1,2,3] — [1]Complexity Science Hub, Vienna, Austria — [2]Medical University of Vienna, Austria — [3]Santa Fe Institute, NM, US

We model bipartisan elections where voters are exposed to two forces: local homophilic interactions and external influence from two political campaigns. The model is mathematically equivalent to the random field Ising model with a bimodal field. When both parties exceed a critical campaign spending, the system undergoes a phase transition to a highly polarized state where homophilic influence becomes negligible, and election outcomes mirror the proportion of voters aligned with each campaign, independent of total spending. The model predicts a hysteresis region, where the election results are not determined by campaign spending but by incumbency. Calibrating the model with historical data from US House elections between 1980 and 2020, we find the critical campaign spending to be ~1.8 million USD. Campaigns exceeding critical expenditures increased in 2018 and 2020, suggesting a boost in political polarization.

SOE 11.4 Wed 16:45 GÖR/0226

Information Saturation in the Political Center Drives the Spread of Extreme Content — •Markus Hofer[1,2], Jan Korbel[2], and Stefan Thurner[1,2,3] — [1]Center for Medical Data Science, Institute of the Science of Complex Systems, Medical University of Vienna, Vienna 1090, Austria — [2]Complexity Science Hub Vienna, Vienna 1030, Austria — [3]Santa Fe Institute, Santa Fe, NM 87501

Although most voters hold moderate opinions, online discourse is increasingly dominated by ideological extremes. To understand this phenomenon, we employ an agent-based model in which post-sharing mediates all opinion dynamics. First, agents filter posts based on ideological distance to update their own opinions. Then they select one of the received posts based on novelty, quantified as the local information-theoretic surprisal. Here we show that empirically consistent opinion distributions with moderate polarization naturally emerge alongside a disproportionate sharing of extreme content. We identify the underlying mechanism as a density-dependent competition for novelty: high post density in the political center leads to information saturation, effectively suppressing surprisal and resharing. In contrast, extreme content maintains high surprisal, increasing its resharing probability. This mechanism explains the heavy-tailed cascade distributions observed on Twitter/X and points toward interventions that reduce the informational novelty advantage of extreme content.

SOE 11.5 Wed 17:00 GÖR/0226

The role of antagonization in political discourse on social media — •Armin Pournaki and Eckehard Olbrich — Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany

Antagonization is a central discursive strategy in political narratives. The creation of an enemy allows for political mobilization through powerful affective mechanisms. It is commonly assumed that social media, through a combination of platform affordances and algorithmic amplification, reward and therefore enhance antagonizing content. However, it is an open empirical question whether the prevalence and nature of antagonization as a discursive strategy depends on the political leaning, or whether different political camps antagonize equally.

The present work aims to address those questions by presenting a novel computational approach to systematically extract traces of antagonization from text, including potential targets of antagonization. On a corpus of 1M tweets from the German Twittersphere, we observe a strong prevalence of antagonizing content, confirming common hypotheses by which social media tend to facilitate such discourse. By combining the method with a large-scale estimation of ideological positions of users based on their retweet behaviour, we show that antagonization is significantly more prevalent in the online discourse of right-leaning than of left-leaning actors. Finally, a systematic analysis of the various antagonized targets provides novel insights into how different political factions employ this strategy to mobilize their audience.

SOE 12: Statistical Physics of Politics

Time: Wednesday 17:15–18:00 Location: GÖR/0226

SOE 12.1 Wed 17:15 GÖR/0226

Critical Dynamics govern the Evolution of Political Regimes — •Joshua Uhlig[1], Paula Pirker-Díaz[1], Matthew Wilson[2], Ralf Metzler[1], and Karoline Wiesner[1] — [1]University of Potsdam, Potsdam, Germany — [2]University of South Carolina, Columbia, SC, USA

The emergence and decline of democratic systems worldwide raises fundamental questions about the dynamics of political change. Contrary to the idea of a stable end point of liberal democracy, recent backsliding towards less democratic regimes highlights the non-stationary nature of regime evolution [1]. Here, we analyse the historical trajectories of countries within a two-dimensional regime space derived from the principal components of the Varieties of Democracy dataset [2]. We observe weakly non-ergodic dynamics unfolding in an effective landscape characterised by sparse and shifting basins of stability. Step sizes and waiting times follow heavy-tailed distributions near the critical regime, in which mean values appear to diverge, indicating intermittent and heterogeneous regime change. A continuous time random walk model [3] reproduces the dynamics of the three most recent decades with remarkable accuracy. Together, these results suggest that some aspects of political regime evolution follow universal stochastic principles, while remaining punctuated by unique historical pathways.

[1] P Pirker-Díaz et al., R Soc Open Sci. 12, 250457 (2025) [2] K Wiesner et al., R. Soc. Open Sci. 11, 240262 (2024) [3] R Metzler et al., Phys. Chem. Chem. Phys. 16, 24128 (2014)

SOE 12.2 Wed 17:30 GÖR/0226

The Statistical Physics of Political Voting in German Parliament — •Moritz Marpe[1] and Carolin Dylla[2] — [1]Technical University Berlin — [2]Freie Universität Berlin

We propose a singular value decomposition (SVD) of the German parliament voting records from 2021-2024 to answer the question of how polarised was the legislature during the Ampel administration? Arguably, political polarisation is expressed most prominently between elected representatives who can be stylised in a system of their behavioural voting patterns. We built on the work by Sirovich (2003) and Rees & Lee (2025) who analyse the partisan divide and political voting patterns in the US institutions using frameworks borrowed from statistical physics to investigate the degree of polarisation. Likewise we use the median voter theorem to identify *pivotal voters* tipping collective outcomes along mulidimensional political issues. We propose a SVD to identify the most common voting coalitions following Sirovich (2003) for the last full term of the German Bundestag. Our contribution transfers insights from the bipartisan US-system to a multiparty system in general and the German Bundestag in particular filling a vital gap in the quantitative research on political polarisation.

SOE 12.3 Wed 17:45 GÖR/0226

Analyzing political spaces to understand political realignment: The case of Switzerland — •Eckehard Olbrich[1] and Peter Achermann[2] — [1]Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany — [2]University Zürich, Zürich, Switzerland

The rise of right-wing populist parties and the preceding emergence of new left and ecological parties beginning at the end of the 70s in the last century if often as the emergence of a new conflict line ("cleavage") [1] related to the transition from industrial societies to post-industrial societies. A fully developed political cleavage corresponds to an alignment of divisions in three layers: 1) the sociodemographic structure (structural layer), 2) the prevalent attitudes, narratives and ideologies (ideological layer) and 3) the political parties and social movements. We will test the theory of new cleavage for the case of Switzerland by analyzing political spaces derived from geographically resolved data on public votes and elections. We would expect the appearance of a new cleavage to be reflected as a new dimension in the political space, thus roughly speaking increasing the dimensionality of the political space (de-alignment) while a subsequent decline of the dimensionality could represent a re-alignment in the sense that the older cleavage gets replaced. While we observe that re-alignment as a decrease of dimensionality in the data, the picture for the de-alignment appears more complicated.

[1] S. Bornschier et al. Cleavage Formation in the 21st Century: How Social Identities Shape Voting Behavior in Contexts of Electoral Realignment. Cambridge University Press, 2024.

SOE 13: Members' Assembly

Time: Wednesday 18:00–19:30 Location: GÖR/0226

All members of the Physics of Socio-economic Systems Division are invited to participate.

SOE 14: Focus Session: Physics of AI I (joint session SOE/DY)

The focus session is organized by Claudius Gros (Goethe-Universität Franfurt), Moritz Helias (Forschungszentrum Jülich), Peter Sollich (Georg-August-Universität Göttingen)

This focus session brings together experts in the field of physics-inspired theory of machine learning and artificial intelligence, who aim to supplement the engineering-driven success of AI by a principled theory of neural information processing. Contributions will address how statistical and dynamical perspectives explain learning in modern AI systems and how these insights support interpretability as well as prediction of performance, generalization, and the required resources.

Time: Thursday 9:30–11:15 Location: GÖR/0226

Invited Talk SOE 14.1 Thu 9:30 GÖR/0226

Generative AI and diffusion models: a statistical physics approach — •Giulio Biroli — Ecole Normale Superieure, Paris, France

Generative AI represents a groundbreaking development within the broader *Machine Learning Revolution,* significantly influencing technology, science, and society. In this colloquium, I will focus on the state-of-the-art *diffusion models*, which are currently used to generate images, videos, and sounds. They are very fascinating algorithms for physicists, as they are very much connected to concepts from stochastic thermodynamics, particularly time-reversed Langevin dynamics. These diffusion models start from a simple white noise input and make it evolve through a Langevin process to generate complex outputs such as images, videos, and sounds. I will show that statistical physics provides principles and methods to characterise this generation process. Specifically, I will discuss how phenomena such as the transition from memorization to generalization and the emergence of features can be understood through the lens of symmetry breaking, phase transitions, slow dynamics, and methods used to study disordered systems.

SOE 14.2 Thu 10:00 GÖR/0226

Statistical Physics of Classifier-free Diffusion Guidance — •Enrico Ventura[1], Beatrice Achilli[1], Carlo Lucibello[1], and Luca Ambrogioni[2] — [1]Bocconi University, Milan, Italy — [2]Radboud University, Nijmegen, The Netherlands

Classifier-free Guidance (CFG) is a simple yet effective technique that helps diffusion models better follow a user's prompt. By combining standard unconditional diffusion with diffusion conditioned on a specific class of the data, it steers generation toward samples (e.g. images, videos or text) that more clearly reflect the intended content. We propose a description of the sampling dynamics of a diffusion model under CFG based on the statistical mechanics of disordered systems. Specifically, we study the time-dependent transformation of the diffusion potential providing a quantitative prediction of the way a complex target distribution is deformed to improve data generation. Moreover, we leverage our results to propose alternative theory-based guidance schedules that enhance such beneficial effects.

SOE 14.3 Thu 10:15 GÖR/0226

Fundamental operating regimes, hyper-parameter fine-tuning and glassiness: towards an interpretable replica-theory for trained restricted Boltzmann machines — •Alberto Fachechi[1], Elena Agliari[1], Miriam Aquaro[1], Anthony Coolen[2], and Menno Mulder[2] — [1]Department of Mathematics, Sapienza University of Roma, P. le A. Moro 5, 00185 Roma, Italy — [2]Theoretical Biophysics, DCN Donders Institute, Faculty of Science, Radboud University, 6525 AJ Nijmegen, The Netherlands

Since the seminal work by Amit, Gutfreund and Sompolinsky, statistical mechanics of spin-glasses with structural disorder has acquired a crucial role in theoretical investigations of artificial neural networks, as it enables the representation of their generalization and information processing capabilities as phases within the space of parameters. We study the relaxation towards equilibrium of the training procedure of restricted Boltzmann machines with a binary visible layer and a Gaussian hidden layer with an unlabelled dataset consisting of noisy realizations of a single ground pattern. We develop a statistical mechanics framework to describe the network generative capabilities by exploiting replica theory. We outline the effective control parameters (e.g., the relative number of weights to be trained, the regularization parameter), whose tuning can yield qualitatively different operative regimes. We also provide analytical and numerical evidence for the existence of a sub-region in the space of the hyperparameters where replica-symmetry breaking occurs.

SOE 14.4 Thu 10:30 GÖR/0226

Mirror, Mirror of the Flow: How Does Regularization Shape Implicit Bias? — •Tom Jacobs, Chao Zhou, and Rebekka Burkholz — CISPA Helmholtz Center, Saarbrucken, Germany

Implicit bias plays an important role in explaining how overparameterized models generalize well. Explicit regularization like weight decay is often employed in addition to prevent overfitting. While both concepts have been studied separately, in practice, they often act in tandem. Understanding their interplay is key to controlling the shape and strength of implicit bias, as it can be modified by explicit regularization. To this end, we incorporate explicit regularization into the mirror flow framework and analyze its lasting effects on the geometry of the training dynamics, covering three distinct effects: positional bias, type of bias, and range shrinking. The mirror flow framework relies on Noether style parameter symmetry preservation, the regularization controls them. Our analytical approach encompasses a broad class of problems, including sparse coding, matrix sensing, single-layer attention, and LoRA, for which we demonstrate the utility of our insights. To exploit the lasting effect of regularization and highlight the potential benefit of dynamic weight decay schedules, we propose to switch off weight decay during training, which can improve generalization, as we demonstrate in experiments.

SOE 14.5 Thu 10:45 GÖR/0226

Generalization performance of narrow one-hidden layer networks in the teacher-student setting — Rodrigo Pérez Ortiz[1], •Gibbs Nwemadji[2], Jean Barbier[3], Federica Gerace[1], Alessandro Ingrosso[4], Clarissa Lauditi[5], and Enrico Malatesta[6] — [1]Alma Mater Studiorum * Università di Bologna (Unibo), Bologna, Italy — [2]International School of Advanced Studies (SISSA), Trieste, Italy — [3]The Abdus Salam International Centre for Theoretical Physics, Trieste, Italy — [4]Radboud University, Nijmegen, The Netherlands — [5]Harvard University, Cambridge, US — [6]Bocconi University, Milano, Italy

Generalization on simple input-output distributions is best studied in the teacher-student setting, but fully connected one-hidden-layer networks with generic activations still lack a complete theory. We develop such a framework for networks with a large but finite number of hidden neurons, using statistical-physics tools to obtain closed-form predictions for both Bayesian and ERM estimators through a few summary statistics. We also identify a specialization transition when the sample size matches the number of parameters. The resulting theory accurately predicts generalization errors for networks trained with Langevin dynamics or standard full-batch gradient descent.

SOE 14.6 Thu 11:00 GÖR/0226

Testing generalization through tiny task switching frameworks — •Daniel Henrik Nevermann and Claudius Gros — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Deutschland

With an ever-growing interest in advancing the performance and efficiency of large language models (LLMs), and therein particularly the transformer architecture, the need for tiny testing frameworks is pressing, as many researchers cannot afford to train models on large GPU clusters. We here propose a tiny testing framework, extending the recently published IARC task switching framework, that despite being trivial to implement offers suitable complexity to be non-trivial to learn for small scale transformer models with a few million parameters or less. Beyond model benchmarking, the framework is also suitable for probing phenomena relevant to problems arising in physics of AI, where controlled, interpretable testbeds are essential. The proposed training and evaluation scheme relies on integer sequences to be predicted by the model. These integer sequences are generated by simple deterministic tasks designed to abstract typical challenges arising in natural language processing, such as short and long range correlations, or context awareness. Within the sequences, tasks are randomly switched, where a switch is indicated by a control token. An important quality of LLMs is the ability to generalize at inference time. We here extend the existing task switching framework with new tasks able to probe models generalization capacities in a tiny, yet meaningful manner.

SOE 15: Networks: From Topology to Dynamics III (joint session DY/SOE)

Time: Thursday 11:15–12:45 Location: ZEU/0118

SOE 15.1 Thu 11:15 ZEU/0118

Remote Tipping in Networks — •Philip Marszal[1], Malte Schröder[1], and Marc Timme[1,2] — [1]Chair of Network Dynamics, Center for Advancing Electronics Dresden (cfaed) and Institute of Theoretical Physics, TUD Dresden University of Technology, 01062 Dresden, Germany — [2]Lakeside Labs, Lakeside B04b , 9020 Klagenfurt, Austria

Tipping of a single unit in a complex networked system can trigger large-scale cascades that shift the system's macroscopic state. Typically, such cascades propagate diffusively, with each tipping event destabilizing adjacent units.

Here we report a novel form of tipping cascade in systems of coupled bistable oscillators, that results in the tipping of non-adjacent nodes. One node can trigger transitions in distant nodes while intermediate neighbors remain unaffected. Which nodes tip and which ones remain unaffected depends intricately on the local oscillator dynamics and the underlying network structure. We study the transition between locally spreading and non-local cascades and characterize the conditions necessary for the emergence of non-local cascades.

SOE 15.2 Thu 11:30 ZEU/0118

Ponderomotive Route to Tipping in Open Networks — Seungjae Lee[1], •Marisa Fischer[1], and Marc Timme[1,2,3] — [1]Chair for Network Dynamics, Institute of Theoretical Physics and Center for Advancing Electronics Dresden (cfaed), Technische Universität Dresden, 01062 Dresden, Germany — [2]Center Synergy of Systems, Technische Universität Dresden, 01062 Dresden, Germany — [3]Lakeside Labs, Lakeside B04b, 9020 Klagenfurt, Austria

External fluctuations impact the dynamics of complex networked systems, from cells and ecosystems to engineered infrastructures. Strong external forcing may cause tipping that compromises such systems' functionality. Here, we identify a generic ponderomotive route to tipping in open, periodically driven systems. Upon increasing the driving amplitude, the time-average of the oscillatory responses persistently shifts away from the original system's operating point – a system-level ponderomotive effect. We characterize the shift as the fixed-point solution of a slow dynamics resulting from a two-time-scale analysis. A bifurcation point of the shift defines the tipping point beyond which the system settles into another collective state, diverges gradually, or exhibits finite-time blow-up. The ponderomotive shift together with its bifurcation yields the novel type of *ponderomotive tipping*. It generically emerges across disparate systems from science and engineering and is independent of their diverse post-tipping dynamics.

SOE 15.3 Thu 11:45 ZEU/0118

Linear dynamics on infinite networks — •Bernd Michael Fernengel — HIFMB, Oldenburg, Germany

Linear evolutionary equations are often used to describe the time evolution of a physical system. Their solution operator can be written in an exponential form of exp(t A), with some generator A. When the generator is a finite dimensional matrix, we can interpret its time evolution as a hopping dynamics on a finite network, where the dynamics of the network can be transferred to the dynamics of the solution operator.

In order to study special types of solution operators for non-interacting systems of countable dimensions, we construct countable, infinitely large networks using the iterated Cartesian product of finite graphs, where the dynamics is known. We discuss the possibilities to infer properties like the time evolution and the stationary solution of the infinite network from finite approximations via the thermodynamic limit. This is closely related to the question, under which conditions it is possible to approximate a countable, infinite system by finite subsystems.

SOE 15.4 Thu 12:00 ZEU/0118

Localizing sparse perturbation sources in driven nonlinear networks — •Julian Luca Fleck, Jose Casadiego, and Marc Timme — Chair of Network Dynamics, Center for Advancing Electronics Dresden (cfaed) and Institute of Theoretical Physics, TUD Dresden University of Technology, 01062 Dresden, Germany

Network dynamical systems under the influence of external perturbations abound in nature and engineered systems, ranging from neural circuits to electrical power grids. The external driving can drastically change the system's operating mode and be fatal for system stability. Localizing sources of perturbations in a network is crucial to mitigate systems failure. We present a linear response approach to infer the location from a multivariate time series of a recorded subset of nodes. We employ a compressed-sensing algorithm to locate one or multiple perturbation sources utilizing the sparsity of such locations. The approach additionally yields the time series of the unmeasured nodes and the external driving. We test for random linear systems, and illustrate the applicability to electrical power grids.

SOE 15.5 Thu 12:15 ZEU/0118

Elucidating structure-function relationships in physical networks via ensnarlment — •Yu Tian[1,2,3,4], Chinmayi Subramanya[1,3,4], and Carl Modes[1,3,4] — [1]Center for Systems Biology Dresden, Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems — [3]Max Planck Institute of Molecular Cell Biology and Genetics — [4]Dresden University of Technology, Dresden, Germany

Understanding physical networks – whose structure is constrained by the physical properties of their nodes and links – is a growing interdisciplinary challenge, especially in biological systems. Physical constraints such as volume exclusion and non-crossing conditions, along with biological functionality, can drive these networks into non-optimal spatial configurations. One prominent feature is that cycles may go through each other's interior space, which may not be unraveled without removing edges, leading to an ensnarled state. Characterizing the ensnarlment in the space, and its interplay with the functional behaviours of the network, is essential for revealing structure-function relationships in such systems. In this work, we introduce a graph-theoretic framework based on the linking operator, obtained by the Gauss linking integral applied to the cycles in the network. This approach enables a multiscale analysis of entanglement, spanning local, intermediate, and global structures. Our goal is to reveal how topological complexity shapes, and is shaped by, biological functions, providing new insights into the organizational principles of physical and biological networks.

SOE 15.6 Thu 12:30 ZEU/0118

Transient stability properties for transitions between stationary power flows — •Leo Heidweiler[1,2] and Frank Hellmann[2] — [1]TU Dresden — [2]Potsdam Institute for Climate Impact Research

The increasing incorporation of renewable energy sources into electrical power grids fundamentally changes their dynamical behaviour and introduces new challenges for system stability. While network expansion and operation are traditionally based on stationary power flow analysis, dynamical effects following line faults, such as loss of synchronization of a single generator or whole part of the network, may occur even when a stable post-fault power flow exists and operational constraints are fulfilled. Direct assessment of transient stability, however, requires time-resolved simulations that are computationally expensive and unsuitable for large-scale planning and real-time applications. This motivates the question of whether transient stability properties can be inferred from static characteristics of the network, such as power flow solutions and topology.

In this work, we develop stability indicators for the IEEE39 Bus power system and investigate their predictability using PowerDynamics.jl, a Julia Library for numerical Power Grid simulations. In particular, we make use of the complex oscillator formulation of Power Systems and machine learning. This helps us assess whether stability margins can be predicted from stationary quantities alone or whether intrinsically dynamical information is indispensable. If so, we can deduce what minimal dynamical information is sufficient for reliable prediction.

SOE 16: Tipping Points in Social and Climate Systems (accompanying session for SYTP)

Accompanying session to the Symposium in Tipping Points in Social and Climate Systems

Time: Thursday 11:30–12:45 Location: GÖR/0226

Invited Talk SOE 16.1 Thu 11:30 GÖR/0226

Tipping in Strongly Perturbed Open Networks — •Marc Timme[1,2], Georg Börner[1], Marisa Fischer[1], Julian Fleck[1], Seungjae Lee[1], Philip Marszal[1], Gwendolyn Quasebarth[1], Malte Schröder[1], and Moritz Thümler[1] — [1]Network Dynamics, TU Dresden, http://networkdynamics.info — [2]Lakeside Labs, Klagenfurt, Austria

Strong fluctuations impacting open systems may induce tipping and system-wide cascading failure, yet it remains unclear under which conditions, how, and

at which point fluctuation-driven systems tip. Here we report theoretical and methodological progress about tipping and its precursors in a range of externally driven nonlinear networked systems, substantially generalizing and going beyond work on one- and two-dimensional systems [1,2]. We combine self-consistency conditions, insights from periodically driven systems in electrodynamics and tools from harmonic balance and asymptotic analysis to uncover generic routes to tipping, to predict intrinsically nonlinear response dynamics before tipping and estimate the tipping point semi-analytically. We highlight several application directions and a broad range of unsolved questions.

I acknowledge generous support by the German Science Foundation (DFG) through a Koselleck project (2025-2029, proj. # 544800752).

[1] M. Thümler et al., Nonlinear and divergent responses of fluctuation-driven systems, IFAC-PapersOnLine 55:254 (2022).

[2] G. Börner et al., Perturbation-response dynamics of coupled nonlinear systems, Chaos 34:103149 (2024).

SOE 16.2 Thu 12:00 GÖR/0226

Stability and decay of socio-political systems — •Vaishnavi Jayakumar[1], Matthew Wilson[2], and Karoline Wiesner[1] — [1]Institute for Physics and Astronomy, University of Potsdam, Germany — [2]Department of Political Science, University of South Carolina, Columbia, SC, USA

The government is a fundamental unit of modern societies. There have been many efforts to quantify different styles of governance, one of the most prominent being the V-Dem project. V-Dem provides a comprehensive set of indicators on governance quality, including the Electoral Democracy Index (EDI). Governing styles can be classified in various ways based on such indicators; this has led to many studies on the feasibility, stability, and resilience of such socio-political institutions. In our present work, we analyze the V-Dem database, spanning across 195 countries, and examine the effective lifetimes and decay dynamics of various governments and regimes. Using survival analysis methods, we model regime longevity in terms of half-life and mortality rates. We find that countries with an EDI > 0.5 approximate a fairly straightforward decay function with a well-defined half-life, whereas countries with an EDI < 0.5 display irregular lifetimes, with a trajectory that evades a simple steady-state description. This heterogeneity can be understood by accounting for the underlying drivers of both regime endurance and collapse. We further investigate how economic and institutional factors shape regime lifetimes and contribute to the observed variability. Our study thus sheds new light on the key ingredients that underpin regime stability and mortality.

SOE 16.3 Thu 12:15 GÖR/0226

Generating Representative Social Networks for modeling social tipping points — •Kamiel Gülpen and Vítor Vasconcelos — University of Amsterdam, Amsterdam, The Netherlands

Addressing some of today's most pressing challenges, from climate change to public health crises, requires triggering collective behavioral shifts through social tipping points (STPs). These phenomena have been extensively modeled using synthetic network topologies, which provide valuable theoretical insights but often incompletely represent the mixing patterns that influence tipping dynamics in real populations. Understanding when STPs occur thus requires real-world network data. While such data remains scarce, government agencies possess rich information on household, family, neighborhood, and work/school connections, but often in aggregated form due to privacy constraints. This aggregated data reveals group-level mixing patterns but lacks the individual network topology necessary for modeling diffusion processes. To bridge this gap, we present the Aggregated Social Network Unfolding (ASNU) framework, which generates representative multiplex social networks from aggregated demographic data. Applied to Amsterdam's population, ASNU reconstructs networks across social layers while preserving key structural properties. We also introduce the Social Relational Attachment (SRA) model for generating realistic social networks when aggregated edge data is unavailable. Unlike previous models relying solely on homophily, SRA incorporates both homophilic and heterophilic bonding through tunable demographic distance parameters.

SOE 16.4 Thu 12:30 GÖR/0226

Jacobian Reconstruction from Time-Series of an Opinion Dynamical Network Model and its Applicability as an Early Warning Signal for Tipping Points — •Tim Mauch — Helmholtz Institute for Functional Marine Biodiversity (HIFMB), Im Technologiepark 5, 26129 Oldenburg, Germany — Carl-von-Ossietzky University, Institute for Chemistry and Biology of the Marine Environment, Carl-von-Ossietzky Str. 9-11, 26129 Oldenburg, Germany

In social dynamical systems the early identification of critical transitions is a significant challenge. To address this, we formulate a new opinion model to enhance the understanding of tipping mechanisms in opinion dynamics and adopt a method for reconstructing the Jacobian matrix of the model from time-series data, testing its applicability for detecting critical transitions.

Inspired by meta community models from ecology, we study opinion formation using a network-based model in which nodes represent communities of interacting agents holding one of two competing opinions, and links represent avenues of migration. We analytically derive conditions for diffusion-driven pattern formation and identify a mechanism facilitating opinion diversity, where the minority opinion can reach local majority, thus creating regions of differing opinion dominance.

We then generate synthetic time series of the model and reconstruct the Jacobian matrix using only the time series data and the underlying network structure. We show that the reconstructed eigenvalues correctly capture the trend of the analytical eigenvalues when changing the model parameters towards critical transitions.

SOE 17: Focus Session: Physics of AI II (joint session SOE/DY)

Time: Friday 9:30–12:45 Location: GÖR/0226

Invited Talk SOE 17.1 Fri 9:30 GÖR/0226

What can we learn from neural quantum states? — Brandon Barton[10], Juan Carrasquilla[10], Anna Dawid[9], Antoine Georges[3,6,7,8], Megan Schuyler Moss[1,2], Alev Orfi[3,4], Christopher Roth[3], Dries Sels[3,4], Anirvan Sengupta[3,5], and •Agnes Valenti[3] — [1]Perimeter Institute for Theoretical Physics, Waterloo — [2]University of Waterloo, Waterloo — [3]Flatiron Institute, New York — [4]New York University, New York — [5]Rutgers University, New Jersey — [6]Collège de France, Paris — [7]École Polytechnique, Paris — [8]Université de Genève, Genève — [9]Universiteit Leiden, The Netherlands — [10]ETH Zürich, Switzerland

Neural quantum states (NQS) provide flexible parameterizations of quantum many-body wave-functions that serve as powerful tools for the ground-state search. At the same time, NQS offer something that standard machine-learning tasks and datasets fundamentally lack: a known underlying Hamiltonian and quantum-physics tools that allow direct examination of the encoded wavefunction. This additional structure makes NQS an interesting platform for probing the behavior of classical neural networks themselves. I will first show how pruning and scaling-law phenomena change when the learning task is the quantum wavefunction itself, and link effects depend on the underlying Hamiltonian. I will then discuss generalization and double descent through the lens of quantum observables, by analyzing how NQS fail at the interpolation threshold. Finally, I will discuss how these results relate back to practical consequences for training and architecture search in the context of the ground state search for quantum many-body systems.

SOE 17.2 Fri 10:00 GÖR/0226

The NN/QFT correspondence — •Ro Jefferson — Utrecht University

Exciting progress has recently been made in the study of neural networks by applying ideas and techniques from theoretical physics. In this talk, I will discuss a precise relation between quantum field theory and deep neural networks, the NN/QFT correspondence. In particular, I will go beyond the level of analogy by explicitly constructing the QFT corresponding to a class of networks encompassing both vanilla feedforward and recurrent architectures. The resulting theory closely resembles the well-studied O(N) vector model, in which the variance of the weight initializations plays the role of the 't Hooft coupling. In this framework, the Gaussian process approximation used in machine learning corresponds to a free field theory, and finite-width effects can be computed perturbatively in the ratio of depth to width, T/N. These provide corrections to the correlation length that controls the depth to which information can propagate through the network, and thereby sets the scale at which such networks are trainable by gradient descent. If time permits, I will discuss more recent work incorporating layerwise permutation symmetry. This analysis provides a non-perturbative description of networks at initialization, and opens several interesting avenues to the study of criticality in these models.

SOE 17.3 Fri 10:15 GÖR/0226

Online Learning Dynamics and Neural Scaling Laws for a Perceptron Classification Problem — •Yoon Thelge, Marcel Kuhn, and Bernd Rosenow — Institute for Theoretical Physics, University of Leipzig, 04103 Leipzig, Germany

Understanding neural scaling laws and emergence of power law generalisations remains a central challenge in learning dynamics. A natural setting for analysing this behaviour is the online-learning dynamics of a perceptron trained in a teacher*student scenario, where in the thermodynamic limit, the generalisation error exhibits characteristic power-law decay. In realistic classification problems, the teacher is a discrete classifier, while standard gradient-based training requires the student to have continuous outputs. Thus, in practically relevant settings the student is necessarily mismatched to the discrete teacher, a regime that is less well understood. We study this regime for a perceptron with a sign-activation

teacher and an error-function student. We derive coupled differential equations for the evolution of the relevant order parameters and verify them via numerical integration and SGD simulations. For fixed learning rates, the generalisation error converges to zero as a power-law with respect to the number of training examples with an exponent of -1/3. The onset of this asymptotic regime shifts with the learning rate, and the generalisation at the onset scales with exponent -1/2, motivating the use of learning-rate schedules to enhance the effective asymptotic decay.

SOE 17.4 Fri 10:30 GÖR/0226

Power-Law Correlations in Language: Criticality vs. Hierarchical Generative Structure — •Marcel Kühn[1,2], Max Staats[1,2], and Bernd Rosenow[2] — [1]ScaDS.AI Dresden/Leipzig, Germany — [2]Institute for Theoretical Physics, University of Leipzig, 04103 Leipzig, Germany

Natural language shows power-laws beyond Zipf: the mutual information between words as a function of separation — a two-point correlation — decays approximately as a power-law, a constraint for predictive language models. In autoregressive architectures like transformers, the softmax temperature of the output controls how sharply next-word probabilities concentrate, acting as a thermodynamic knob that might tune correlations. Since phase transitions are a well-known mechanism that generate such scale-free correlations, we ask whether the observed power-law mutual information requires tuning to a critical softmax temperature. Analyzing a Markov (bigram) model, we show that, in a large-system limit, power-law mutual information emerges only at a fine-tuned critical temperature, below correlations decay exponentially. Motivated by the fact that faithful language models must go beyond bigrams and that hierarchical generative processes introducing long range interactions are more representative, we analyze an autoregressive model that perfectly emulates a specific probabilistic context-free grammar. We demonstrate that simple versions of this model preserve power-law mutual information without temperature fine-tuning, and we discuss the generality of this result for variants of the model in which deviations from the grammatical rules may occur.

SOE 17.5 Fri 10:45 GÖR/0226

Dynamics of neural scaling laws in random feature regression — •Jakob Kramp[1,2], Javed Lindner[1,2], and Moritz Helias[1,2] — [1]Institute for Advanced Simulation (IAS-6), Computational and Systems Neuroscience, Jülich Research Centre, Jülich, Germany — [2]Department of Physics, RWTH Aachen University, Aachen, Germany

Training large neural networks reveals signs of universality that hold across architectures. This holds also for overparameterized networks which converge to effective descriptions in terms of Gaussian process regression. Those simplified models, already show one ingredient of universality in form of neural scaling laws. An important ingredient are power-law distributed principal component spectra of the training data.

Past work has therefore studied the dynamics of deterministic gradient flow in linear regression with and without consideration of power-law distributed spectra. Previously, dynamics of gradient flow with power law data in a type of linear random feature model were able to mimic effects of feature learning. Our work differs from the former by presenting an approach that holds for Bayesian inference on Gaussian processes obtained by stochastic Langevin training as well as for deterministic gradient flow with or without regularization by weight decay. We obtain interpretability from an effective mean-field theory that requires fewer order parameters than previous works.

15 min. break

Invited Talk SOE 17.6 Fri 11:15 GÖR/0226

Creativity in generative AI — •matthieu wyart — JHU & EPFL

Is AI creative? Generative AI such as chatGPT or diffusion models can create new texts or images from a finite training set of examples. I will argue that AI can achieve this magical by learning how compose observed low-level elements into a new whole. I will discuss the type of correlations the model can exploit to do so, how many data are needed for that, and how it relates to a hierarchical construction of latent variables. The analysis is based on the introduction of synthetic languages, and comparison with experiments performed on modern AI architectures trained on real text and images.

SOE 17.7 Fri 11:45 GÖR/0226

Understanding Generative Models via Interactions — •Claudia Merger[1,2,3], Alexandre Rene[2,4], Kirsten Fischer[2,3], Peter Bouss[2,3], Sandra Nestler[2,3], David Dahmen[2], Carsten Honerkamp[3], Moritz Helias[2,3], and Sebastian Goldt[1] — [1]SISSA, Trieste, Italy — [2]Jülich Research Centre, Jülich, Germany — [3]RWTH Aachen University, Aachen, Germany — [4]University of Ottawa, Ottawa, Canada

Generative models have become remarkably powerful at reproducing complex data distributions. They can infer the characteristic statistics of a system from comparatively small datasets and even generate new, realistic samples. Yet, our understanding of what these models learn remains limited: which statistics do they capture, and how accurately? To address the first question, we translate the statistics learned by generative models into a central concept of statistical physics: interactions between degrees of freedom that describe how pairs, triplets, and higher-order groups coact to produce the observed statistics of a system. Using invertible neural networks, we extract these interactions directly from trained models, providing a microscopic description of their learned data structure. To assess how accurately these interactions are learned, we use an analytic theory of diffusion models that predicts the precision with which pairwise interactions can be inferred from finite datasets, quantifying how generalization depends on sample size, data hierarchy, and regularization. Together, these results provide a framework grounded in statistical physics to interpret and predict the behavior of modern generative models.

SOE 17.8 Fri 12:00 GÖR/0226

From Kernels to Features: A Multi-Scale Adaptive Theory of Feature Learning — •Javed Lindner[1,2], Noa Rubin[5], Kirsten Fischer[1,6], David Dahmen[1], Inbar Seroussi[4], Zohar Ringel[5], Michael Krämer[3], and Moritz Helias[1,2] — [1]Institute for Advanced Simulation (IAS-6), Computational and Systems Neuroscience, Jülich Research Centre, Jülich, Germany — [2]Department of Physics, RWTH Aachen University, Aachen, Germany — [3]Institute for Theoretical Particle Physics and Cosmology, RWTH Aachen University, Aachen, Germany — [4]Department of Applied Mathematics, School of Mathematical Sciences, Tel-Aviv University, Tel-Aviv, Israel — [5]he Racah Institute of Physics, The Hebrew University of Jerusalem, Jerusalem, Israel — [6]RWTH Aachen University, Aachen, Germany

Feature learning in neural networks is crucial for their expressive power and inductive biases, moti- vating various theoretical approaches. Some ap- proaches describe network behavior after train- ing through a change in kernel scale from initial- ization, resulting in a generalization power com- parable to a Gaussian process. Conversely, in other approaches training results in the adapta- tion of the kernel to the data, involving directional changes to the kernel. The relationship and re- spective strengths of these two views have so far remained unresolved. This work presents a theo- retical framework of multi-scale adaptive feature learning bridging these two views. Using methods from statistical mechanics, we derive analytical expressions for network output statistics which are valid across scaling regimes and in the continuum between them.

SOE 17.9 Fri 12:15 GÖR/0226

Statistical physics of deep learning: Optimal learning of a multi-layer perceptron near interpolation — Jean Barbier[1], Francesco Camilli[1], Minh-Toan Nguyen[1], Mauro Pastore[1], and •Rudy Skerk[2] — [1]The Abdus Salam International Centre for Theoretical Physics, Strada Costiera 11, 34151 Trieste, Italy — [2]International School for Advanced Studies, Via Bonomea 265, 34136 Trieste, Italy

We address a long-standing question in statistical physics by analysing the supervised learning of a multi-layer perceptron, beyond narrow models and kernel methods. Crucially, (i) the width scales with input dimension, making the model more prone to feature learning than ultra-wide networks and more expressive than narrow ones; and (ii) we work in the interpolation regime where trainable parameters and data are comparable, forcing task-specific adaptation. In a matched teacher-student setting we establish the fundamental limits for learning random deep-network targets and identify the sufficient statistics that an optimally trained network acquires as data increases. A rich phenomenology appears with multiple learning transitions: with enough data optimal performance arises via model "specialisation", yet practical algorithms can be trapped in theory-predicted suboptimal solutions. Specialisation occurs inhomogeneously across layers, propagating from shallow towards deep ones, but also across neurons in each layer. The Bayesian-optimal analysis thus clarifies how depth, nonlinearity and finite (proportional) width shape feature learning, with implications beyond this idealised setting.

SOE 17.10 Fri 12:30 GÖR/0226

Phase Transitions as Rank Transitions: Connecting Data Complexity and Cascades of Phase Transitions in analytically tractable Neural Network Models — •Björn Ladewig, Ibrahim Talha Ersoy, and Karoline Wiesner — Institute of Physics and Astronomy, University of Potsdam, Germany

Tuning the L2-regularization strength in neural networks can result in a cascade of (zero-temperature) phase transitions between regimes of increasing accuracy. This phenomenology was previously numerically observed and linked to a basin structure of the error landscape formed by the underlying data [1]. At the level of analytically tractable models, we (i) establish the existence of cascades of transitions for those models, (ii) give meaning to the transitions in terms of the ordered onset of "learned eigendirections" of the underlying data distribution; and (iii) link the phase transitions and corresponding accuracy regimes to saddle points of the error landscape.

[1] I. Talha Ersoy and Karoline Wiesner. Exploring l2-phase transitions on error landscapes. In ICML, Workshop on High-dimensional Learning Dynamics 2025. https://openreview.net/forum?id=AkQNtAw09u

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Overview of Invited Talks and Sessions

(Lecture halls HSZ/0003, HSZ/0101, HSZ/0103, HSZ/0105, CHE/0089, and CHE/0091; Poster P1 and P4)

Invited Talks

TT 27.1	Tue	9:30–10:00	HSZ/0105	**Simulating high-temperature superconductivity in a triangular moiré lattice** — •Kin Fai Mak

Topical Talks in Focus Sessions

Topical Talks of the Focus Session "New Routes to Localization and Quantum Non-Ergodicity" (joint session TT/DY)

TT 1.1	Mon	9:30–10:00	HSZ/0003	**Eigenstate thermalization in thermal first-order phase transitions** — •Maksym Serbyn
TT 1.2	Mon	10:00–10:30	HSZ/0003	**Stabilizing Floquet orders to infinite time** — •Anushya Chandran
TT 1.3	Mon	10:30–11:00	HSZ/0003	**Dynamical landscape of out of equilibrium emergent lattice gauge theories in two dimensions** — •Nilotpal Chakraborty
TT 1.4	Mon	11:15–11:45	HSZ/0003	**Interference, topology, and new Hilbert-space routes to quantum non-ergodicity** — •Yi-Ping Huang
TT 1.5	Mon	11:45–12:15	HSZ/0003	**Fock-space cages and their spectral signatures** — •Cheryne Jonay

Topical Talks of the Focus Session "Tunable Correlations in van der Waals Quantum Materials" (joint session TT/DS/HL)

TT 12.1	Mon	15:00–15:30	HSZ/0003	**Charge confinement in twisted bilayer graphene** — •Christoph Stampfer
TT 12.2	Mon	15:30–16:00	HSZ/0003	**Tuning Coulomb interactions and Hubbard bands in 1T-TaS_2** — •Anna Galler
TT 12.3	Mon	16:00–16:30	HSZ/0003	**Optical signatures of interlayer electron coherence in a bilayer semiconductor** — •Nadine Leisgang
TT 12.4	Mon	16:45–17:15	HSZ/0003	**Faithful modeling of quantum geometry and electronic correlations in van der Waals heterostructures** — •Ammon Fischer
TT 12.5	Mon	17:15–17:45	HSZ/0003	**Mesoscale Atomic Engineering in a Crystal Lattice** — •Julian Klein

Topical Talks of the Focus Session "Relaxation Timescales in Open Quantum Systems" (joint session TT/DY)

TT 18.1	Mon	15:00–15:30	CHE/0089	**Markovian and non-Markovian approaches to quantum relaxation** — •Heinz-Peter Breuer
TT 18.2	Mon	15:30–16:00	CHE/0089	**Asymptotic relaxation in quantum Markovian dynamics** — •Susana Huelga
TT 18.3	Mon	16:00–16:30	CHE/0089	**Floquet engineering of open quantum Systems** — •André Eckardt
TT 18.4	Mon	16:45–17:15	CHE/0089	**Nonequilibrium thermodynamics of time-dependent quantum transport** — •Janine Splettstoesser
TT 18.5	Mon	17:15–17:45	CHE/0089	**Connecting time-nonlocal and time-local quantum master equations** — •Maarten Wegewijs

Topical Talks of the Focus Session "Quantum Sensing with Solid State Spin defects" (joint session TT/MA)

TT 24.1	Tue	9:30–10:00	HSZ/0003	**Exploring nanoscale van der Waals magnetism using single spin microscopy** — •Patrick Maletinsky
TT 24.2	Tue	10:00–10:30	HSZ/0003	**Optically addressable spin defects in two-dimensional materials** — •Vladimir Dyakonov
TT 24.3	Tue	10:30–11:00	HSZ/0003	**Nitrogen vacancy centers in diamond as novel sensing and imaging tool for magnetic nanostructures, in life science and chemistry** — •Elke Neu-Ruffing
TT 24.4	Tue	11:15–11:45	HSZ/0003	**Electron spin, nuclear spin, and optical properties of transition-metal defects in silicon carbide with perspectives for quantum technologies** — •Guido Burkard
TT 24.5	Tue	11:45–12:15	HSZ/0003	**Statics and dynamics of complex magnetic states in microstructures** — •Aurore Finco

Topical Talks of the Focus Session "Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects" (joint session TT/DS/MA)

TT 39.1	Wed	9:30–10:00	HSZ/0003	**Unconventional Superconductivity in Infinite-layer Samarium Nickelates** — •Danfeng Li
TT 39.2	Wed	10:00–10:30	HSZ/0003	**Recent insights into infinite-layer nickelate heterostructures from x-ray spectroscopy** — •Eva Benckiser
TT 39.3	Wed	10:30–11:00	HSZ/0003	**Theory of infinite-layer nickelate superconductors** — •Karsten Held
TT 39.4	Wed	11:15–11:45	HSZ/0003	**Disorder and distortions: what electrons tell us about nickelate superconductivity** — •Berit H. Goodge
TT 39.5	Wed	11:45–12:15	HSZ/0003	**Superconducting gap structure and bosonic mode in $La_2PrNi_2O_7$ thin films at ambient pressure** — •Hai-Hu Wen

Topical Talks of the German-French Focus Session "Superconducting Junctions and Quantum Circuits"

TT 50.1	Wed	15:00–15:30	HSZ/0003	**Josephson Quantum Tunneling at Odd Parity** — •Julia S. Meyer
TT 50.2	Wed	15:30–16:00	HSZ/0003	**Superconducting qubits and amplifiers resilient to Tesla-scale magnetic fields** — •Ioan Pop
TT 50.3	Wed	16:00–16:30	HSZ/0003	**Josephson metamaterials as near-quantum-limited microwave amplifiers** — •Nicolas Roch
TT 50.4	Wed	16:45–17:15	HSZ/0003	**Second Order Topological Insulators probed with mesoscopic physics** — •Sophie Gueron
TT 50.5	Wed	17:15–17:45	HSZ/0003	**Proximity superconductivity in chiral Kagome antiferromagnets** — •Piet Brouwer

Topical Talks of the Focus Session "High-Temperature Superconductivity in Hydride Materials at High Pressures" (joint session TT/DS)

TT 80.1	Thu	15:00–15:30	HSZ/0003	**Computational searches for conventional high temperature superconductivity** — •Chris Pickard
TT 80.2	Thu	15:30–16:00	HSZ/0003	**High-pressure synthesis of hydrides and their characterisation by single-crystal X-ray diffraction** — •Natalia Dubrovinskaia
TT 80.3	Thu	16:00–16:30	HSZ/0003	**Electrical Transport Studies in bulk and thin-film hydride high-temperature superconductors** — •Sven Friedemann
TT 80.4	Thu	16:45–17:15	HSZ/0003	**Near room-temperature conventional superconductivity in hydrogen-rich compounds at high pressures: Experimental evidences** — •Vasily Minkov
TT 80.5	Thu	17:15–17:45	HSZ/0003	**Predictive T_c Calculations in Hydride Superconductors** — •Christoph Heil

Invited Talks of the joint Symposium SKM Dissertation Prize 2026 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	HSZ/0002	**Stochastic-Calculus Approach to Non-equilibrium Statistical Physics** — •Cai Dieball
SYSD 1.2	Mon	10:00–10:30	HSZ/0002	**Nonuniform magnetic spin textures for sensing, storage and computing applications** — •Sabri Koraltan
SYSD 1.3	Mon	10:30–11:00	HSZ/0002	**Anomalous Quantum Oscillations beyond Onsager's Fermi Surface Paradigm** — •Valentin Leeb
SYSD 1.4	Mon	11:00–11:30	HSZ/0002	**Coherent Control Schemes for Semiconductor Quantum Systems** — •Eva Schöll
SYSD 1.5	Mon	11:30–12:00	HSZ/0002	**On stochastic thermodynamics under incomplete information: Thermodynamic inference from Markovian events** — •Jann van der Meer

Invited Talks of the joint Symposium Designing Quantum Materials with Light: From Floquet to Cavity Engineering (SYFC)

See SYFC for the full program of the symposium.

SYFC 1.1	Mon	9:30–10:00	HSZ/AUDI	**Subcycle videography of strong-field controlled band structures** — •Rupert Huber
SYFC 1.2	Mon	10:00–10:30	HSZ/AUDI	**Engineering Quantum Materials through Structured Cavity Vacuum Fluctuations** — •Angel Rubio
SYFC 1.3	Mon	10:30–11:00	HSZ/AUDI	**Floquet engineering of quantum materials: from semiconductors to semimetals** — •Shuyun Zhou
SYFC 1.4	Mon	11:15–11:45	HSZ/AUDI	**(Quantum) Light Control of Materials** — •Dante Kennes
SYFC 1.5	Mon	11:45–12:15	HSZ/AUDI	**Lightwave-driven electrons in a Floquet topological insulator** — •Peter Hommelhoff

Invited Talks of the joint Symposium Fluids with Broken Time-Reversal Symmetry: Odd/Hall Viscosity between Active Matter and Electron Flows (SYBS)

See SYBS for the full program of the symposium.

SYBS 1.1	Tue	9:30–10:00	HSZ/AUDI	**Odd viscosity in three-dimensional fluids: flows, wakes, and eddies** — •Tali Khain
SYBS 1.2	Tue	10:00–10:30	HSZ/AUDI	**Odd viscosity in two-dimensional hydrodynamic electron transport** — •Igor Gornyi
SYBS 1.3	Tue	10:30–11:00	HSZ/AUDI	**Odd slip on chiral active surfaces** — •Andrej Vilfan
SYBS 1.4	Tue	11:15–11:30	HSZ/AUDI	**Parity-odd transport in electron fluids** — •Johanna Erdmenger
SYBS 1.5	Tue	11:30–11:45	HSZ/AUDI	**Curved Odd Elasticity** — •Piotr Surówka

Invited Talks of the joint Symposium Interacting Degrees of Freedom in Ultrathin Quantum Films (SYQF)

See SYQF for the full program of the symposium.

SYQF 1.1	Fri	9:30–10:00	HSZ/AUDI	**Exciton dressing by extreme nonlinear magnons in a layered semiconductor** — •Geoffrey M. Diederich
SYQF 1.2	Fri	10:00–10:30	HSZ/AUDI	**A tale of demons and decay in two-dimensional (alter)magnets** — •Alexander Mook
SYQF 1.3	Fri	10:30–11:00	HSZ/AUDI	**Magnetism, light and matter - Role of excitons in two-dimensional magnets** — •Florian Dirnberger
SYQF 1.4	Fri	11:15–11:45	HSZ/AUDI	**Advantages and challanges of resonance Raman scattering with infrared excitation energy** — •Leonetta Baldassarre
SYQF 1.5	Fri	11:45–12:15	HSZ/AUDI	**Shining light on 2D antiferromagnets** — •Dmytro Afanasiev

Sessions

TT 1.1–1.5	Mon	9:30–12:15	HSZ/0003	**Focus Session: New Routes to Localization and Quantum Non-Ergodicity I (joint session TT/DY)**
TT 2.1–2.11	Mon	9:30–12:30	HSZ/0101	**Quantum-Critical Phenomena (joint session TT/DY)**
TT 3.1–3.5	Mon	9:30–10:45	HSZ/0103	**Correlated Electrons: Electronic Structure Calculations**
TT 4.1–4.12	Mon	9:30–12:45	HSZ/0105	**Graphene, 2D and Twisted Materials**
TT 5.1–5.11	Mon	9:30–12:30	CHE/0089	**Superconductivity: Sample Preparation and Characterization**
TT 6.1–6.6	Mon	9:30–11:00	CHE/0091	**Topological Superconductors**
TT 7.1–7.9	Mon	9:30–12:00	POT/0351	**Surface Magnetism and Topological Insulators (joint session MA/TT)**
TT 8.1–8.1	Mon	9:30–10:15	TRE/PHYS	**Topical Talk Wulfhekel (joint session O/TT)**
TT 9.1–9.7	Mon	10:30–12:30	TRE/MATH	**2D Materials: Electronic structure, excitations, etc. I (joint session O/HL/TT)**
TT 10.1–10.7	Mon	11:00–12:45	HSZ/0103	**Correlated Electrons: Other Theoretical Topics**
TT 11.1–11.5	Mon	11:15–12:30	CHE/0091	**$PtBi_2$**
TT 12.1–12.7	Mon	15:00–18:15	HSZ/0003	**Focus Session: Tunable Correlations in van der Waals Quantum Materials I (joint session TT/DS/HL)**
TT 13.1–13.13	Mon	15:00–18:30	HSZ/0101	**Correlated Electrons: Method Development I**
TT 14.1–14.12	Mon	15:00–18:15	HSZ/0103	**Superconductivity: Properties and Electronic Structure**
TT 15.1–15.13	Mon	15:00–18:30	HSZ/0105	**Topology: Majorana Physics**
TT 16.1–16.11	Mon	15:00–17:45	HSZ/0204	**2D Materials beyond graphene: Growth, structure and substrate interaction (joint session O/HL/TT)**
TT 17.1–17.11	Mon	15:00–18:30	BEY/0245	**Quantum Manybody Systems (joint session QI/TT)**
TT 18.1–18.6	Mon	15:00–18:00	CHE/0089	**Focus Session: Relaxation Timescales in Open Quantum Systems (joint session TT/DY)**
TT 19.1–19.9	Mon	15:00–17:30	CHE/0091	**Focus Session: New Routes to Localization and Quantum Non-Ergodicity II (joint session TT/DY)**
TT 20.1–20.6	Mon	15:00–16:30	POT/0081	**2D Materials II – Electronic and Transport Properties (joint session HL/TT)**
TT 21.1–21.11	Mon	15:00–18:00	POT/0151	**Electron Theory of Magnetism and Correlations (joint session MA/TT)**
TT 22.1–22.37	Mon	18:00–20:00	P1	**Superconductivity – Poster I**
TT 23.1–23.35	Mon	18:00–20:00	P1	**Correlated Electrons – Poster I**
TT 24.1–24.7	Tue	9:30–12:45	HSZ/0003	**Focus Session: Quantum Sensing with Solid State Spin defects I (joint session TT/MA)**
TT 25.1–25.11	Tue	9:30–12:30	HSZ/0101	**f-Electron Systems**
TT 26.1–26.10	Tue	9:30–12:15	HSZ/0103	**Correlated Magnetism – Frustrated Systems**
TT 27.1–27.4	Tue	9:30–10:45	HSZ/0105	**Focus Session: Tunable Correlations in van der Waals Quantum Materials II (joint session TT/DS/HL)**
TT 28.1–28.12	Tue	9:30–12:45	CHE/0089	**Superconducting Electronics: SQUIDs and other Josephson Circuits and Components**
TT 29.1–29.12	Tue	9:30–12:45	CHE/0091	**Unconventional Superconductors**
TT 30.1–30.7	Tue	9:30–11:30	POT/0151	**Caloric Effects in Ferromagnetic Materials (joint session MA/TT)**
TT 31.1–31.11	Tue	9:30–12:30	POT/0361	**Frustrated Magnets I (joint session MA/TT)**
TT 32.1–32.10	Tue	10:00–12:45	POT/0051	**Nanomechanical systems (joint session HL/TT)**
TT 33.1–33.6	Tue	11:00–12:30	HSZ/0105	**Correlated Magnetism – Dynamics and Spectroscopy**
TT 34	Tue	14:00–15:30	HSZ/0101	**Members' Assembly**
TT 35.1–35.6	Tue	14:00–15:30	POT/0151	**Cooperative Phenomena: Spin Structures and Magnetic Phase Transitions (joint session MA/TT)**
TT 36.1–36.6	Tue	14:00–15:30	POT/0361	**Weyl Semimetals (joint session MA/TT)**
TT 37.1–37.21	Tue	14:00–16:00	P2	**Ultrafast electron dynamics at surface and interfaces – Poster (joint session O/TT)**
TT 38.1–38.4	Tue	14:00–16:00	P2	**Topology and symmetry protected materials & Topological insulators – Poster (joint session O/TT)**
TT 39.1–39.7	Wed	9:30–12:45	HSZ/0003	**Focus Session: Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects I (joint session TT/DS/MA)**
TT 40.1–40.4	Wed	9:30–10:30	HSZ/0101	**Focus Session: Quantum Sensing with Solid State Spin defects II (joint session TT/HL/MA)**
TT 41.1–41.11	Wed	9:30–12:30	HSZ/0103	**Topological Semimetals**
TT 42.1–42.12	Wed	9:30–12:45	HSZ/0105	**Other Transport Topics**
TT 43.1–43.12	Wed	9:30–12:45	CHE/0089	**Superconducting Electronics: Qubits**
TT 44.1–44.12	Wed	9:30–12:45	CHE/0091	**Nonequilibrium Quantum Systems I (joint session TT/DY)**
TT 45.1–45.12	Wed	9:30–12:45	HÜL/S186	**Many-body Systems: Equilibration, Chaos, and Localization (joint session DY/TT)**

TT 46.1–46.11	Wed	9:30–12:45	POT/0112	**Spin Transport and Orbitronics, Spin-Hall Effects I (joint session MA/TT)**
TT 47.1–47.12	Wed	9:30–12:45	POT/0361	**Frustrated Magnets II (joint session MA/TT)**
TT 48.1–48.8	Wed	10:30–12:30	TRE/MATH	**2D Materials: Electronic structure, excitations, etc. II (joint session O/HL/TT)**
TT 49.1–49.8	Wed	10:45–12:45	HSZ/0101	**Correlated Electrons: Charge Order**
TT 50.1–50.8	Wed	15:00–18:30	HSZ/0003	**German-French Focus Session: Superconducting Junctions and Quantum Circuits**
TT 51.1–51.12	Wed	15:00–18:15	HSZ/0101	**Correlated Electrons: Method Development II**
TT 52.1–52.6	Wed	15:00–16:30	HSZ/0103	**Heavy Fermions**
TT 53.1–53.9	Wed	15:00–17:30	HSZ/0105	**Nonequilibrium Quantum Systems II (joint session TT/DY)**
TT 54.1–54.11	Wed	15:00–17:45	HSZ/0204	**Graphene: Electronic structure, excitations, etc. (joint session O/TT)**
TT 55.1–55.11	Wed	15:00–17:45	HSZ/0401	**Topology and symmetry protected materials & Topological insulators (joint session O/HL/TT)**
TT 56.1–56.13	Wed	15:00–18:30	CHE/0089	**Superconductivity: Theory I**
TT 57.1–57.12	Wed	15:00–18:15	CHE/0091	**Correlated Magnetism – Kagome Systems**
TT 58.1–58.5	Wed	15:00–16:15	POT/0006	**Quantum Transport and Quantum Hall effects (joint session HL/TT)**
TT 59.1–59.7	Wed	15:00–17:15	POT/0081	**2D Materials V – Magnetic, spintronic, and topological properties (joint session HL/TT)**
TT 60.1–60.10	Wed	15:00–18:00	POT/0112	**Spintronics (other effects) (joint session MA/TT)**
TT 61.1–61.14	Wed	15:00–17:00	P4	**Topology – Poster**
TT 62.1–62.12	Wed	15:00–17:00	P4	**Correlated Electrons – Poster II**
TT 63.1–63.15	Wed	15:00–18:00	P5	**Quantum Dynamics and Many-body Systems – Poster (joint session DY/TT)**
TT 64.1–64.6	Wed	16:45–18:15	HSZ/0103	**BKT Physics**
TT 65.1–65.7	Wed	18:00–20:00	P2	**2D materials: Stacking and heterostructures – Poster (joint session O/TT)**
TT 66.1–66.23	Wed	18:00–20:00	P2	**2D Materials: Electronic structure, excitations, etc. – Poster (joint session O/TT)**
TT 67.1–67.6	Wed	18:00–20:00	P2	**2D Materials beyond graphene: Growth, structure and substrate interaction – Poster (joint session O/TT)**
TT 68.1–68.9	Wed	18:00–20:00	P2	**Graphene: Electronic structure, excitations, etc. – Poster (joint session O/TT)**
TT 69.1–69.11	Thu	9:30–12:30	HSZ/0003	**Focus Session: Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects II (joint session TT/DS/MA)**
TT 70.1–70.5	Thu	9:30–10:45	HSZ/0101	**Correlated Electrons: Method Development III**
TT 71.1–71.7	Thu	9:30–11:15	HSZ/0103	**Ultrafast Phenomena**
TT 72.1–72.9	Thu	9:30–12:00	HSZ/0105	**Correlated Magnetism – Spin Liquids I**
TT 73.1–73.12	Thu	9:30–12:45	CHE/0089	**Superconductivity: Tunneling and Josephson Junctions**
TT 74.1–74.12	Thu	9:30–12:45	CHE/0091	**Topological Insulators**
TT 75.1–75.12	Thu	9:30–12:45	HÜL/S186	**Many-body Quantum Dynamics I (joint session DY/TT)**
TT 76.1–76.8	Thu	9:30–13:00	POT/0151	**Focus Session: Curvilinear magnetism: Magnetics with nanoscale curved geometries (joint session MA/TT)**
TT 77.1–77.1	Thu	9:30–10:15	TRE/PHYS	**Topical Talk Bibes (joint session O/TT)**
TT 78.1–78.7	Thu	11:00–12:45	HSZ/0101	**Quantum Dots and Point Contacts (joint session TT/HL)**
TT 79.1–79.5	Thu	11:30–12:45	HSZ/0103	**Correlated Magnetism – Transport**
TT 80.1–80.9	Thu	15:00–18:45	HSZ/0003	**Focus Session: High-Temperature Superconductivity in Hydride Materials at High Pressures (joint session TT/DS)**
TT 81.1–81.8	Thu	15:00–17:15	HSZ/0101	**Correlated Electrons: Other Materials**
TT 82.1–82.6	Thu	15:00–16:30	HSZ/0103	**Cryogenic Detectors and Sensors**
TT 83.1–83.13	Thu	15:00–18:30	HSZ/0105	**Topology: Quantum Hall Systems**
TT 84.1–84.11	Thu	15:00–17:45	HSZ/0204	**2D Materials: Electronic structure, excitations, etc. III (joint session O/HL/TT)**
TT 85.1–85.8	Thu	15:00–17:15	CHE/0089	**Superconductivity: Yu-Shiba-Rusinov and Andreev Physics**
TT 86.1–86.7	Thu	15:00–16:45	CHE/0091	**Correlated Magnetism – Spin Liquids II**
TT 87.1–87.6	Thu	15:00–16:30	HÜL/S186	**Many-body Quantum Dynamics II (joint session DY/TT)**
TT 88.1–88.8	Thu	15:00–17:00	POT/0361	**Spin Transport and Orbitronics, Spin-Hall Effects II (joint session MA/TT)**
TT 89.1–89.4	Thu	16:45–17:45	HSZ/0103	**Cryotechnique: Refrigeration**
TT 90.1–90.6	Thu	17:00–18:30	CHE/0091	**Quantum Impurities and Kondo Physics**
TT 91.1–91.4	Thu	17:30–18:30	HSZ/0101	**Superconductivity: Theory II**
TT 92.1–92.19	Thu	18:00–20:00	P4	**Transport – Poster**
TT 93.1–93.19	Thu	18:00–20:00	P4	**Superconductivity – Poster II**
TT 94.1–94.9	Fri	9:30–12:00	HSZ/0101	**Correlated Magnetism – Low-Dimensional Systems**

TT 95.1–95.8	Fri	9:30–11:45	HSZ/0103	**Fe-based Superconductors**
TT 96.1–96.12	Fri	9:30–12:30	HSZ/0401	**2D Materials: Stacking and heterostructures (joint session O/HL/TT)**
TT 97.1–97.9	Fri	9:30–12:00	CHE/0089	**Superconducting Diodes and Ratchets**
TT 98.1–98.8	Fri	9:30–11:45	CHE/0091	**Altermagnets**
TT 99.1–99.11	Fri	9:30–12:45	HÜL/S186	**Quantum Chaos and Coherent Dynamics (joint session DY/TT)**

Members' Assembly of the Low Temperature Physics Division

Tuesday 14:00–15:30 HSZ/0101

- Report
- Elections
- Outlook 2026
- Miscellaneous

Sessions

– Invited, Topical, Contributed Talks, and Posters –

TT 1: Focus Session: New Routes to Localization and Quantum Non-Ergodicity I (joint session TT/DY)

This session explores how quantum many-body systems can fail to thermalize through mechanisms that extend beyond conventional many-body localization. Recent work has discovered new mechanisms that lead to non-ergodic behavior, including Hilbert-space fragmentation, disorder-free localization, and confinement effects that arise from destructive interference in Fock space. At the same time, experiments with ultracold atoms, trapped ions, Rydberg platforms, and superconducting qubits directly reveal many-body scars, slow relaxation, and unusual transport. This session highlights these developments and identifies the central open questions that are now driving the field forward.

Coordinators: Roderich Moessner (MPI PKS Dresden), Frank Pollmann (TU München)

Time: Monday 9:30–12:15 Location: HSZ/0003

Topical Talk TT 1.1 Mon 9:30 HSZ/0003

Eigenstate thermalization in thermal first-order phase transitions — •Maksym Serbyn — IST Austria, Am Campus 1, 3400 Klosterneuburg

In my talk I will discuss the fate of eigenstates in quantum systems in vicinity of thermal first order phase transition. The eigenstate thermalization hypothesis (ETH) posits how isolated quantum many-body systems thermalize, assuming that individual eigenstates at the same energy density have identical expectation values of local observables in the limit of large systems. In my talk I will show that ETH requires generalization in the presence of thermal first-order phase transitions. I will argue that for energies in the vicinity of the thermal phase transition, eigenstate expectation values do not need to converge to the same thermal value. The system has a regime with coexistence of two classes of eigenstates corresponding to the two branches with distinct expectation values at the same energy density, and another regime with Schrodinger-cat-like eigenstates that are inter-branch superpositions; these two regimes are separated by an eigenstate phase transition. I will also discuss potential extensions of these results to more physical models, and outline how the special structure of eigenstates near first order phase transition can be probed via quench dynamics.

Topical Talk TT 1.2 Mon 10:00 HSZ/0003

Stabilizing Floquet orders to infinite time — •Anushya Chandran[1], Shreyas Raman[2], Robin Schäfer[3], and Alicia Kollàr[4] — [1]Boston University, Boston, USA — [2]Boston University, Boston, USA — [3]Helmholtz-Zentrum Berlin, Berlin, Germany — [4]University of Maryland, College Park, USA

Floquet engineering, in which the properties of a quantum system are modified through the application of strong periodic drives, is an indispensable tool in atomic and condensed matter systems. It enables quantum simulation, the dynamic stabilization of unstable states, and the realization of exotic topological order and time crystals. However, it is inevitably limited by intrinsic heating processes, so that the engineered states are, at best, pre-thermal. I will describe a general-purpose dissipative scheme that autonomously cools a strongly driven system to close to a desired Floquet engineered state. I will demonstrate this stabilization in a driven many-body spin chain, that either spontaneously breaks a symmetry or exhibits discrete time-crystalline order in the steady state.

Topical Talk TT 1.3 Mon 10:30 HSZ/0003

Dynamical landscape of out of equilibrium emergent lattice gauge theories in two dimensions — •Nilotpal Chakraborty — University of Cambridge

Many-body models with local constraints, such as dimer, ice or generally quantum link type models often are described as emergent gauge theories. I will describe a range of recent results, comprising classical and quantum dynamics of different kind, highlighting the rich dynamical phenomenology present in these models. In line with the session's topic, I will focus more on the two-dimensional U(1) quantum link model, and highlight its potential as a new route toward localisation and non-ergodicity in the absence of quenched disorder. In doing so, I will also present spectral signatures of such localization. Finally, I will end by discussing possibilities of realising the different constrained models and their dynamics in quantum simulators, for which there appears to be palpable current interest.

15 min. break

Topical Talk TT 1.4 Mon 11:15 HSZ/0003

Interference, topology, and new Hilbert-space routes to quantum non-ergodicity — •Yi-Ping Huang[1,2,3] and Tao-Lin Tan[1] — [1]Department of Physics, National Tsing Hua University, Hsinchu 30013, Taiwan — [2]Physics Division, National Center for Theoretical Sciences, Taipei 10617, Taiwan — [3]Institute of Physics, Academia Sinica, Taipei 115, Taiwan

A central challenge in nonequilibrium quantum physics is to understand why certain many-body systems fail to thermalize even in the absence of disorder or integrability. In this talk, I will outline a different perspective in which non-ergodicity is governed by hidden geometric structures in Hilbert space rather than by conventional real-space mechanisms. This viewpoint leads to the concept of interference-caged quantum many-body scars (ICQMBS), where exact many-body destructive interference confines eigenstates to small regions of the Fock-space graph. Remarkably, interference zeros and graph automorphisms emerge as universal organizing principles, revealing a class of topological ICQMBS whose robustness originates from local Fock-space topology rather than symmetries or constraints. This framework not only explains diverse non-ergodic phenomena from one-dimensional systems to two-dimensional gauge models but also provides new tools for systematically identifying them. I will end with a brief look at stabilizing QMBS through the lens of Kramers-Wannier duality, illustrating the challenges and possibilities that arise when studying QMBS under duality.

Topical Talk TT 1.5 Mon 11:45 HSZ/0003

Fock-space cages and their spectral signatures — •Cheryne Jonay — University of Ljubljana

Generic quantum many-body systems thermalize. Yet several mechanisms can prevent this, notable examples include integrability, many-body localization, Hilbert-space fragmentation, and scars. We will discuss a new mechanism of ergodicity breaking that arises from destructive interference in Fock space. This leads to exact eigenstates localized on polynomially many configurations within an exponentially large, fully connected Hilbert space sector. We call these states Fock-space cages. They emerge naturally in kinetically constrained models with chiral symmetry. We will present graph-theoretic methods to explicitly construct cages with support ranging from O(1) to O(L) sites, and examine how their dynamical signatures, such as return probabilities and magnetization, resist thermalization. Finally, we will explore the spectral statistics through the lens of chiral random matrix theory. The exponentially degenerate zero-energy manifold produces distinctive signatures, yet the agreement with random matrix predictions varies across energy scales - a direct consequence of localized and thermal eigenstates coexisting within the same Hilbert space sector. We will also probe the stability of these phenomena: the gap between the zero-energy manifold and the spectral bulk may give rise to protected slow dynamics.

TT 2: Quantum-Critical Phenomena (joint session TT/DY)

Time: Monday 9:30–12:30 Location: HSZ/0101

TT 2.1 Mon 9:30 HSZ/0101

Possible Quantum Criticality Tuned by Pressure in $CeVGe_3$ — Rong-Zhu Lin[1], Po-Yuan Cheng[1], Yusei Shimizu[2], Timothée Vasina[3], Daniel Braithwaite[3], Hanshang Jin[4], Peter Klavins[4], Valentin Taufour[4], and •Chien-Lung Huang[1] — [1]Department of Physics, National Cheng Kung University and Center for Quantum Frontiers of Research & Technology, Tainan 701, Taiwan — [2]International Research Center for Nuclear Materials Science, Institute for Materials Research (IMR-Oarai), Tohoku University, Ibaraki 311-1313, Japan — [3]Univ. Grenoble Alpes, CEA, Grenoble INP, IRIG, PHELIQS, 38000, Grenoble, France — [4]Department of Physics and Astronomy, University of California, Davis, California 95616, USA

In this work, we focus on the helical antiferromagnetic (AFM) $CeVGe_3$ to explore whether an AFM quantum critical point (QCP) can be approached. By performing resistivity measurements under pressure, we construct the pressure-temperature-field phase diagram and track the evolution of multiple field-induced phases. The AFM ordering temperature is suppressed at the critical pressure p_c = 0.7 GPa. The coefficient A in the temperature-dependent resistivity $\rho = \rho_0 + AT^2$ exhibits a maximum at p_c and gradually decreases at higher pressures, indicating enhanced electron-electron correlations near the critical point. These results reveal how the competition between Ruderman-Kittel-Kasuya-Yosida (RKKY) and Kondo interactions evolves under pressure, leading to a plausible pressure-induced QCP in $CeVGe_3$.

TT 2.2 Mon 9:45 HSZ/0101

Spin and charge criticality in the pseudogap two-impurity Anderson model — •Charlotte Beneke and Matthias Vojta — Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

The Kondo effect originates from spin screening of localized impurities by conduction electrons. This Kondo screening can be suppressed by a fermionic bath following a pseudogap (i.e. power-law) density of states, by inter-impurity interactions, or by coupling to multiple conduction channels. We investigate the two-impurity Anderson model in various limits, and establish mappings to known Kondo and Anderson models. This leads to rich phase diagrams with Kondo-breakdown transitions of distinct universality classes giving rise to non-Fermi-liquid behavior. We analyze the phase diagram, and critical exponents of the pseudogap two-impurity Anderson model in the particle-hole symmetric, SU(2)-invariant case using perturbative renormalization-group techniques. We recover the transitions of the pseudogap single-impurity Anderson model, and find additional Kondo-breakdown quantum transitions to inter-impurity singlet-, triplet- and charge-ordered phases. At the quantum critical points, superconducting-pairing susceptibilities can be enhanced depending on the type of spin- and charge criticality. We discuss connections to heavy-fermion systems and two-quantum-dot realizations where quantum dots act as tunable magnetic impurities.

TT 2.3 Mon 10:00 HSZ/0101

Stability of Deconfined Quantum Critical Points Coupled to Quantum Phonons — •Anton Romen[1,2], Josef Willsher[1,2,3], David Hofmeier[4], Johannes Knolle[1,2,5], and Michael Knap[1,2] — [1]Technical University of Munich, Garching, Germany — [2]Munich Center for Quantum Science and Technology, München, Germany — [3]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [4]University of Southern Denmark, Odense M, Denmark — [5]Imperial College London, London, United Kingdom

Deconfined quantum criticality (DQC) describes continuous transitions beyond the Landau-Ginzburg paradigm. A typical example is the VBS-Néel transition in frustrated antiferromagnets. Since the VBS order parameter breaks lattice symmetries, it can couple to lattice distortions (phonons). Field-theory (PRB 110, 125130 (2024)) predicts that static lattice vibrations induce strong first-order character. A full quantum treatment, however, indicates that DQC survives above a critical phonon frequency. In this work, we provide a detailed study on the stability of 1D DQC under spin-phonon coupling resorting to a frustrated anisotropic J1-J2 model as a paradigmatic example. Using large-scale tensor network simulations, we determine the flow of the continuously varying critical exponents with phonon frequency and the critical phonon frequency, at which the transition becomes strongly first-order. By relating the critical theory to an Ashkin-Teller type model, we argue that the critical endpoint is in the four-state Potts universality class. We further compute dynamical phonon spectral functions that provide a powerful experimental signature of DQC.

TT 2.4 Mon 10:15 HSZ/0101

Inducing extraordinary-log criticality in the Heisenberg spin chain — •Grigorios Makris, Francesco Parisen Toldin, and Stefan Wessel — Institute for Theoretical Solid State Physics, RWTH Aachen University, Germany

We examine the ground state correlations emerging in a spin-1/2 Heisenberg chain upon coupling it to a quantum critical two-dimensional bilayer Heisenberg model. Based on the quantum-to-classical mapping and recent findings of unconventional surface criticality of three-dimensional classical Heisenberg models, extraordinary-log criticality is expected to become accessible within this setup along the coupled chain, which serves as a line defect. In particular, such a defect corresponds, through the quantum-to-classical mapping, to a planar defect in the classical case which exhibits extraordinary-log criticality. We use large-scale quantum Monte Carlo simulations to systematically explore this scenario, based on measurements of correlations and the spin stiffness, using the stochastic series expansion methods.

TT 2.5 Mon 10:30 HSZ/0101

Kibble-Zurek Dynamics in the Anisotropic Ising Model of the Si(001) Surface — •Gernot Schaller[1], Friedemann Queisser[1], Parya Katoorani[1], Christian Brand[2], Christian Kohlfürst[1], Mark Freeman[3], Alfred Hucht[2], Peter Kratzer[2], Björn Sothmann[2], Michael Horn-von Hoegen[2], and Ralf Schützhold[1,4] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [2]Fakultät für Physik, Universität Duisburg-Essen and CENIDE, Lotharstraße 1, 47057 Duisburg, Germany — [3]Department of Physics, University of Alberta, 4-181 Centennial Center for Interdisciplinary Science Edmonton, Alberta T6G 2E1, Canada — [4]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

As a simplified description of the nonequilibrium dynamics of buckled dimers on the Si(001) surface, we consider the anisotropic two-dimensional (2D) Ising model [1,2] and study the freezing of spatial correlations during a cooling quench across the critical point. Depending on the cooling rate, we observe a crossover from one-dimensional (1D) to 2D behavior [3]. For rapid cooling, we find effectively 1D behavior in the strongly coupled direction, for which we provide an exact analytic solution of the nonequilibrium dynamics. For slower cooling rates, we start to see 2D behavior where our numerical simulations show an approach to the usual Kibble-Zurek scaling in 2D.

[1] C. Brandt *et al.*, Phys. Rev. Lett. **130**, 126203 (2023).
[2] C. Brandt *et al.*, Phys. Rev. B **109**, 134104 (2024).
[3] G. Schaller *et al.*, Phys. Rev. Lett. **134**, 246202 (2025).

TT 2.6 Mon 10:45 HSZ/0101

Frustration effects and self-consistent matter description in the Dicke-Ising model on the sawtooth chain — •Jonas Leibig, Max Hörmann, Anja Langheld, Andreas Schellenberger, and Kai Phillip Schmidt — Department of Physics, Staudtstraße 7, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

We investigate how the exact thermodynamic-limit mapping of the Dicke-Ising model to a self-consistent effective matter Hamiltonian applies to the geometrically frustrated sawtooth chain. The mapping, established in Ref. [2], was recently solved with NLCE+DMRG for the unfrustrated chain in our work [1]. Using the same method, we obtain the zero-temperature phase diagram of the sawtooth geometry and identify frustration-induced features absent in the unfrustrated case. In the frustrated Ising limit, an infinitesimal effective transverse field lifts the classical degeneracy and produces a disorder-by-disorder transition, analogous to the transverse-field Ising model [3].

[1] J. Leibig, M. Hörmann, A. Langheld, A. Schellenberger, and K. P. Schmidt, *to be published* (2025).
[2] J. Román-Roche, Á. Gómez-León, F. Luis, and D. Zueco, *Physical Review B* **111**, 035156 (2025).
[3] D. J. Priour, M. P. Gelfand, and S. L. Sondhi, *Phys. Rev. B* **64**, 134424 (2001).

15 min. break

TT 2.7 Mon 11:15 HSZ/0101

Potts nematic quantum phase transition in Dirac fermion systems — •Max Fornoville[1,2], Kilian Fraboulet[1], Michael M. Scherer[3], and Laura Classen[1,2] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]School of Natural Sciences, Technische Universität München, 85748 Garching, Germany — [3]Theoretische Physik III, Ruhr-Universität Bochum, 44801 Bochum, Germany

With the advent of 2D moiré materials, Dirac fermion models have yet again emerged as promising candidates to describe putative quantum critical points in these systems. The presence of gapless fermions provides an avenue towards criticality beyond the conventional universality classes because it profoundly alters the quantum critical behavior, also giving rise to non-Fermi liquid behavior. We investigate the onset of nematic order in Dirac systems with hexagonal symmetry. Owing to the sixfold rotational symmetry, the nematic director selects among three equivalent orientations and the associated order parameter is described by a 3-state Potts model coupled to the Dirac fermions via a Yukawa interaction. In the ordered phase, the fermions remain gapless but the Dirac points split, dynamically breaking rotational symmetry. At the mean-field level,

the transition is of first order, which we demonstrate using a minimal lattice model. We further employ a functional renormalization group approach to investigate the influence of the Dirac fermions on the Potts model and the nature of the transition due to a possible fermion-induced continuous quantum critical point.

TT 2.8 Mon 11:30 HSZ/0101

Chiral Quantum Phase Transition in Moiré Dirac Materials at finite density — •Ana Garcia-Page[1] and Laura Classen[1,2] — [1]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [2]Technical University of Munich, Munich, Germany

Chiral quantum phase transitions in Dirac materials at finite density: Strong enough interactions induce a semimetal-to-insulator transition in Dirac materials, which can be viewed as the solid-state analogue of the chiral phase transition in quantum chromodynamics. Moiré Dirac materials such as twisted bilayer graphene offer a new opportunity to study this transition because they facilitate tuning the effective interaction via a twist angle. Motivated by this, we explore the quantum phase transition of a (2+1) dimensional Dirac material at T = 0K which spontaneously develops a gap that breaks an Ising symmetry. It is still an open question what is the structure of the phase diagram at finite chemical potential. To explore it, we study a Gross-Neveu-Yukawa model for the phase transition using both a mean-field theory and a functional renormalization group approach. Interestingly, we find an intermediate state between semi-metal and insulator where a homogeneous solution appears to be unstable.

TT 2.9 Mon 11:45 HSZ/0101

Pseudo-first-order transition from competing Dirac masses in one dimension — •Manuel Weber — Institut für Theoretische Physik and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, Germany

Emergent symmetries and slow crossover phenomena are central themes in quantum criticality and manifest themselves in the pseudocritical scaling experienced in the context of deconfined criticality. Here we discover its conceptual counterpart, i.e., a symmetry-enhanced *pseudo-first-order transition*. It emerges from a one-dimensional realization of deconfined criticality between charge- and bond-ordered states driven by competing Holstein and Su-Schrieffer-Heeger electron-phonon couplings, for which quantum fluctuations and thereby the nature of the transition can be tuned systematically via the phonon frequency ω_0. In the classical limit $\omega_0 \to 0$, a low-energy Dirac theory predicts a direct first-order transition with emergent U(1) symmetry. Using exact quantum Monte Carlo simulations, we provide strong evidence for symmetry enhancement and even finite-size scaling on intermediate length scales but in the thermodynamic limit it turns into a narrow intermediate phase where both order parameters are finite, as chiral U(1) symmetry is weakly broken on the lattice. Including quantum lattice fluctuations diminishes the width of the intermediate phase, gradually restores the U(1) symmetry, and eventually tunes the system to a deconfined quantum critical point.

TT 2.10 Mon 12:00 HSZ/0101

Spectral Optimization of the 2-Sphere and Applications to Classical and Quantum Interacting Spin Systems — •Jonas Völler[1], Grigorios Makris[1], Fabian Hassler[2], and Stefan Wessel[1] — [1]Institute for Theoretical Physics, RWTH Aachen University, Germany — [2]Institute for Quantum Information, RWTH Aachen University, Germany

We investigate discretizations of the 2-sphere using non-uniform simplicial lattices. Starting from an icosahedral seed, we optimize the lattice by solving the free-particle tight-binding model and applying gradient descent to reduce spectral degeneracy breaking, with the goal of restoring the $2\ell + 1$-fold degeneracy of an $SO(3)$-symmetric system. We then perform Monte Carlo simulations of the critical Ising and Potts models and quantify the rotational symmetry breaking by projecting the two-point correlation function onto spherical harmonics. For sufficiently fine discretizations, we successfully recover the expected $SO(3)$-symmetric behavior. Finally, we carry out quantum Monte Carlo simulations of the transverse-field Ising model and locate its critical point by studying Binder-cumulant crossings.

TT 2.11 Mon 12:15 HSZ/0101

Hybrid Monte Carlo on the fuzzy sphere for conformal critical phenomena — •Lidia Stocker[1], Zheng Zhou[2], Yin-Chen He[3], Emilie Huffmann[4], and Johannes Stephan Hofmann[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Perimeter Institute for Theoretical Physics, Waterloo, Ontario N2L 2Y5, Canada — [3]C. N. Yang Institute for Theoretical Physics, Stony Brook University, Stony Brook, NY, USA — [4]Department of Physics, Wake Forest University, Winston-Salem, NC, USA

The fuzzy sphere regularization was recently introduced to study conformal symmetry in the 3D Ising transition [1]. Preliminary analysis with this approach showed excellent agreement with the state*operator correspondence, even though the size of the system considered was particularly restricted. Building on a sign-problem-free formulation of quantum many-body models on the fuzzy sphere [2], we extend the study to significantly larger system sizes using a hybrid Monte Carlo (HMC) scheme. In contrast to microscopic lattice models, we study the deconfined quantum critical point from a low-energy perspective and address whether the transition is of first- or second-order nature, assuming SO(5) symmetry. Our results demonstrate that HMC on the fuzzy sphere is a powerful and scalable framework for exploring conformal critical phenomena in models with many degrees of freedom.

[1] Phys. Rev. X 13, 021009 (2023)
[2] SciPost Phys. Core 7, 028 (2024)

TT 3: Correlated Electrons: Electronic Structure Calculations

Time: Monday 9:30–10:45 Location: HSZ/0103

TT 3.1 Mon 9:30 HSZ/0103

Electronic structure, effective model and electron correlation in Ruddlesden-Popper Cobalt Oxychloride — •xiaolong feng[1], Yang Zhang[2,3], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA — [3]Min H. Kao Department of Electrical Engineering and Computer Science, University of Tennessee, Knoxville, Tennessee 37996, USA

Recent advances in Ruddlesden-Popper(RP)-layered nickelates have revealed a remarkable superconducting transition above the boiling point of liquid nitrogen under high pressure. Here, we report a theoretical investigation of RP cobalt oxychloride, which shows a correlation-driven metal-insulator transition. Strong hybridization between Co-d orbitals and O-p orbitals is identified close to the Fermi level. Upon incorporating enhanced electronic correlations, the Co-d orbital emerges as the dominant component at the Fermi level with partial filling. To further explore the ground state, we construct a minimal effective model via Wannier downfolding, capturing the essential physics of the system. Notably, our results predict an insulator-metal transition under high pressure, positioning RP cobalt oxychloride as a compelling candidate for studying correlated transition metal compounds with potential magnetism and superconductivity.

TT 3.2 Mon 9:45 HSZ/0103

Imaging the $3d$ orbitals in V_2O_3 across the AFI-PM-PI transitions — •Paulius Dolmantas[1], Chun-Fu Chang[1], Martin Sundermann[1,2], Hlynur Gretarsson[2], Jonathan Denlinger[3], Maurits Haverkort[4], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]DESY, Hamburg, Germany — [3]ALS, Berkeley, USA — [4]Institute for Theoretical Physics, Heidelberg University, Heidelberg, Germany

V_2O_3 exhibits a rich phase diagram in which the transitions between the antiferromagnetic insulating (AFI), paramagnetic metallic (PM) and paramagnetic insulating (PI) phases are all 1^{st} order. The presence of c-axis V-V dimers in the crystal structure is the reason for proposing the standard model for V_2O_3 in which a_{1g}-a_{1g} molecular singlets are formed, leaving each V ion with an S=1/2 electron to generate the complex phase diagram. Numerous *ab-initio* electronic structure calculations and spectroscopy studies have been carried out to determine the mechanism of the phase transitions, with contradicting results. The main problem underlying this issue is that the actual valence charge density in V_2O_3 has not yet been determined with sufficient reliability, a quantity that forms the very basis for modeling the properties. Here we utilized a newly developed experimental method with which we can make a direct image of the active orbital. The method is non-resonant inelastic X-ray scattering using an s-core level. Our experimental results unveiled that the a_{1g}-a_{1g} molecular singlets have not materialized and that instead, subtle changes changes in the orbital occupations across the transitions must be considered.

TT 3.3 Mon 10:00 HSZ/0103

$Ni_{1/3}NbS_2$: A correlated impurity-lattice with Ni^{2+} in a metallic Van der Waals magnet — •Sheng-Huai Chen[1], Chun-Fu Chang[1], Yu-Chih Ku[2,3], Po-Yu Cho[2], Chang-Yang Kuo[2,3], Marcus Schmidt[1], Antoine Maignan[4], Atsushi Hariki[5], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Germany — [2]Natl. Synchrotron Radiation Research Center, Taiwan — [3]Dep. of Electrophysics, Natl. Yang Ming Chiao Tung University, Taiwan — [4]CRISMAT, Normandie Univ., CNRS, France — [5]Dep. of Phys. and Electronics, Osaka Metropolitan University, Japan

Ni-intercalated NbS_2 has attracted considerable attention as a chiral metallic van der Waals magnet that couples helical antiferromagnetism to a conducting

Nb-4d/S-3p host, exhibiting current-driven spin-texture control, and showing pocket-selective Fermi surface doping. Our objective is to investigate the specific role of the Ni ions in here. In particular, we would like to know as to what extent electron correlations play a role, and if so, what the actual valence and electronic configurations the Ni has. By combining Ni $L_{2,3}$ XAS, Ni $2p$ XPS, valence band and resonant PES with material-specific DFT+DMFT calculations, we establish that the Ni has a strongly correlated local electronic structure with the Ni^{2+} ($3d^8$) as the main configuration. The NiS_6 octahedra thus set the existence and scale of the local moment and single-ion anisotropy that are the ingredients for the helical state. The interplay between the correlated Ni states with the dispersing bands forming the Fermi surface is the subject of ongoing study.

TT 3.4 Mon 10:15 HSZ/0103

Origin of orbital and magnetic transitions in rare-earth perovskites — •Xuejing Zhang[1], Erik Koch[2], and Eva Pavarini[1] — [1]Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Jülich Supercomputing Centre, Forschungszentrum Jülich, 52425 Jülich, Germany

Strongly-correlated transition-metal oxides are characterized by complex phase diagrams, which result from the interplay of orbital, charge, lattice and spin degrees of freedom. Recently, we introduced an efficient scheme to investigate these phenomena [1-3]. It combines the LDA+DMFT method with a analysis scheme based on the decomposition of the order parameter into its irreducible components. Thanks to this approach, we could explain the origin of the inversion of orbital and magnetic order observed with increasing rare-earth (R) radius in the t_{2g}^2 series RVO_3 [3]. Here we present results for these as well as for other systems.

[1] X. J. Zhang, E. Koch, E. Pavarini, PRB **105** (2022) 115104
[2] X. J. Zhang, E. Koch, E. Pavarini, PRB **106** (2022) 115110
[3] X. J. Zhang, E. Koch, E. Pavarini, PRL **135** (2025) 026508

TT 3.5 Mon 10:30 HSZ/0103

Real-frequency DMFT for multi-orbital models with the neural network configuration interaction impurity solver — •Alexander Kowalski[1], Philipp Hansmann[2], Giorgio Sangiovanni[1], and Adriana Pálffy[1] — [1]Institute for Theoretical Physics and Astrophysics, Universität Würzburg, 97074 Würzburg, Germany — [2]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

The numerical solution of an auxiliary Anderson Impurity Model is usually the most resource-intensive part of the dynamical mean-field treatment of strongly correlated lattice models. Among the variety of approaches with different trade-offs that have been developed, the problem with exact diagonalization is that the exponential scaling of the Hilbert space constrains it to describing the infinite bath in terms of only a small finite number of sites. Selected Configuration Interaction (CI) methods try to achieve more favorable scaling by performing an a priori restriction of the basis used for diagonalization to try to capture only the most important subspace of the desired size. Neural networks have been shown to be remarkably suitable for performing the CI basis selection [1] and we have previously previewed the integration of such a CI algorithm as impurity solver in DMFT. Further developments since then have allowed us to do DMFT calculations with self-consistency directly on the real frequency axis for multi-orbital models with numbers of bath sites well beyond the reach of exact diagonalization.

[1] P. Bilous, L. Thirion, H. Menke, M. W. Haverkort, A. Pálffy, P. Hansmann, Phys. Rev. B 111, 035124 (2025)

TT 4: Graphene, 2D and Twisted Materials

Time: Monday 9:30–12:45 Location: HSZ/0105

TT 4.1 Mon 9:30 HSZ/0105

Toward electron lensing in graphene — Yi-Chen Tsai[1,2], Yu-En Wu[3], Chung-Ting Ke[2,4], and •Ming-Hao Liu[3] — [1]Institute of Physics, Academia Sinica, Taipei, Taiwan — [2]Department of Engineering and System Science, National Tsing Hua University, Hsinchu, Taiwan — [3]Department of Physics and Center for Quantum Frontiers of Research and Technology (QFort), National Cheng Kung University, Tainan, Taiwan — [4]Research Center for Critical Issues, Academia Sinica, Tainan, Taiwan

Electron lensing in graphene based on the combined effects of Klein collimation and negative refraction was theoretically proposed in [1]. The proposal promises striking phenomena that could advance the emerging field of electron optics in graphene. Yet, the original design requiring a parabolic pn junction and a point-like injector at the focal point has remained experimentally demanding and unverified. Here, we present recent progress toward realizing electron lensing in state-of-the-art ultraclean graphene devices. These devices feature multiple contacts—point injectors, narrow collectors, and wide drains—engineered to probe the lensing regime. Low-temperature transport measurements are systematically compared with fully ballistic quantum transport simulations at zero temperature. This combined experimental-theoretical approach enables us to assess how closely current devices approach the envisioned lensing regime described in [1] and to identify critical steps still needed for its experimental confirmation.

[1] M.-H. Liu, C. Gorini, and K. Richter, PRL **118**, 066801 (2017).

TT 4.2 Mon 9:45 HSZ/0105

Non-collinear magnetism of flat bands in magic-angle twisted bilayer graphene — •Maxime Lucas[1], Arnaud Ralko[2], Andreas Honecker[1], and Guy Trambly de Laissardière[1] — [1]Laboratoire de Physique Théorique et Modélisation, CY Cergy Paris Université / CNRS, France — [2]Institut Néel, Université de Grenoble Alpes / CNRS, France

Recent advances of twisted bilayer graphene (and related moiré materials) have been stimulated by the discovery of strong electronic correlations [1] between flat-band states due to a moiré pattern [2]. It is shown experimentally and theoretically that the filling of the flat bands affects their magnetic properties significantly. Similar to what we have done in monolayer graphene [3], we investigate how electronic filling and on-site interactions drive magnetic ordering by studying a Hubbard model on the moiré lattice within an unrestricted Hartree-Fock framework. We mapped out a rich magnetic ground-state phase diagram and uncover a variety of exotic non-collinear spin textures.

[1] Y. Cao et al., Nature 556, 43 (2018); Nature 556, 80 (2018).
[2] G. Trambly de Laissardière et al., Physica E 175, 116362 (2026)
[3] M. Lucas et al., arXiv:2511.22714 [cond-mat.str-el] (2025)

TT 4.3 Mon 10:00 HSZ/0105

Quantum diffusion in twisted bilayer graphene — •Taher Rhouma and Guy Trambly de Laissardière — LPTM, CY Cergy Paris Univ / CNRS, Cergy-Pontoise, France.

The discovery of correlated insulating and superconducting phases arising from the flat bands of magic-angle twisted bilayer graphene (TBG) [1] has stimulated intense interest in their electronic properties. We present a theoretical study of the electronic structure and quantum transport in these flat-band states, incorporating the structural effects of local defects such as non-resonant scatterers. Our real-space method [2,3,4,5] fully accounts for the modification of the electronic structure by defects and for multiple-scattering effects in the conductivity. It shows, in particular, that because of the extremely low Fermi velocity in the flat bands, standard semiclassical Bloch–Boltzmann approaches break down. We present the impact of non-resonant short-range disorder, modeled as diagonal Anderson disorder [4,5] with on-site energies $\varepsilon_i = \varepsilon_0 \pm \Delta W$, on the bandwidth, conductivity, focusing on the impact of filling on the quantum diffusion of twisted bilayer graphene close to the magic angle.

[1] Y. Cao, et al., Nature **556**, 43 (2018); Nature **556**, 80 (2018).
[2] F. Triozon, et al., Phys. Rev. B **65**, 220202, (2002).
[3] O. Faizy Namarvar, et al., Phys. Rev. B **101**, 245407 (2020).
[4] P. Guerrero, et al., Phys. Rev. Lett. **134**, 126301, (2025).
[5] G. Trambly de Laissardière, et al., Physica E **175** 116362 (2026).

TT 4.4 Mon 10:15 HSZ/0105

Quasiparticle Interference as a Probe of Electron's Form Factor in Twisted Bilayer Graphene — D.-H.-Minh Nguyen[1], Francisco Guinea[1,2], and •Dario Bercioux[1,3] — [1]Donostia International Physics Center, 20018 Donostia-San Sebastián, Spain — [2]IMDEA Nanoscience, C/ Faraday 9, 28049 Madrid, Spain — [3]IKERBASQUE, Basque Foundation for Science, Euskadi Plaza, 5, 48009 Bilbao, Spain

We show that characteristics of the electron's form factor in two-dimensional materials are observable in the quasiparticle interference (QPI) spectrum. We study QPI in twisted bilayer graphene using real-space tight-binding calculations combined with the kernel polynomial method, which agrees excellently with the form-factor norm obtained from the continuum Hamiltonian. The QPI signals, displaying a chiral structure, reveal all distinct interference processes between states near the Dirac points. We propose pseudospin textures of twisted bilayer graphene to explain all the interference mechanisms. Our results provide microscopic insights into the electronic eigenstates of twisted bilayer graphene and suggest that QPI could be a promising method for probing the form factor, which governs the material's quantum geometry and many-body states.

[1] D.-H.-M. Nguyen, F. Guinea, D. Bercioux, arXiv:2509.11223.

TT 4.5 Mon 10:30 HSZ/0105

Charge neutrality phase diagram of twisted bilayer graphene from sign-free Monte Carlo simulations — •Johannes S. Hofmann[1], Jong Yeon Lee[2], Patrick Ledwith[3], Eslam Khalaf[4], Ashvin Vishwanath[4], and Erez Berg[5] — [1]Max Planck Institute for the physics of complex systems, Dresden, Germany — [2]University of Illinois at Urbana-Champaign, Urbana, USA — [3]Massachusetts Institute of Technology, Cambridge, USA — [4]Harvard University, Cambridge, USA — [5]Weizmann Institute of Science, Rehovot, Israel

We study the phase diagram of twisted bilayer graphene at charge neutrality as a function of twist angle θ, uniaxial heterostrain ε, and temperature T using sign-problem-free quantum Monte Carlo simulations. At $T = 0$ and zero strain, we find a continuous transition from a Dirac semimetal to a gapped Kramers intervalley coherent (KIVC) phase as θ decreases toward the magic angle. With finite strain, the KIVC phase undergoes a further continuous transition at smaller θ into an anisotropic semimetal with gapless excitations near the center of the moiré Brillouin zone. In the KIVC regime, the entropy rises sharply with temperature and plateaus at $15\,\mathrm{K} \lesssim T \lesssim 40\,\mathrm{K}$ near the value expected from a Mott-like regime of localized electrons with nearly uncorrelated spin, valley, and orbital degrees of freedom. The spectral function evolves continuously with θ: at low T, a gap opens at the K points and the minimal gap shifts to Γ as θ decreases; at intermediate T, the spectral function smoothly interpolates between a Dirac semimetal spectrum with coherent K-point quasiparticles and a spectrum with gapless Γ-centered quasiparticles near the magic angle.

TT 4.6 Mon 10:45 HSZ/0105

Probing doping profiles in large-angle twisted bilayer graphene by Fabry-Perot interference — •Alina Mrenca-Kolasinska[1], Curtis McDowell[2], Thiti Taychatanapat[2], and Ming-Hao Liu[3] — [1]AGH University of Krakow, Faculty of Physics and Applied Computer Science, Poland — [2]Chulalongkorn University, Department of Physics, Faculty of Science, Patumwan, Bangkok, Thailand — [3]National Cheng Kung University, Department of Physics, Tainan, Taiwan

In graphene, p-n junctions can be induced by electrostatic gating. Fabry-Perot (FP) interferometers formed in gate-defined bipolar cavities have been used to probe Klein tunneling [1], miniband structure in moire superlattices [2], and transport in decoupled bilayer graphene [3]. In this work, we investigate a decoupled large-angle twisted bilayer graphene device that shows rich fringe patterns that resemble FP oscillations. We postulate that they originate from extra electronic cavities created by unintentional local doping in the device. Our quantum transport simulations incorporating this assumption reproduce the observed patterns. Our findings demonstrate that disorder can lead to unexpected and rich structures that can be probed by transport.

[1] A.F. Young, P. Kim, Nat. Phys. 5 (2009) 222.
[2] C. Handschin et al. , Nano Lett. 17 (2017) 328.
[3] P. Rickhaus et al. , Sci. Adv. 6 (2020) eaay8409.

15 min. break

TT 4.7 Mon 11:15 HSZ/0105

Theory for optical control of correlated states in moiré transition metal dichalcogenide heterostructures — •Haoyang Tian and Urban F.P. Seifert — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77a, 50937 Köln, Germany

In recent years, moiré transition metal dichalcogenide (TMD) heterostructures have emerged as highly versatile platforms for investigating phases and phenomena of strongly correlated electrons on emergent lattice scales. However, experimental characterization of the precise nature of some interaction-driven orders, in particular antiferromagnetism, and their excitations has remained a challenge. Given strong light-matter couplings and valley selection rules in TMD materials, ultrafast optical methods may constitute a promising avenue for probing and controlling these states and their collective modes.

In this work, we develop a theoretical framework to describe the coherent light-driven dynamics of type-II moiré TMD heterobilayers under circularly polarized laser irradiation. We construct a moiré-Floquet Hamiltonian for the electronic states under periodic driving. In the off-resonant regime, we find that the moiré valence band flattens due to hybridization with the photon-dressed conduction band and derive an effective low-energy model for the Floquet valence band. By incorporating electron-electron interactions via a Hartree-Fock framework, we analyze the impact of optical driving on the phase structure and collective excitations (e.g., magnons).

TT 4.8 Mon 11:30 HSZ/0105

Unveiling structural transitions in the van der Waals multiferroic $CuCrP_2S_6$ under pressure and temperature — •Swarnamayee Mishra[1,3], Gaston Garbarino[2], Alexander Mistonov[1,3], Steven Gebel[1], and Jochen Geck[1,3] — [1]Institute for Solid State and Materials Physics, TU Dresden, Dresden, Germany — [2]European Synchrotron Radiation Facility (ESRF), Grenoble, France — [3]Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, Dresden, Germany

Two-dimensional (2D) crystals with strong in-plane covalent bonds and weak van der Waals interlayer interactions have garnered significant attention following the discovery of graphene and its remarkable properties. $CuCrP_2S_6$ (CCPS) is a promising 2D material exhibiting antiferromagnetic behavior due to the collective ordering of Cr3+ spins and antiferroelectric properties driven by Cu+ ion ordering. These ferroic properties arise from spin-orbit coupling associated with crystal symmetry breaking. Despite its potential, a detailed pressure-dependent crystallographic study of CCPS remains unexplored. In this work, high-resolution single crystal x-ray diffraction is employed to explore its response to variations in pressure and temperature. Our measurements reveal a clear pressure-driven change of lattice symmetry at low temperatures from monoclinic Pc to monoclinic C2/c, together with signatures of charge ordering that point to strong coupling between structure and electronic degrees of freedom. In addition, a pressure-induced reorientation of a structural modulation is found, shifting it from the ac plane at low pressure to the ab plane at higher pressure.

TT 4.9 Mon 11:45 HSZ/0105

Switching Magnetic Anisotropy by Chemical Substitution in Single Crystals of the 2D van der Waals System $(Fe_{1-x}Ni_x)_2P_2S_6$ — •Yuliia Shemerliuk[1], Anja U. B. Wolter[1], Bernd Büchner[1,2], and Saicharan Aswartham[3] — [1]The Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [2]Institute for Solid State and Materials Physics and Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, Germany — [3]International Center for Interfacing Magnetism and Superconductivity with Topological Matter - MagTop, Institute of Physics, Polish Academy of Sciences: Warsaw, Poland

During recent years, layered quasi-two-dimensional van der Waals materials have attracted considerable attention in fundamental science due to their intrinsic low-dimensional crystal structure, which affects their physical properties. Among these materials, layered thiophosphates $M_2P_2S_6$ (M= Ni, Co, Fe, Mn, V) stand out as a versatile platform for exploring the interplay between structure and magnetic exchange interactions. In this talk, we will show how chemical substitution and structural tuning influence magnetic ground states in the quasi-2D system $(Fe_{1-x}Ni_x)_2P_2S_6$. This series combines two structurally compatible parent compounds with fundamentally different magnetic behaviors, interlayer couplings, and ordering temperatures. Our magnetization measurements on single crystals across the substitution series reveal antiferromagnetic ground states throughout. Importantly, we observe a continuous reorientation of magnetic anisotropy from out-of-plane to in-plane with increasing Ni content.

TT 4.10 Mon 12:00 HSZ/0105

Tuning surface resonance states on black phosphorus — •Dongming Zhao[1], Byeongin Lee[2], Junho Bang[2], Claudia Felser[1], Jian-Feng Ge[1], and Doohee Cho[2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Department of Physics, Yonsei University, Seoul 03722, Republic of Korea

Surface resonance states can significantly alter how semiconductors respond to external electric fields. When present, such states can accommodate charge accumulation at the surface, reducing the response from bulk carriers and thereby suppressing band bending. In this work, we show that surface-resonance states near the band edge of black phosphorus couple strongly to the tip-induced electrostatic potential in scanning tunneling spectroscopy. This coupling produces a characteristic dip in the tunneling conductance spectrum. Our simulations indicate that this dip arises from a field-driven change in the tunneling probability into surface resonance states. By effectively tuning the electric field in the junction, we drive the surface-resonance band across the Fermi level, enhancing its contribution to the tunneling current. Our results illustrate how localized surface resonances under an external field dominate electrostatic screening, highlighting their importance in designing and operating semiconductor devices.

TT 4.11 Mon 12:15 HSZ/0105

Quantifying Twist Angles in Cuprate Heterostructures with Anisotropic Raman Signatures — •Flavia Lo Sardo[1,2], Marina Esposito[3,4], Tommaso Confalone[1,5], Kornelius Nielsch[1,2,5], Nicola Poccia[1,3], and Haider Golam[1] — [1]Leibniz Institute for Solid State and Materials Research Dresden (IFWDresden), 01069 Dresden, Germany — [2]Institute of Materials ScienceTechnische Universität DresdenDresden 01062, Germany — [3]Department of PhysicsUniversity of Naples Federico IINaples 80126, Italy — [4]National Institute for Nuclear Physics (INFN) - Sezione di NapoliNaples 80126, Italy — [5]Institute of Applied PhysicsTechnische Universität Dresden, 01062 Dresden, Germany

Artificially engineered twisted van der Waals (vdW) heterostructures have unlocked new pathways for exploring emergent quantum phenomena and strongly correlated electronic states. Many of these phenomena are highly sensitive to the twist angle, which can be deliberately tuned to tailor the interlayer interactions which makes the twist angle a critical tunable parameter. In particular, twisted cuprate heterostructures based on $Bi_2Sr_2CaCu_2O_{8+x}$ (BSCCO) have demonstrated angle-dependent superconducting properties, positioning the twist angle as a key tunable parameter. In this work, a fully non-invasive, polarization-resolved Raman spectroscopy approach is introduced for determining twist angles in artificially stacked BSCCO heterostructures. By analyzing

twist-dependent anisotropic vibrational Raman modes, clear optical fingerprints of the rotational misalignment between cuprate layers are identified.

TT 4.12 Mon 12:30 HSZ/0105

Polaritonic near-field effects on the metal-to-insulator transition of the Hubbard model — •Paul Fadler[1], Marios Michael[2], Katharina Lenk[3], Michael Sentef[1], and Martin Eckstein[3] — [1]Institute for Theoretical Physics, University of Bremen — [2]Max-Planck-Institut für Physik komplexer Systeme, Dresden — [3]Department of Physics, University of Hamburg

The influence of the dielectric environment on material properties has been studied theoretically mostly within two different contexts: Within Coulomb engineering one uses electrostatic screening of the longitudinal electromagnetic field to renormalize interactions [1]. In contrast, within cavity material engineering one tries to shape the transverse electromagnetic field to produce desired material properties [2]. For certain settings, such as in the near-field of materials hosting phonon- or plasmon-polaritons, this separation is no longer possible as the longitudinal and transverse components of the electromagnetic field mix. We investigate the resulting effect on the metal-to-insulator phase transition of a 2-D Hubbard model suspended above a polariton-hosting material using DMFT + GW treating the longitudinal and transverse fields consistently. Lastly, we consider the gauge dependence introduced by our scheme for the Coulomb [3] and Weyl gauge [4].

[1] E. van Loon et al., npj 2D Mater. Appl. **7**, 47 (2023)
[2] F. Schlawin et al., Appl. Phys. Rev. **9**, 011312 (2022)
[3] K. Lenk et al., Phys. Rev. B **106**, 245124 (2022)
[4] C. Eckhardt et al., Phys. Rev. Lett. **135**, 156902 (2025)

TT 5: Superconductivity: Sample Preparation and Characterization

Time: Monday 9:30–12:30 Location: CHE/0089

TT 5.1 Mon 9:30 CHE/0089

Dielectric properties of NbN-films at the insulating side of the superconductor-insulator-transition — •Max Reinhart[1], Lea Pfaffinger[1], Sven Linzen[2], Evgenii Il'ichev[2], Alexander Weizel[1], and Christoph Strunk[1] — [1]Experimental and Applied Physics, Uni Regensburg, Germany — [2]Leibniz Institute of Photonic Technology, Jena, Germany

In 2D strongly disordered thin films the superconductor-insulator-transition (SIT) occurs [1]. The resistive behavior of the insulating side of this transition is well studied, as it has been observed in various materials [2,3]. For the imaginary part of the impedance the situation is less clear. To obtain information on the dielectric properties of 3nm thin NbN in the insulating regime at $R_{sq}(2\ \mathrm{K}) = 60\ \mathrm{k\Omega}$ we deposited interdigitated gold fingers as capacitor within an LC-circuit on SiOx and NbN. On SiOx, we obtained $C \approx 6$ pF. On insulating NbN, the measured capacitance was 6.6 pF. In the latter case the capacitance has a contribution, that depends non-monotonically on temperature, magnetic field and DC bias voltage.

[1] D.B. Haviland et al., Phys. Rev. Lett. 62 (1989) 2180
[2] V.F. Gantmakher and V.T. Dolgopolov, Phys. Usp. 180 (2010) 3
[3] N. G. Ebensperger, Dielectric properties on the insulating, side of the superconductor-insulator-transition [PhD thesis], Universität Stuttgart, 2021

TT 5.2 Mon 9:45 CHE/0089

Gap smearing and sub-gap states in disordered nitride superconductors — •Frederik Bolle[1], Yayi Lin[1], Heidemarie Krüger[2], Martin Dressel[1], and Marc Scheffler[1] — [1]1. Physikalisches Institut, Universität Stuttgart — [2]Leibniz IPHT, Jena

In recent years nitride-based superconductors have gathered a lot of attention due to their high critical temperatures, large kinetic inductances, and ease of manufacturing. According to the BCS theory, at temperatures far below the critical transition temperature, the superconducting s-wave state is characterized by a hard gap Δ and a coherence peak above the gap. In the case of substantial disorder, subgap states emerge and the coherence peak is suppressed.

We present the quasiparticle dynamics of ultra-thin NbN and MoN films with various levels of disorder, probed at energies comparable to the energy gap using THz spectroscopy (0.2 meV – 10 meV). To quantify the additional pair-breaking we employ the phenomenological Dynes model for the optical conductivity. We find in the case of NbN, a temperature-independent pair-breaking rate, which suggests magnetic impurities, while MoN shows a strongly temperature-dependent pair-breaking rate, which we attribute to inhomogeneities of the local gap function. The understanding of this excess quasiparticle density plays an important role for decoherence and loss mechanisms in quantum circuits at millikelvin temperatures.

TT 5.3 Mon 10:00 CHE/0089

Superconducting resonators from ultrathin NbN films — •meenakshi sharma[1], hrishikesh borah[1], surinder singh[2], sandeep singh[2], haolin jin[1], yejin lee[1], and uri vool[1] — [1]MPI CPFS, Dresden, Germany — [2]CSIR NPL, Delhi, India

We investigate superconducting microwave resonators fabricated from ultrathin niobium nitride (NbN) films with thicknesses down to 3 nm. Such films show extremely high kinetic inductance values of 298 pH per square, approaching the regime where disorder strongly influences superconductivity. However, they remain robust and exhibit a critical temperature of 7.8 K, making them suitable for high-impedance circuit applications. The resonators achieve internal quality factors of approximately 10^4-10^5, demonstrating that reliable device performance can be sustained even at such critical thicknesses. By monitoring the resonance frequency as a function of temperature, we probe the electrodynamic response of the ultrathin superconducting state. The superfluid density departs from the exponential temperature dependence expected for conventional BCS superconductors and instead follows a power-law behavior at low temperatures, indicating spatial inhomogeneity in the superconducting condensate. At millikelvin temperatures, dissipation is dominated by two-level systems, but the large kinetic inductance suppresses their influence on the resonance frequency, thereby enabling stable and reproducible devices. These results establish ultrathin NbN as both a practical platform for high-impedance quantum circuits and an accessible system for studying unconventional superconducting physics.

TT 5.4 Mon 10:15 CHE/0089

Tuning Superconductivity and Vortex Dynamics in NbRe Films via Grain-Size Control — •Zahra Makhdoumi Kakhaki[1], Francesco Avitabile[2], Abhishek Kumar[2], Francesco Colangelo[2], Carla Cirillo[3], Carmine Attanasio[2], and Oleksandr Dobrovolskiy[1] — [1]Cryogenic Quantum Electronics, EMG and LENA, Technische Universität Braunschweig, Germany — [2]Università degli Studi di Salerno, Italy — [3]CNR-SPIN, Università di Salerno, Italy

NbRe, a non-centrosymmetric superconductor with strong antisymmetric spin-orbit coupling and relatively high Tc, is of interest for superconducting spintronics and single-photon detectors. Yet, it poses a challenge: understanding how its order parameter evolves in thin films as crystallite size changes. Here, we induce a significant structural transformation in 20 nm-thick NbRe films through thermal an-nealing, increasing the average crystallite size from about 2 nm to approximately 8 nm across as-grown and annealed conditions [1]. We probe superconducting pairing via upper critical field measurements and quantify vortex dynamics through current-voltage curves under varying temperatures and magnetic fields. The annealed films exhibit discrete resistive states and traces of normal-conducting domains at- tributed to dissipative vortex motion and local overheating [2]. In addi- tion to spin-triplet correlations in NbRe-based hybrids [3], the annealed films show indications of two superconducting gaps.

[1] Makhdoumi Kakhaki et al., SUST 37 (2024) 125002
[2] Bezuglyj et al., PRB 99 (2019) 174518
[3] Colangelo et al., PRL (2025), arXiv:2510.08110

TT 5.5 Mon 10:30 CHE/0089

Superconductivity of $[(SnSe)_{1+\delta}]_m$[NbSe2] superlattices with varying $NbSe_2$ interlayer spacing — •Olivio Chiatti[1], Linus P. Stahlberg[1], Wieland G. Stoffel[1], Tom Herter-Lehmann[1], Willi Vallant[1], Alina Dietrich[1], Danielle Hamann[2], David C. Johnson[2], and Saskia F. Fischer[1,3] — [1]Novel Materials Group, Humboldt-Universität zu Berlin, 10099 Berlin, Germany — [2]Department of Chemistry and Materials Science Institute, University of Oregon, Eugene OR 97403, USA — [3]Center for the Science of Materials Berlin, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

In layered superconductors the coupling betwee superconducting layers is crucial due to its strong impact on their properties [1]. We investigate the properties of $[(SnSe)_{1+\delta}]_m$[NbSe2] superlattices, which allow for nearly arbitrary stacking sequences due to the growth technique [2]. With this degree of freedom we study how coupling mechanisms enable the occurrence of superconductivity.

Temperature-dependent resistance measurements show superconductivity for $NbSe_2$ interlayer distances of 2.4 nm or smaller. This is explained by the interplay of grain boundaries, crossplane tunneling and proximity effect in the SnSe spacer layer. Additionally, current-voltage characteristics provide insights into the coupling mechanisms of 2D superconductors.

[1] Chiatti *et al.*, J. Phys.: Condens. Matter **35**, 215701 (2023)
[2] Grosse *et al.*, Sci. Rep. **6**, 33457 (2016)

TT 5.6 Mon 10:45 CHE/0089

Characterization and superconducting properties of $SrBi_2Se_4$ — •Max Brückner[1], Jule Kirschke[1], Ashiwini Balodhi[1], Cedric Schmitt[2], Lukas Gehrig[2], Kilian Strauss[2], Christoph Flathmann[3], Dina I. Fazlizhanova[4], Christian Liebscher[3], Ilya Eremin[5], Simon Moser[1,2], Andreas Kreyssig[1], and Anna E. Böhmer[1] — [1]Experimental Physics IV, Ruhr-University Bochum, Bochum — [2]Physikalisches Institut and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Würzburg — [3]Faculty of Physics and Astronomy, Ruhr-University Bochum, Bochum — [4]private — [5]Theoretical Physics III, Ruhr-University Bochum, Bochum

$SrBi_2Se_4$ is a newly discovered quasi-one-dimensional superconductor that offers a promising platform for exploring exotic superconductivity in low-dimensional systems. We present the growth of free-standing single crystals using a Bi-Se-rich self-flux method and characterize their structure and composition via x-ray diffraction, transmission electron microscopy, and energy-dispersive x-ray spectroscopy. Heat-capacity and magnetization measurements confirm bulk superconductivity below $T_c = 2.9$ K, while magnetotransport reveals an anisotropic upper-critical field. Additionally, we present angle-resolved photoemission spectroscopy and density-functional theory calculations, that provide insight into the electronic structure and lay the groundwork for understanding possible unconventional superconductivity in $SrBi_2Se_4$.

We acknowledge funding from the European Research Council through Project 101040811, Distort-to-Grasp.

15 min. break

TT 5.7 Mon 11:15 CHE/0089

Structural transition and emergent bulk superconductivity in Te-doped $PtBi_2$ — •Soumen Ash[1,2], Kilian Srowik[1,2], Pablo Pedrazzini[1,3], Oksana E. Kvitnitskaya[1], Andrii Kuibarov[1], Susmita Changdar[1], Rui Lou[1], Alexander Fedorov[1], Swarnamayee Mishra[4], Alexander Mistonov[4], Saicharan Aswartham[1], Jochen Geck[4], Sergey Borisenko[1], Laura T. Corredor[1], and Bernd Büchner[1,4] — [1]Institute for Solid State Research, Leibniz IFW Dresden, 01069 Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [3]Lab. Bajas Temperaturas, Centro Atómico Bariloche, CNEA-CONICET, 8400 San Carlos de Bariloche, Argentina — [4]Institute of Solid State and Materials Physics, TU Dresden, 01062 Dresden, Germany

Noncentrosymmetric trigonal $PtBi_2$ has emerged as a topological system exhibiting signatures of unconventional surface superconductivity, while sub-Kelvin superconductivity, as revealed by resistivity measurements, makes it a promising platform for studying chemical-tuning effects. We have carried out Te doping at the Bi sites of $PtBi_2$ and grown plate-like crystals with nominal compositions of $PtBi_{2-x}Te_x$ (x = 0.02 - 0.05) using a stoichiometric-melt-growth method. Detailed structural, electrical transport, magnetic, thermodynamic, and spectroscopic studies reveal that doping of Te at Bi-sites results in a transition from noncentrosymmetric (space group: $P31m$) to centrosymmetric (space group: $P\bar{3}m1$) crystal structure and gives rise to a bulk superconductivity with comparatively higher $T_c \approx 2.4$ K.

TT 5.8 Mon 11:30 CHE/0089

High-pressure high-temperature synthesis of uranium-silver compounds — •Jordan Tierney[1], Julia-Maria Hübner[2], Ulrich Schwarz[1], Andreas Leithe-Jasper[1], Ulrich Burkhardt[1], Markus König[1], Anamaria Ghihor[1], Yurii Prots[1], and Eteri Svanidze[1] — [1]MPI CPfS, Dresden — [2]TU Dresden

Uranium-based quantum materials have recently entered a renaissance. Evidence of correlated topological states, spin-liquid behavior, hidden order phases, and spin-triplet superconductivity prove that these materials are exceptionally interesting. Because of their complex chemistry and fragile stability, many potentially fascinating uranium-based systems are currently entirely beyond the reach of conventional synthesis methods. In this talk, we will show how simultaneous high-pressure high-temperature synthesis, combined with micro-scale specimen isolation, can reach previously unattainable phases. We will discuss the uranium-silver system, in which no binary compounds have been previously reported; the two elements have appeared to be immiscible during conventional synthesis. By employing simultaneous high-pressure high-temperature synthesis instead, we have discovered several new materials. In particular, we were able to identify new magnetic and superconducting phases, with the detailed analysis of chemical and physical properties still currently underway. This proof-of-principle work shows that by implementing this methodology we can access high-purity materials and study their novel crystallographic arrangements and exotic quantum states. Supported by DFG grant number 553528746.

TT 5.9 Mon 11:45 CHE/0089

From superconductivity to unusual magnetic behaviour in noncentrosymmetric mercurides — •R. Nixon[1,2], N. Zaremba[1], S. Adegboyega[3], A. Leithe-Jasper[1], M. Krnel[1], Yu. Prots[1], L. Akselrud[1,4], M. Schmidt[1], U. Burkhardt[1], J. Sichelschmidt[1], L. Amidani[5,6], F. La Mattina[7], M. Shatruk[3], A. Shengelaya[8], M. Brando[1], Yu. Grin[1], and E. Svanidze[1] — [1]MPI CPfS, Dresden — [2]Uni. of St Andrews, UK — [3]Florida St. Uni., US — [4]Ivan Franko Lviv National Uni., Ukraine — [5]ESRF, Grenoble, France — [6]HZDR, Dresden — [7]Lab. for Transport at Nanoscale Interfaces, Duebendorf, Switzerland — [8]Ivane Javakhishvili Tbilisi State Uni., Georgia

Mercury and superconductivity are forever linked due to the discovery of zero resistivity (Onnes 1911), yet superconductivity in elemental Hg remains non-trivial (Tresca 2022). Here we examine superconductivity in noncentrosymmetric mercurides, $A_{11-x}Hg_{54+x}$, (A = Na, Ca, Sr). Due to their complexity, these structures were refined over many years (Tambornino 2015), the Ca and Sr adopt $A_{11-x}Hg_{54+x}$ (Tkachuk 2008), and Na forms a 3-fold superstructure, $Na_{11}Hg_{52}$ (Hoch 2012). Mercurides are often structurally characterised, but physical properties are rarely reported. We previously identified $Sr_{11-x}Hg_{54+x}$ to superconduct (Nixon 2024), motivated by growing interest of unconventional pairing in noncentrosymmetric superconductors (Bauer 2004), we extend to the Na and Ca analogues, also identified to superconduct (Nixon in prep.). Moving to rare-earths, we obtain the related $Eu_{11-x}Hg_{54+x}$ phase, however, multiple Eu sites give several magnetic phases (Nixon 2025). Research funded by DFG - No. 528628333.

TT 5.10 Mon 12:00 CHE/0089

Atomic scale imaging of the effect of chemical pressure in $Sr_{2-x}Ba_xRuO_4$ — •Siri A. Berge[1], Rebecca Bisset[1], Daniel Halliday[1], Carolina de Almeida Marques[1], Luke C. Rhodes[1], Alexander C. Komarek[2], Phil D. C. King[1], and Peter Wahl[1,3] — [1]SUPA, School of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews, KY16 9SS, United Kingdom — [2]Max Planck Institute for Chemical Physics of Solids Nöthnitzer Strasse 40, Dresden 01187, Germany — [3]Physikalisches Institut, Universitat Bonn, Nussallee 12, 53115 Bonn, Germany

Tuning the electronic structure of layered perovskites is a powerful pathway to control their properties for future applications. Structural distortion in Sr_2RuO_4 affects the electronic structure, moving the van Hove singularity across the Fermi level, with significant consequences for physical properties such as superconductivity [1-2]. Here, we study the effect of chemical pressure by substitution with isovalent Ba atoms in $Sr_{2-x}Ba_xRuO_4$ for $x = 0$, 0.2, and 0.4 by Scanning Tunnelling Microscopy (STM). We report changes in the electronic structure with rotation of the surface RuO octahedra as well as surface inhomogeneity with regions of varying degrees of rotation. Our results highlight the connection between electronic and lattice degrees of freedom and demonstrate control of the electronic structure.

[1] C.A. Marques et al. Advanced Materials 33 (2021) 2100593
[2] J.B. Profe et al. Phys. Rev. Research 6 (2024) 043057

TT 5.11 Mon 12:15 CHE/0089

Multiple superconducting transitions in $Yb_{3+x}Co_4Sn_{13-x}$ — •Roman Gumeniuk[1], Meret Orlob[1], Volodymyr Levytskyi[1], Alexander A. Tsirlin[2], Bohdan Kundys[3], and Andreas Leithe-Jasper[4] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg, 09596 Freiberg, Germany — [2]Felix-Bloch-Institut für Festkörperphysik, Universität Leipzig, 04103 Leipzig, Germany — [3]Université de Strasbourg, CNRS, Institut de Physique et Chimie des Matériaux, Strasbourg F-67000, France — [4]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany

$Yb_{3+x}Co_4Sn_{13-x}$ is shown to posses homogeneity range within $0 \leq x \leq 0.5$. For all x a primitive cubic [space group $Pm\bar{3}n$, $a \approx 9.54$ Å] structure of strongly disordered $Sc_3Ir_4Si_{13+x}$ type is found. Despite showing no signatures of presence of additional phases, different pieces of the same stoichiometric $Yb_3Co_4Sn_{13}$ sample revealed multiple superconducting transitions of varying intensity at $T_c = 3.1(2)$ K and $T_c = 2.4(2)$ K in temperature dependence of specific heat. On the other hand, $Yb_{3.2}Co_4Sn_{12.8}$ is found to be a strongly coupled superconductor with single transition at $T_c = 2.4(2)$ K and enhanced critical magnetic field $B_{c2} = 4.79(9)$ T. To shed light on superconducting behaviors in both stannides diverse models were applied to describe $B_{c2}(T_c)$ and $c_{el}(T)$ dependencies. Both $Yb_{3+x}Co_4Sn_{13-x}$ ($x = 0, 0.2$) compounds reveal bosonic peaks in specific heat and thus, possible 'rattling' behavior. They are also metallic systems, some aspects of which are described by a free electron gas model [1].

[1] M. Orlob et al., Phys. Rev. B 112 (2025) 174513

TT 6: Topological Superconductors

Time: Monday 9:30–11:00 Location: CHE/0091

TT 6.1 Mon 9:30 CHE/0091

Experimental Signatures of Gate-Tuneable One-Dimensional Edge Channels in Bi_2Se_3 Josephson Junctions — •Feike van Veen[1], Femke Witmans[1], Jara Vliem[2], Daniel Vanmaekelbergh[2], Chuan Li[1], and Alexander Brinkamn[1] — [1]MESA+ Institute for Nanotechnology, University of Twente, Hallenweg 15, 7522 NH Enschede, The Netherlands — [2]Debye Institute for Nanomaterials Science, Utrecht University, Princetonplein 1, 3584 CC Utrecht, The Netherlands

The quantum spin Hall (QSH) effect exhibits helical edge channels that can be utilized in the development of quantum computing [1]. Such QSH states are expected to be present in the hybridization gap that opens at the Dirac point in ultrathin 3D topological insulators (TIs) when opposite topological surface states hybridize [2]. In a previous study, an enhanced density of states has been probed at the edges of ultrathin colloidal Bi_2Se_3 nanoplatelets (NPLs) with scanning tunnelling spectroscopy [3]. Here, we study superconducting transport properties of these Bi_2Se_3 NPLs and reveal strong signatures of a 1D edge state contribution. Moreover, we found experimental evidence of a thickness dependence as is described by theoretical frameworks [2]. We can deplete the NPLs, hereby destroying the supercurrent, allowing for an "on" or "off" mode of the JJs. These observations contribute to the understanding and development of (non)-topological JJs made of ultrathin 3D TIs and shed new light on previous studies on superconductivity induced in QSH states.

[1] 10.1103/RevModPhys.82.3045
[2] 10.1103/PhysRevB.97.075419
[3] 10.1021/acs.nanolett.3c04460

TT 6.2 Mon 9:45 CHE/0091

Higher-order topological states in antiferromagnet/superconductor interface — •Ignacio Sardinero[1,4], Yuriko Baba[2], Rubén Seoane-Souto[3], and Pablo Burset[1,4] — [1]Department of Theoretical Condensed Matter Physics, Universidad Autónoma de Madrid, 28049 Madrid, Spain — [2]Instituto de Estructura de la Materia (IEM-CSIC), Serrano, 121, 28006 Madrid, Spain — [3]Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Sor Juana Inés de la Cruz, 3, 28049 Madrid, Spain — [4]Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049 Madrid, Spain

Topological superconductors (TSs) are promising candidates for reliable quantum information processing. While field-free platforms often rely on ferromagnets, their stray magnetization hinders scalability. Antiferromagnets (AFMs) offer a novel approach by providing local time-reversal symmetry breaking without macroscopic magnetization. Motivated by recent experiments [1], we investigate TS in van der Waals AFM/superconductor hybrid structures. We show that trivial Andreev bound states can localize at uncompensated magnetic edges, which could explain the recent experiment [1]. Then, we propose a pathway to nontrivial topological phases driven by the interplay of AFM with Rashba or Ising spin-orbit couplings. We demonstrate that specific crystalline symmetries, particularly mirror symmetry combined spin-flip operations, stabilize second-order topological superconducting phases, characterized by a finite quadrupole moment.

[1] C. González-Sánchez et al., arXiv:2505.18578

TT 6.3 Mon 10:00 CHE/0091

Topological superconductivity induced by atomic-scale skyrmion lattices — •Felix Nickel and Stefan Heinze — Institute of Theoretical Physics and Astrophysics, University of Kiel

Topological superconductivity, which can host Majorana zero modes with potential applications in topological quantum computing, relies on unconventional superconductors not known to exist in nature. However, magnet*superconductor hybrid systems (MSHs), built from ultra-thin magnetic layers on conventional superconductors, can induce such unconventional pairing [1]. While much research has focused on ferromagnetic systems with substantial spin*orbit coupling (SOC), non-collinear magnetic structures have been only sparsely investigated. Among them, atomic-scale skyrmion lattices are particularly interesting, as they lead to topological orbital moments and a topological Hall effect. They also offer a promising platform for MSHs, since their non-coplanar spin arrangement, characterized by the scalar spin chirality, induces spin mixing naturally, even in the absence of SOC.

We present a systematic study based on a tight-binding model of various collinear, non-collinear, and non-coplanar spin textures and analyze their effect on the superconducting substrate. We relate the scalar spin chirality to the topological phase of the superconductor, characterized by its Chern number. For magnetic textures with finite scalar spin chirality, we find topological superconductivity, indicating a direct link between both properties [2].

[1] R. Lo Conte *et al.*, Riv. Nuovo Cim. **47**, 453 (2024)
[2] F. Nickel *et al.*, npj Spintronics **3**, 13 (2025)

TT 6.4 Mon 10:15 CHE/0091

Topologically enabled superconductivity in 2D quantum materials — •Francesca Paoletti[1], Daniele Guerci[2], Giorgio Sangiovanni[1], Urban F. P. Seifert[3], and Elio J. König[4] — [1]JMU Würzburg — [2]Massachusetts Institute of Technology — [3]Universität zu Köln — [4]University of Wisconsin-Madison

We investigate the role of Green's function zeros in strongly interacting topological Mott insulators, focusing on their meaning and physical interpretation. Recent advancements, particularly through slave rotor calculations of the Kane-Mele-Hubbard model, have established a connection between zeros and spinons and with U(1) gapped spin liquids. We find a macroscopic spin-charge separation resulting from the non-trivial interplay with the conventional boundary modes of the topological insulator. We further employ our method to an attractive Hubbard-Haldane honeycomb model. In this context, the extensive slave-rotor mean-field calculations are used as a microscopic foundation to determine the phase diagram of the model as well as important phenomenological properties, such as the coherence length and penetration depth (Pearl length) within a topologically enabled mechanism of superconductivity.

TT 6.5 Mon 10:30 CHE/0091

Euler band topology in superfluids and superconductors — •Shingo Kobayashi[1], Manabu Sato[2], and Akira Furusaki[1] — [1]RIKEN Center for Emergent Matter Science, Wako, Saitama, Japan — [2]Department of Applied Physics, University of Tokyo, Bunkyo, Tokyo, Japan

Real band topology often appears in systems with space-time inversion symmetry and is characterized by invariants such as the Euler and second Stiefel-Whitney classes. Here, we examine the generic band topology of Bogoliubov de-Gennes (BdG) Hamiltonians with $C_{2z}T$ symmetry, where C_{2z} and T are twofold rotation about the z axis and time-reversal symmetries, respectively. We discuss the Euler band topology of superfluids and superconductors in the DIII and CI Altland-Zirnbauer symmetry classes. We demonstrate our theory with two examples: the superfluid ^{3}He B phase in magnetic field and the nodal lines of multi-orbital s-wave superconductors in class CI. These results provide a theoretical framework for exploring Euler band topology in superfluids and superconductors and offer a unified understanding of the robustness of topological phases under TRSB perturbations, including Majorana Ising physics and higher-order topology.

TT 6.6 Mon 10:45 CHE/0091

Topology of non-normalizable physical vector fields — •Philipp Gessler, Alessandro Pignedoli, Alexander Neuhaus, Pascal Dreher, Frank Meyer zu Heringdorf, Maria Azhar, and Karin Everschor-Sitte — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47048 Duisburg, Germany

Topological classification of physical vector fields typically relies on normalizing the field and using homotopy groups to classify them. When field amplitudes vanish, normalization becomes impossible, preventing a direct topological classification. We resolve this by mapping the d-dimensional vector field into a (d+1)-dimensional space, enabling a general classification scheme for non-normalizable fields. Applying this method to the transverse electric mode of a classical electromagnetic waveguide, we reveal their topological nature. This approach extends topological analysis to a broad range of physical systems, including magnetism, water waves, and ferroelectrics.

TT 7: Surface Magnetism and Topological Insulators (joint session MA/TT)

Time: Monday 9:30–12:00 Location: POT/0351

TT 7.1 Mon 9:30 POT/0351

Impact of keV He-ion bombardment on the magnetic proximity effect in Pt/Fe bilayers — •Mika Ossenschmidt[1], Arne Vereijken[1], Yahya Shubbak[1], Varun Vanakalapu[1], Maik Gaerner[2], Arno Ehresmann[1], and Timo Kuschel[2] — [1]University of Kassel, Germany — [2]Bielefeld University, Germany

The static magnetic proximity effect (MPE) describes the occurrence of spin polarization at the interface of nominally paramagnetic materials caused by its ad-

jacency to a ferromagnetic material. KeV-He light ion bombardment (IB) of thin-film interfaces offers the opportunity to modify the interface properties of thin-film systems without destroying the thin films, e.g., as shown for exchange-bias systems [1].

Samples of Pt 4 nm/Fe 10 nm//MgO(001) were fabricated by sputter deposition and the subsequent IB was performed with 10 keV He^+ ions with a varying ion dose from 10^{15} to 10^{17} ions/cm^2 in a few steps. To analyze the strength of the MPE in Pt, x-ray resonant magnetic reflectivity measurements were performed at the Pt L_3 absorption edge (11.567 keV) at DESY beamline P09 [2].

The fits of the x-ray reflectivity measurements provide a significant difference for the roughness σ of the Pt-Fe interface due to IB while substrate and surface roughnesses as well as layer thicknesses remained nearly unchanged. The resulting maximum Pt moment at the interface for the sample with IB is higher than without IB, due to the increasing intermixing of Pt and Fe atoms at the Pt-Fe interface.

[1] Ehresmann et al., J. Phys. D: Appl. Phys. 38, 801 (2005)
[2] Kuschel et al., Phys. Rev. Lett. 115, 097401 (2015)

TT 7.2 Mon 9:45 POT/0351

Exchange splitting at surfaces: a new paradigm for spin-polarization in antiferromagnets — •William Schaarman and Sophie Weber — Chalmers University of Technology, Göteborg, Sweden

There has been recent interest in combining the robustness and ultrafast dynamics of antiferromagnets with the transport properties of spin-polarized band structures. While antiferromagnetic bands are typically spin-degenerate, exceptions to this rule such as the altermagnets have demonstrated the possibility to obtain spin polarization in bulk antiferromagnets via selective symmetry lowering. Here, we use symmetry analysis and density functional theory to examine a ferromagnetic-like exchange splitting at certain surfaces. Such spin polarization of the surface-projected band structure can occur for surface orientations with a net two-dimensional magnetization which can emerge via symmetry-lowering at the antiferromagnet's surface. By analyzing the band structure of a slab geometry projected onto a single surface, we confirm surface spin polarization in two representative materials, magnetoelectric Cr2O3 and altermagnetic FeF2. We rationalize the magnitudes of exchange splitting on distance surface orientations in these two materials as a complex interplay between the exchange and crystal field splittings of individual magnetic atoms making up the surface. Notably, our analysis shows the effect of surface exchange splitting can in some cases be of the order of eV which has important implications for spintronic devices.

TT 7.3 Mon 10:00 POT/0351

Image-potential states on a 2D Gr-ferromagnet hybrid: enhancing spin and stacking sensing — Maciej Bazarnik[1,2] and •Anika Schlenhoff[1,2] — [1]Institute of Physics, University of Münster, Germany — [2]Department of Physics, University of Hamburg, Germany

With the increasing research interest in 2D materials, image-potential states (IPSs) have regained attention as sensitive probes, e.g. for a charge transfer at buried graphene(Gr)-metal interfaces. For a Gr-ferromagnet hybrid, the question arises how IPSs sense a respective spin transfer laterally varying within the moiré heterostructure.

Here, we present spin-resolved scanning tunneling microscopy and spectroscopy studies on Fe intercalated Gr/Ir(111), that show the IPSs' sensitivity to the spatial variation of the Gr-Fe distance, and of the interfacial charge and spin transfer within the moiré unit cell [1]. A stacking contrast between fcc and hcp sites, indistinguishable in the direct tunneling mode, is provided by the IPSs. We observe a moiré-site- and energy-dependent spin-polarization of the IPSs that can be mapped across the entire moiré unit cell. Unlike the electronic states around the Fermi energy, the lowest IPSs are found to exhibit a high spin-polarization on the on-top sites attributed to their interfacial character at the respective Gr-Fe distance. Since the physisorbed Gr is only weakly spin-polarized on these sites, our work demonstrates that the lowest order IPSs can be used to locally sense the spin density at magnetic interfaces buried by a nonmagnetic passivation layer.

[1] M. Bazarnik and A. Schlenhoff, ACS Nano 19, 25812 (2025).

TT 7.4 Mon 10:15 POT/0351

Theoretical Investigation of Intrinsically Patterned 2D Transition Metal Halides: Defects, Structure, and Magnetic Phenomena — •Neeta Bisht[1], Andreas Görling[1], Feifei Xiang[2], Binbin Da[2], Mohammad Sajjan[2], Sabine Maier[2], and Christian Neiss[1] — [1]Lehrstuhl für Theoretische Chemie, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen

— [2]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen

In the quest for complex structured functional materials, defect engineering and patterning in two-dimensional (2D) systems are critical for tuning material properties and enabling new functionalities. Herein, we report on intrinsically patterned 2D transition metal dihalides (TMDs) on a gold surface, featuring periodic halogen vacancies in the upper and bottom halide layers that result in alternating coordination of the transition metal atoms throughout the film.

We explore the formation pathways leading to periodic halogen vacancies and their role in modifying the electronic and magnetic structure of TMDs. Our calculations also explores the possibility of non-collinear magnetic textures through the magnetic anisotropy calculations. The excellent match between the experimental findings and the DFT calculations, confirms the intrinsic vacancy lattice. By coupling our theoretical results with experimental observations, we provide a comprehensive framework for understanding the structure formation and magnetic properties of 2D materials.

TT 7.5 Mon 10:30 POT/0351

Magnetic domain structure of holmium films at low temperatures — •Patrick Härtl[1], Vijayalaxmi Sankeshwar[2], and Matthias Bode[1] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Indian Institute of Science Education and Research(IISER), Pune, Maharashtra 411008, India

Rare-earth metals play a central role in modern magnetism, with their behavior largely governed by the element-specific sign and oscillation period of the RKKY interaction. However, real-space investigations of their complex magnetic domain structures remain scarce. Here, we present a systematic study of the structural and magnetic properties of epitaxial holmium (Ho) films grown on W(110), using low-temperature spin-polarized scanning tunneling microscopy (SP-STM).

Bulk Ho crystallizes in a hexagonal close-packed structure and exhibits an exceptionally large magnetic moment of approximately 10 μ_B, forming a helical spin spiral below $T_C = 20$ K. In our films, we find predominantly ferromagnetic in-plane domains for thicknesses up to about 50 atomic layers (AL), with domain walls strongly pinned to crystalline defects. For coverages above 50 AL, additional out-of-plane stripe domains emerge, which we attribute to the uncompensated c-axis magnetization of the helical cone state. Domain wall analysis reveals Néel-capped Bloch-type walls with characteristic widths of roughly ≈ 1.2 nm (60°), ≈ 3 nm (120°), and ≈ 4 nm (180°). The stripe domains are suppressed by out-of-plane magnetic fields of $\mu_0 H = \pm 300$ mT.

Published in: P. Härtl et al., Phys. Rev. B **112**, 174402 (2025).

TT 7.6 Mon 10:45 POT/0351

Electronic bounds in magnetic crystals — •Daniel Passos[1] and Ivo Souza[1,2] — [1]Centro de Física de Materiales, Universidad del País Vasco, 20018 San Sebastián, Spain — [2]Ikerbasque Foundation, 48013 Bilbao, Spain

A quantum system in its ground-state must display non-negative optical absorption. This simple statement forms the basis for a string of inequalities between moments of the absorptive conductivity. Through the use of sum rules, these inequalities provide bounds on quantities of physical interest. Recent discoveries include new constraints on the electronic localization length in insulators, and an upper bound on the bandgap of topological insulators. Current research focuses on finding inequalities relating ground-state properties such as the quantum metric to more directly measurable quantities.

We present a systematic study of bound relations between different electronic properties of magnetic crystals: electron density, effective mass, orbital magnetization, localization length, Chern invariant, and electric susceptibility. New results include a lower bound on the electric susceptibility of Chern insulators, and an upper bound on the sum-rule part of the orbital magnetization. In addition, bounds involving the Chern invariant are generalized from two dimensions (Chern number) to three (Chern vector). Bound relations are established for metals as well as insulators, and are illustrated for model systems. The manner in which they approach saturation in a model Chern insulator with tunable flat bands is analyzed in terms of the optical absorption spectrum.

15 min break

TT 7.7 Mon 11:15 POT/0351

Hidden Dirac-Like Crossings in a Prototypical Topological Insulator — •Wei-Sheng Chiu[1,2], Ina Marie Verzola[3], Ying-Jiun Chen[1], Rovi Angelo Beloya Villaos[3], Claus Michael Schneider[1,2], Feng-Chuan Chuang[3], and Christian Tusche[1,2] — [1]Forschungszentrum Jülich, Germany — [2]Universität Duisburg-Essen, Germany — [3]National Sun Yat-sen University, Taiwan

The prototypical topological insulator Bi_2Se_3 has been extensively studied for its topological surface state characterized by a $\mathbb{Z}_2$ topological invariant. By using spin-resolving momentum microscopy with an Au passivated Ir(100) imaging spin filter, we simultaneously recorded the spin-resolved momentum maps (k_x, k_y) over entire surface Brillouin zone of Bi_2Se_3. In addition to the well-known Dirac cone near Fermi energy, we observe a sequence of several Dirac-like spin textures and crossings spanning binding energies down to 4 eV at the $\overline{\Gamma}$ point. Moreover, a Dirac-like crossing is also found at a binding energy 2.3 eV at the $\overline{M}$ point. Our first-principles calculations indicate that those overlooked bands are attributed to surface states. The Dirac-like crossing at the $\overline{M}$ point arises from crystalline-symmetry-enforced degeneracy at the high symmetry point, showing that Bi_2Se_3 has a more complex surface electronic structure than previously expected.

TT 7.8 Mon 11:30 POT/0351

Single domain spectroscopic signatures of a magnetic Kagome metal — •Lukasz Plucinski[1], Gustav Bihlmayer[1], Yuriy Mokrousov[1], Yishui Zhou[2], Yixi Su[2], Jonathan Denlinger[3], Aaron Bostwick[3], Christopher Jozwiak[3], Eli Rotenberg[3], Dmitriy Usachov[4], and Claus M. Schneider[1] — [1]FZ Jülich — [2]JCNS/MLZ Garching — [3]ALS/LBNL Berkeley — [4]DIPC San Sebastian

We investigate the magnetic Kagome metal $DyMn_6Sn_6$ using high-resolution micro-focused circular-dichroic angle-resolved photoemission (μ-CD-ARPES) to probe its magnetic and electronic properties. By tuning the kinetic energy to various features of the Dy $4f$ multiplet, we resolve magnetic domains in samples cryo-cooled down to 20 K. Smaller, but clear signatures are detected in the Mn $3p$ levels. The behavior of both Dy $4f$ and Mn $3p$ features are in remarkable agreement with our modeling based on the Hartree-Fock method, revealing ferrimagnetic alignment of Dy and Mn local moments, and further strengthening our interpretation. Adjusting the energy to the Mn $3d$-dominated valence bands reveals signatures which we relate to the orbital magnetization through a comparison to *ab initio* electronic structure calculations. Our study establishes the spectroscopic access to a single magnetic domain in a Kagome metal, paving the way for further research into imaging magnetic phases of novel magnetic materials using μ-CD-ARPES. Preprint is available at https://arxiv.org/abs/2507.12085.

TT 7.9 Mon 11:45 POT/0351

Topologically non-trivial Kondo insulating state in graphene nanoribbons — •Amogh Kinikar[1,2], Guangze Chen[3], Yanwei Gu[4], David Jacob[5,6], Joaquín Fernández-Rossier[7], Gonçalo Catarina[2], António T. Costa[7], Oliver Gröning[2], Carlo Antonio Pignedoli[2], Klaus Müllen[4], Pascal Ruffieux[2], Jose L. Lado[8], Akimitsu Narita[4], and Roman Fasel[2,9] — [1]KIT, Karlsruhe, Germany — [2]Empa, Dübendorf, Switzerland — [3]Chalmers University of Technology, Gothenburg, Sweden — [4]MPIP, Mainz, Germany — [5]UPV/EHU, San Sebastián, Spain — [6]Basque Foundation for Science,Bilbao, Spain — [7]INL, Braga, Portugal — [8]Aalto University, Espoo, Finland — [9]University of Bern, Bern, Switzerland

Metallic rare-earth alloys display characteristic correlated electron phenomena due to interactions between electrons which give rise to a narrow heavy-fermion band near the Fermi level that hybridizes with the metallic band and opens a hybridization gap. When the Fermi level falls within this gap the system forms a Kondo insulator, which can also acquire a topologically non-trivial character. Here we provide evidence for a topological Kondo insulating state in a specific atomically precise graphene nanoribbon synthesized on Au(111) by on surface methods and characterized by scanning probe microscopy. We observe a sharp resonance near the Fermi level and a pronounced zero-bias peak at the ribbon termini. We show that these spectroscopic signatures are a fingerprint of a topological Kondo insulating state in this graphene nanoribbon.

TT 8: Topical Talk Wulfhekel (joint session O/TT)

Time: Monday 9:30–10:15 Location: TRE/PHYS

Topical Talk TT 8.1 Mon 9:30 TRE/PHYS

Vortices, inter-band coupling and inelastic QPI in two band superconductors — •Wulf Wulfhekel — Physikalisches Institut, Karlsruhe Institute of Technology

The majority of superconductors have more than one Fermi surface, on which the electrons pair below the critical temperature, yet their behavior can be well described by a single-band Bardeen-Cooper-Schrieffer theory. This is mostly due to interband scattering, especially in superconductors in the dirty limit, rigidly linking the pairing amplitude of the bands. We here lift this constrain and study the behavior of the ultra-pure two-band superconductor Pb. We show that at low temperatures, it is neither of type I nor type II and superconducting vortices of arbitrary flux quanta can be formed. We show that on the non-spherical Fermi surfaces, a modified index theory is needed for the description of in gap states in vortices. Further, the two condensates are only weakly coupled and can be individually manipulated. By studying stacking fault tetrahedra, we demonstrate local tuning of interband coupling ranging from weak to strong and the modification of the superconducting order parameters from two well separated gaps to one merged gap around defects. The experiments critically test the theory of multiband superconductors and give a route to access a wide range of predicted quantum effects in these systems. Finally, we demonstrate that quasi particle interference is also possible in the inelastic tunneling channel enabling the imaging of standing phonons with STM.

TT 9: 2D Materials: Electronic structure, excitations, etc. I (joint session O/HL/TT)

Time: Monday 10:30–12:30 Location: TRE/MATH

Invited Talk TT 9.1 Mon 10:30 TRE/MATH

Magnetic Order in 2D Materials Beyond Bulk Constraints — •Jeison Fischer — II. Physikalisches Institut, Universität zu Köln

Even though exfoliated microflakes remain widely used in 2D magnetism research, their bulk origin restricts access to many potentially interesting phases, an obstacle that molecular beam epitaxy (MBE) can overcome. MBE enables the controlled synthesis of single-layer materials directly related to, yet often distinct from, their bulk counterparts.

In my talk, I will present structural characterization and discuss the mechanisms behind the formation of such novel 2D materials grown via MBE on graphene. [1-2] The emerging magnetic properties of these new 2D materials will be exemplified with two cases: Cr_2S_3-2D and Fe_2S_2-2D. Cr_2S_3 forms a covalently bonded NiAs-type structure without van der Waals gaps. Using spin-polarized scanning tunneling microscopy (STM) and X-ray magnetic circular dichroism (XMCD), we show that it hosts ferromagnetic coupling within the plane with magnetic moments pointing out-of-plane, combined with A-type antiferromagnetic coupling between different Cr planes. Fe_2S_2 exhibits a unique hexagonal phase, in which Fe atoms occupy tetragonally coordinated sites. Spin-polarized STM reveals that the moments are noncollinear within the plane. We map the in-plane components of two distinct magnetic configurations and find that the moments are confined to the 2D plane, forming a Néel state and a 2Q state.

[1] Knispel et al. Small, 2025 21, 2408044.

[2] Safeer et al. Adv. Funct. Mater. 2025, 202500907.

TT 9.2 Mon 11:00 TRE/MATH

Ab initio modeling of magnons and magnon-phonon coupling in 2D magnetic materials — Ali Esquembre-Kucukalic1[1], Khoa Le[2], Hsiao-Yi Chen[3], Ivan Maliyov[2], Jin-Jian Zhou[4], Davide Sangalli[5], and •Alejandro Molina-Sánchez[1] — [1]ICMUV, University of Valencia, Valencia, Spain — [2]CALTECH, California, USA — [3]Tohoku University, Japan — [4]Beijing Institute of Technology, Beijing, China — [5]ISM-CNR, Roma, Italy

Understanding spin-wave excitations in two-dimensional magnetic materials is essential for advancing spintronic and quantum information technologies. Chromium trihalides and related 2D magnets provide a platform where the choice of halide influences on the magnetic behavior, yet its impact on magnon properties is not completely understood. We present first-principles calculations of magnon dispersions and wave functions in monolayer Cr trihalides using the Bethe-Salpeter equation (BSE), resolving key features such as the topological gap at the Dirac point. The BSE analysis reveals that magnons originate from electronic transitions spanning a wider energy range than excitons, offering new insight magnon character and enabling the extraction of Heisenberg exchange parameters. Building on this framework, we develop an ab initio description of mag-ph coupling by deriving BSE-based mag-ph interaction matrices and applying them to monolayer CrI3 and hydrogenated graphene. We show that mag-ph and electron-phonon couplings differ markedly, identifying specific phonon modes that dominate magnon scattering.

TT 9.3 Mon 11:15 TRE/MATH

Electron-phonon interaction in transition-metal dichalcogenides — •Gerrit Johannes Mann, Thorsten Deilmann, and Michael Rohlfing — Institute of Solid State Theory, University of Münster, Germany

Electron-phonon interaction is a crucial effect in solid state physics, in particular in two-dimensional materials. We developed a generally applicable ab-initio implementation on top of density functional theory using a basis set of localized Gaussian orbitals. It combines finite differences calculations with the perturbative Allen-Heine-Cardona framework in order to calculate the temperature-dependent renormalization of the electronic bandstructure due to electron-phonon interaction. Our implementation circumvents the limiting problems of previous implementations and allows to evaluate Debye-Waller contributions beyond the rigid-ion approximation [1], which are usually neglected.

In addition to the renormalization of the electronic bands, electron-phonon interaction introduces a line broadening due to finite-lifetime effects, which

have recently been incorporated into our implementation. In this presentation, we discuss our results, including those with finite-lifetime effects, for two-dimensional transition-metal dichalcogenides, where the renormalization of the electronic bandstructure due to electron-phonon interaction can be as large as several hundreds of meV.

[1] Mann et al., Phys. Rev. B **110**, 075145 (2024)

TT 9.4 Mon 11:30 TRE/MATH

Surface-state engineering for nonlinear charge and spin photocurrent generation — •Javier Sivianes[1], Peio Garcia-Goiricelaya[2], Daniel Hernangómez-Pérez[3], and Julen Ibañez-Azpiroz[1,4,5] — [1]Centro de Física de Materiales (CSIC-UPV/EHU), Donostia, Spain — [2]University of the Basque Country UPV/EHU, Leioa, Spain — [3]CIC nanoGUNE BRTA, San Sebastián, Spain — [4]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — [5]Donostia International Physics Center (DIPC), Donostia, Spain

We systematically explore the generation of nonlinear charge and spin photocurrents using spin-orbit-split surface states. This mechanism enables net DC flow along the surface plane even in centrosymmetric bulk environments like the Rashba prototype Au(111), where we characterize the main quadratic contributions by combining model predictions with density functional calculations. We further identify the Tl/Si(111) surface as a prime scenario for experimental verification; with slight doping, it develops metallic surface states featuring remarkable relativistic properties deviating from the Rashba paradigm, while the bulk remains semiconducting. Its nonlinear charge photocurrent reveals a distinct angular signature and a magnitude comparable to bulk ferroelectrics, highlighting the potential of surface-state photocurrents for low-bias optoelectronic applications. Moreover, the non-trivial spin texture of its surface states enables the generation of pure out-of-plane spin-polarized currents, offering a highly versatile nonlinear spin-filtering functionality beyond the conventional spin Hall effect.

TT 9.5 Mon 11:45 TRE/MATH

Influence of Vanadium Doping on WSe_2, as seen through ARPES — •Jana Kähler[1,2], Florian K. Diekmann[1,2], Matthias Kalläne[1,2,3], Tim Riedel[1,2], Adina Timm[1,2], Anja Yalim[1,2], Jens Buck[1,2], Meng-Jie Huang[2], Jules M. Knebusch[1,2], Luka Hansen[1,3], Jan Benedikt[1,3], and Kai Rossnagel[1,2,3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Spintronics offers a compelling, energy-efficient alternative to traditional electronics with potential applications in communications, sensing, and information processing. The vanadium-doped layered transition metal dichalcogenide $2H$-WSe_2 is particularly promising as a room-temperature magnetic semiconductor with gate-tunable transport properties. Here, we use a combination of 11 eV laser, 21.2 eV He-lamp, and soft X-ray synchrotron ARPES to highlight the influence of a fairly small vanadium doping on the electronic structure of WSe_2. Both the pristine and doped compounds were grown by chemical vapor transport in our own laboratory.

TT 9.6 Mon 12:00 TRE/MATH

Engineering sulfur vacancy dimers in monolayer WS_2 — •Daniel Jansen[1], Guangyao Miao[1], Jan Keienburg[1], Jeison Fischer[1], Thomas Michely[1], Hannu-Pekka Komsa[2], and Wouter Jolie[1] — [1]Institute of Physics II, University of Cologne, Cologne, Germany — [2]Faculty of Information Technology and Electrical Engineering, University of Oulu, Oulu, Finland

Sulfur vacancies [1] and sulfur vacancy dimers in nearest-neighbor distance [2] in monolayer WS_2 have been experimentally proven to yield bright and stable photon emission, thus holding promises for the development of quantum technologies.

Here we investigate dimers of sulfur vacancies in different configurations in monolayer WS_2 created with the tip of a scanning tunneling microscope [3]. Scanning tunneling spectroscopy reveals strong hybridization of the sulfur vacancy electronic in-gap states, validated by density functional theory calculations. For dimers in nearest-neighbor configuration we find that inelastically tunneling electrons can induce sulfur atom migration, resulting in a rotary motion of the dimer. This motion is studied in detail by analyzing the emerging telegraph noise in the junction. Lastly, we elaborate on scenarios to make use of the dimer motion for the design of vacancy structures and lattices.

[1] Schuler et al., Sci. Adv. **6**, 38 (2020)
[2] Sun et al., Nature Commun. **15**, 9476 (2024)
[3] Jansen et al., Phys. Rev. B **109**, 195430 (2024)

TT 9.7 Mon 12:15 TRE/MATH

Alkali-metal doped transition metal chlorides confined in bilayer graphene: Insights from first-principles calculations — •Munawar Ali[1], Arkady V. Krasheninnikov[2], Giovanni Cantele[1], and Mahdi Ghorbani-Asl[2] — [1]Università degli Studi di Napoli "Federico II," Dipartimento di Fisica "Ettore Pancini," Complesso di Monte S. Angelo, via Cinthia, 80126 Napoli, Italy — [2]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany

The intercalation of atomic and molecular species into layered materials has emerged as a powerful strategy for synthesizing novel two-dimensional systems with tunable electronic, magnetic, and energy-storage properties. Encapsulating transition-metal halides into bilayer graphene has proven effective for stabilizing 2D magnetic phases that are otherwise thermodynamically unstable. Using density functional theory, we systematically investigate the intercalation of metal chlorides (TCl_3, T = Fe, Cu, Mo, Al) doped with alkali metals (Li, Na, K, Rb, Cs) across a range of concentrations. Li- and Na-doped $FeCl_3$, $CuCl_3$, and $MoCl_3$ monolayers exhibit the highest thermodynamic stability, whereas $AlCl_3$ remains unstable even under doping. Bader charge analyses reveal substantial charge transfer from the graphene host to the intercalated layers, particularly in the case of $CuCl_3$, which also shows the strongest binding. These findings provide a theoretical framework for understanding the stability of these heterostructures and highlight alkali-metal-intercalated graphene systems as a platform for engineering tunable 2D magnetic materials.

TT 10: Correlated Electrons: Other Theoretical Topics

Time: Monday 11:00–12:45 Location: HSZ/0103

TT 10.1 Mon 11:00 HSZ/0103

Two site entanglement and maximal correlations in the Hubbard model — Frederic Bippus[1], Anna Kauch[1], •Gergo Roosz[1], Christian Mayrhofer[1], Fakher Assaad[2,3], and Karsten Held[1] — [1]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [2]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg Germany — [3]Würzburg-Dresden Cluster of Excellence ct.qmat, Am Hubland, 97074 Würzburg, Germany

The study of entanglement in strongly correlated electron systems typically requires knowledge of the reduced density matrix. Here, we apply the parquet dynamical vertex approximation to study the two-site reduced density matrix at varying distance, in the Hubbard model at weak coupling. This allows us to investigate the spatial structure of entanglement in dependence of interaction strength, electron filling, and temperature. We compare results from different entanglement measures and benchmark against quantum Monte Carlo. Using the two-site density matrix, we compute the fermionic entanglement negativity, the mutual information between the two sites. We determine the maximal correlation function between the two lattice points.

TT 10.2 Mon 11:15 HSZ/0103

Superconductor-Insulator transition in a two-orbital attractive Hubbard model with Hund exchange — •Laura Torchia and Massimo Capone — International School for Advanced Studies (SISSA), via Bonomea 265, 34136 Trieste, Italy

We study a two-orbital attractive Hubbard model with a repulsive Hund exchange coupling J as an idealized model for a two-band superconductor. This framework is motivated by systems where a strong isotropic electron-phonon coupling drives the on-site Hubbard repulsion U negative while leaving the exchange term unaffected. We solve the model at $T = 0$ and half-filling using DMFT, focusing on the intra-orbital singlet superconducting phase and discarding other possible instabilities, as inter-orbital pairing and a charge-density wave ordering. Already at $J = 0$, the two-orbital model features a superconductor-insulator transition as $|U|$ grows, in contrast with the single-orbital case which remains superconducting for any $U < 0$. We find that a finite J strengthens the effect of the attractive U, both in the normal state and, even more significantly, in the superconducting state. However, this pushes the system towards an effectively stronger coupling, hence to a faster transition to the insulating state.

Similarly to the Mott transition in the repulsive model, the superconductor-insulator transition here is marked by a vanishing quasi-particle weigh Z. This leads to a scenario that recalls strongly correlated superconductivity close to a Mott transition, where pairing is enhanced but phase coherence is rapidly lost, even though the present model is dominated by attractive interactions.

TT 10.3 Mon 11:30 HSZ/0103

Orbital Magnetic Field Driven Metal-Insulator Transition in Strongly Correlated Electron Systems — •Georg Rohringer[1,2] and Anton Markov[3] — [1]Theory and Simulation of Condensed Matter, Department of Physics, King's College London, The Strand, London WC2R 2LS, United Kingdom — [2]I. Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg, Germany — [3]Center for Nonlinear Phenomena and Complex Systems, Université Libre de Bruxelles, CP 231, Campus Plaine, B-1050 Brussels, Belgium

We study the effects of an orbital magnetic field on the Mott metal-insulator transition in the Hubbard-Hofstadter model. We demonstrate that sufficiently large magnetic fields induce a Mott insulator-to-metal phase transition supporting our claim with dynamical mean field theory (DMFT) numerical results. For both competing phases (metal and insulator) we observe a magnetic-field-induced metallization reflected in an enhancement of kinetic and potential energy. We demonstrate that this phenomenon originates from a field-driven redistribution of spectral weight due to the formation of magnetic mini-bands and the Aharonov-Bohm effect experienced by electrons virtually tunneling around an elementary plaquette. Our theoretical results might be relevant for recent experimental studies on magnetic field driven insulator-to-metal transitions in strongly correlated materials such as VO_2,λ-type organic conductors, and moiré multilayers.

TT 10.4 Mon 11:45 HSZ/0103

Probing Green's Function Zeros by Cotunneling through Mott Insulators — •Carl Lehmann[2,3,1], Lorenzo Crippa[4,2,3], Giorgio Sangiovanni[2,3], and Jan Budich[1,2,5] — [1]Technische Universität Dresden, 01069 Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, 97074 Würzburg, Germany — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany — [4]I. Institute of Theoretical Physics, University of Hamburg, Notkestrasse 9, 22607 Hamburg, Germany — [5]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, 01187 Dresden, Germany

Quantum tunneling experiments have provided deep insights into basic excitations occurring as Green's function poles in the realm of complex quantum matter. However, strongly correlated quantum materials also allow for Green's functions zeros (GFZs) that may be seen as an antidote to the familiar poles and have so far largely eluded direct experimental study. Here, we propose and investigate theoretically how cotunneling through Mott insulators enables direct access to the shadow band structure of GFZs. In particular, we derive an effective Hamiltonian for the GFZ that is shown to govern the cotunneling amplitude and reveal fingerprints of many-body correlations clearly distinguishing the GFZ structure from the underlying free Bloch band structure of the system. Our perturbative analytical results are corroborated by numerical data for a one-dimensional model system consisting of a Su-Schrieffer-Heeger-Hubbard model coupled to two single-level quantum dots.

TT 10.5 Mon 12:00 HSZ/0103

Conformal elastic zero modes at isostructural transitions — •Lars Franke[1], Nick Sander[1], and Markus Garst[1,2] — [1]Institute of Theoretical Solid State Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Institute for Quantum Materials and Technology, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

In correlated materials the coupling of the itinerant electrons to the crystal lattice can induce an isostructural instability where the bulk modulus vanishes. This occurs for example at the endpoint of a line of first order Mott metal-insulator transitions or metamagnetic transitions [1]. Interestingly, at such an isostructural instability the acoustic phonons remain non-critical and their velocities are finite. Consequently, the isostructural transition is a genuine mean-field transition without critical microscopic fluctuations. Nevertheless, we demonstrate that four elastic macroscopic zero modes exist. In addition to a soft mode given by a macroscopic volume change, there are three further zero modes corresponding to special conformal transformations. We discuss the consequences for the critical dynamics close to isostructural instabilities as well as realizations in dilational metamaterials.

[1] M. Zacharias, L. Bartosch, M. Garst, PRL 109 (2012) 176401

TT 10.6 Mon 12:15 HSZ/0103

Stabilization of sliding ferroelectricity through exciton condensation — •Matteo D'Alessio[1,2], Daniele Varsano[2], Elisa Molinari[1,2], and Massimo Rontani[2] — [1]University of Modena and Reggio Emilia, Department of Physics, Informatics and Mathematics, Modena, Italy — [2]CNR Nanoscience Institute, Modena, Italy

Sliding ferroelectricity is a phenomenon that arises from the insurgence of spontaneous electronic polarization perpendicular to the layers of two-dimensional (2D) systems upon the relative sliding of the atomic layer constituents. Because of the weak van der Waals (vdW) interactions between layers, sliding and the associated symmetry breaking can occur at low energy cost in materials such as transition-metal dichalcogenides. Here we discuss theoretically this phenomenon by focusing on a prototype structure, the WTe2 bilayer, where sliding ferroelectricity was first experimentally observed. We compute the significant energy band renormalizations of the ground state induced by excitonic effects and show that in the case of bilayer WTe2 - as long as exciton coherence survives - relevant modifications result in the energetics of the system that contribute to stabilize ferroelectricity upon sliding displacement of the layers. We thus show that electron-hole interaction effects can play an important role in sliding ferroelectricity, where they have been neglected up to now.

TT 10.7 Mon 12:30 HSZ/0103

Ising Spin-Orbit Coupling in Three Dimensions — •Tonghua Yu, Eli Gerber, and Benjamin Wieder — Institut de Physique Théorique, Université Paris-Saclay, CEA, CNRS, F-91191 Gif-sur-Yvette, France.

Ising-type spin-orbit coupling (SOC) that produces out-of-plane spin polarization has been extensively explored in nonmagnetic two-dimensional (2D) materials, and has been shown to give rise to intriguing phenomena such as Pauli-limit-violating and spin-triplet superconductivity, SOC-polarized (interacting) topological bands, and high-performance nonvolatile valley spin valve. For 2D systems lying in the xy-plane, Ising SOC enforces that the bulk is nearly S_z-symmetric, in sharp contrast to systems dominated by Rashba or Dresselhaus SOC. Though all known examples of Ising SOC occur in 2D mono- or few-layer systems, there is no mathematical obstruction that restricts three-dimensional (3D) crystals from exhibiting nearly perfect (Ising-like) SOC textures. Using Green's functions and the projected spin spectrum applied to first-principles calculations, we identify 3D materials with Ising SOC that do not decompose into simple van der Waals layers of 2D Ising SOC materials, and we characterize their associated topological properties. Our calculations expand the class of Ising SOC materials and reveal new venues for spintronics and unconventional superconductivity.

TT 11: $PtBi_2$

Time: Monday 11:15–12:30 Location: CHE/0091

TT 11.1 Mon 11:15 CHE/0091

Surface-confined fluctuating superconductivity in the topological semimetal γ-$PtBi_2$ — •Manaswini Sahoo, Luminita Harnagea, Mahdi Behnami, Michele Ceccardi, Sebastian Gass, Sabine Wurmehl, Anja UB Wolter, and Bernd Büchner — Leibniz Institute for Solid State and Materials Research Dresden, Helmholtzstrasse 20, D-01069 Dresden, Germany

$PtBi_2$ has recently emerged as a promising candidate for hosting superconducting topological surface states. While surface-sensitive probes have observed this unique superconductivity, it remains elusive in bulk thermodynamic measurements. Here, we present evidence of superconducting fluctuations at elevated temperatures through AC susceptibility measurements. The real component of the susceptibility exhibits a diamagnetic response below 20 K, accompanied by a finite imaginary component, both indicative of surface-confined superconducting fluctuations. The small superconducting volume fraction supports a surface rather than bulk origin. Complementary magnetoresistance measurements reveal anomalies below this characteristic temperature. These findings establish $PtBi_2$ as a robust platform for exploring topological superconductivity and provide strong motivation for future studies aimed at elucidating the superconducting bulk-surface interplay.

TT 11.2 Mon 11:30 CHE/0091

Engineering Weyl nodes in the nodal-line semimetal $PtBi_2$ — •Ankit Kumar[1,2], Joseph Dufouleur[1], and Bernd Büchner[1,2] — [1]Leibniz Institute for Solid State and Materials Research(IFW) Dresden — [2]Department of Physics, TU Dresden

The nonmagnetic Weyl and nodal-line semimetal $PtBi_2$ has recently been shown an anomalous planar Hall effect (APHE), a phenomenon generated purely by Berry curvature surrounding Zeeman-induced Weyl points. The location of Zeeman-split Weyl nodes along the nodal line can be tuned.

In this work, we investigate the tunability of Weyl physics in $PtBi_2$ through systematic APHE measurements performed under three-dimensional rotations of the magnetic field. By tilting the magnetic field out of plane, we are able to tune the amplitude of the anomalous Hall effect, obtaining a signal stronger or weaker than that measured in-plane. This behaviour provides evidence that the location of Zeeman-induced Weyl nodes can be manipulated by controlling the field orientation.

Our results establish a new pathway to engineer Zeeman-induced Weyl nodes in nodal line semimetals by a magnetic field.

TT 11.3 Mon 11:45 CHE/0091

Low-temperature scanning tunneling spectroscopy on the superconducting Weyl semimetal t-$PtBi_2$ — •Sebastian Schimmel[1], Julia Besproswanny[1], Xiaochun Huang[2], Yanina Fasano[3], Grigory Shipunov[4], Victor Felix Correa[3], José Zabala[3], Luminita Harnagea[5], Sven Hoffmann[1], Bernd Büchner[5], Matthias Bode[2], and Christian Hess[1] — [1]Universität Wuppertal, 42119, Wuppertal, Germany — [2]Universität Würzburg, 97074 Würzburg, Germany — [3]Centro Atómico Bariloche and Instituto Balseiro,8400, Bariloche, Argentina — [4]University of Amsterdam, 1098 XH Amsterdam, The Netherlands — [5]IFW Dresden, 01069, Dresden, Germany

Combining a topologically non-trivial Weyl semimetal nature and surface superconductivity with $T_c > 5$ K, trigonal $PtBi_2$ (t-$PtBi_2$) is a fascinating representative of quantum materials. Intriguingly, large superconducting gaps, comparable to those known from high-T_c superconductors, suggest elevated transition temperatures, and ARPES revealed that the surface superconductivity is confined to Weyl Fermi arcs exhibiting unconventional i-wave symmetry [1,2]. Via low-temperature scanning tunneling spectroscopy, we experimentally address the local electronic properties of the surface of t-$PtBi_2$. Here we report on the temperature dependence of the surface superconductivity and peculiar spectroscopic signatures of its spacially varying electronic structures. The presented results corroborate the unconventional non-trivial electronic properties of t-$PtBi_2$.

[1] A. Kuibarov et al., Nature(2024)
[2] S. Changdar et al., Nature(2025)

TT 11.4 Mon 12:00 CHE/0091

t-$PtBi_2$: Topological Fermi Arcs and Surface Superconductivity from Quasiparticle Interference — •Julia Besproswanny[1], Sebastian Schimmel[1], Sven Hoffmann[1], Gregory Shipunov[2], Saicharan Aswartham[2], Joaquin Puig[3], Yanina Fasano[3], Danny Baumann[2], Riccardo Vocaturo[2], Jorge I. Facio[3], Oleg Janson[2], Jeroen van den Brink[2], Bernd Büchner[2], and Christian Hess[1] — [1]University of Wuppertal, 42119 Wuppertal, Germany — [2]IFW Dresden, 01069 Dresden, Germany — [3]Centro Atómico Bariloche, Instituto Balseiro, 8400 Bariloche, Argentina

Non-centrosymmetric trigonal $PtBi_2$ hosts a rich electronic structure that gives rise to several quantum phenomena. In particular, the coexistence of topological surface states and surface superconductivity suggests that it may be an intrinsic, possibly high-T_c, topological superconductor. ARPES [1] shows that superconductivity in t-$PtBi_2$ is both intertwined with and confined to its topological surface states.

By means of low-temperature scanning tunneling spectroscopy and quasiparticle interference investigations, we probe the local topological and superconducting properties and their interplay on the surface of t-PtBi2. The revealed scattering channels originate from the topological Fermi arcs. These QPI signatures are suppressed in the superconducting state, while re-emerging above B_c – highlighting the close connection between superconductivity and topology.

[1] A. Kuibarov et. al., Nature 626, 294 (2024).

TT 11.5 Mon 12:15 CHE/0091

Phonon and Coulomb mechanism for nodal topological superconductivity on $PtBi_2$ surface — •Kristian Maeland, Giorgio Sangiovanni, and Björn Trauzettel — Institute for Theoretical Physics and Astrophysics, University of Würzburg and Würzburg-Dresden Cluster of Excellence ct.qmat, D-97074 Würzburg, Germany

Experiments show that the Weyl semimetal $PtBi_2$ hosts unconventional superconductivity in its topological surface states. Hence, the material is a candidate for intrinsic topological superconductivity. Measurements indicate nodal gaps in the center of the Fermi arcs. We show that unusually anisotropic electron-phonon coupling on Weyl semimetal surfaces combined with statically screened Coulomb repulsion is a microscopic mechanism for the i-wave pairing. We solve the linearized gap equation close to the critical temperature and find nodal gaps when the surface state bandwidth is comparable to the maximum phonon energy, as is the case in $PtBi_2$.

TT 12: Focus Session: Tunable Correlations in van der Waals Quantum Materials I (joint session TT/DS/HL)

The library of strongly correlated layered materials has intensively grown, giving now access to the full breadth of symmetry broken emergent phases, ranging from excitonic, to magnetic, superconducting, or Mott insulating ground states. At the same time, also the ways of tuning these correlated phases in 2D are steadily developing, e.g, via twisting or stacking, engineered defects, or applied external fields. Taken together, this nowadays allows for sheer endless possibilities to tailor layered correlated quantum materials on demand opening unprecedented avenues towards both deep insights into emergent phenomena and novel functionalization routes based on many-body properties.

This focus session will highlight recent advancements and breakthroughs achieved in this field, which we expect to be of great interest to the broadest audience and to stimulate discussions crossing field boundaries.

Coordinators: Lennart Klebl (Uni Würzburg, Jonas Profe (Uni Frankfurt), Malte Rösner (Uni Bielefeld), Ursula Wurstbauer (Uni Münster)

Time: Monday 15:00–18:15 Location: HSZ/0003

Topical Talk TT 12.1 Mon 15:00 HSZ/0003

Charge confinement in twisted bilayer graphene — •Christoph Stampfer — JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, 52074 Aachen, Germany — Peter Grünberg Institute (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany

Twisted bilayer graphene (tBLG) near the magic angle is a unique platform where the combination of topology and strong correlations gives rise to exotic electronic phases. These phases are gate-tunable and related to the presence of flat electronic bands, isolated by single-particle band gaps. This enables charge confinement and allows to explore the interplay of confinement, electron interactions, band renormalisation and the moiré superlattice, potentially revealing key paradigms of strong correlations. In this talk we will present two experiments where we study charge confinement in tBLG. First, we report on the observation of negative electronic compressibility in tBLG for Fermi energies close to insulating states. To observe this negative compressibility, we take advantage of naturally occurring twist-angle domains that emerge during the fabrication of the samples, leading to the formation of charge islands. Second, we present gate-defined single-electron transistors (SETs) in near-magic-angle tBLG with well-tunable Coulomb blockade resonances. These SETs allow to study magnetic field-induced quantum oscillations in the density of states of the source-drain reservoirs, providing insight into gate-tunable Fermi surfaces of tBLG and open the door to quantum dots and Josephson junction arrays in tBLG.

Topical Talk TT 12.2 Mon 15:30 HSZ/0003

Tuning Coulomb interactions and Hubbard bands in 1T-TaS_2 — •Anna Galler — Institute of Theoretical and Computational Physics, TU Graz, Austria — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany

Monolayer 1T-TaS_2 hosts a star-of-David charge-density wave (CDW) that stabilizes a low-temperature Mott-insulating state. Recent time-resolved spectroscopies indicate a coupling between the CDW amplitude mode and the electronic correlation strength, yet the role of the screened Coulomb interaction remains unclear. Using the constrained random-phase approximation, we show that the CDW amplitude modifies the bare and screened on-site interactions, leading to sizable variations in the effective Hubbard U. Our combined density-functional and dynamical mean-field theory calculations reveal that the Hubbard bands shift in concert with the CDW amplitude, and that a reduced distortion drives a transition from a Mott insulator to a correlated metal. These results demonstrate a direct link between lattice distortions and Coulomb interactions in transition-metal dichalcogenides, providing a microscopic mechanism for light-induced control of correlated phases in two-dimensional quantum materials.

Topical Talk TT 12.3 Mon 16:00 HSZ/0003

Optical signatures of interlayer electron coherence in a bilayer semiconductor — •Nadine Leisgang[1,2], Xiaoling Liu[2], Pavel Dolgirev[2], Philip Kim[2], and Mikhail Lukin[2] — [1]Phillips-Universität Marburg, Germany — [2]Harvard University, United States

Emergent strongly correlated electronic phenomena in atomically thin transition-metal dichalcogenides represent an exciting frontier in condensed matter physics, with examples ranging from bilayer superconductivity and electronic Wigner crystals to the ongoing search for exciton condensation. Here, we take a step towards the latter by reporting experimental signatures of unconventional coupling of interlayer excitons consistent with coherence between interlayer electrons in a transition-metal dichalcogenide bilayer. We investigate naturally-grown MoS_2 homobilayers integrated in a dual-gate device structure allowing independent control of the electron density and out-of-plane electric field. When the bilayer is electron-doped under conditions where tunnelling between layers is negligible, we observe that two interlayer excitons - which normally should not interact - hybridize in a way distinct from both conventional level crossing and anti-crossing. We show that these observations can be explained by quasi-static random coupling between the excitons, which increases with electron density and decreases with temperature. We argue that this phenomenon is indicative of a spatially fluctuating order parameter in the form of interlayer electron coherence - a theoretically predicted many-body state that has yet to be unambiguously established experimentally outside the quantum Hall regime.

15 min. break

Topical Talk TT 12.4 Mon 16:45 HSZ/0003

Faithful modeling of quantum geometry and electronic correlations in van der Waals heterostructures — •Ammon Fischer — Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — Center for Computational Quantum Physics, Flatiron Institute, New York, NY 10010, USA

Moiré materials - twisted stacks of two-dimensional materials - bridge between two influential paradigms of condensed matter research: non-trivial quantum geometry and strong electron-electron interactions. In this talk, I will outline how the construction of faithful low-energy models and their successive treatment by state-of-the-art many-body techniques allows to resolve electronic order in moiré and non-moiré heterostructures from first principles. In twisted bilayers of WSe_2, functional renormalization group techniques allow to unravel the angle evolution of antiferromagnetic order and superconductivity in the crossover regime from weak-to-moderate interactions. In rhombohedral multilayer graphenes, the low-energy theory is naturally described in terms of supercell Wannier functions that span the effective $U(4) \times U(4)$ subspace of the spin, valley and layer degrees of freedom. Electronic correlations give rise to various iso-spin ordered regimes, superconductivity and charge density wave order at low electronic densities bridging to the physics of their twisted counterparts.

Topical Talk TT 12.5 Mon 17:15 HSZ/0003

Mesoscale Atomic Engineering in a Crystal Lattice — •Julian Klein — Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, 02319 MA, USA

Controlling the arrangement of individual atoms with lasers, ion traps, and scanning probe techniques has enabled quantum simulation and computing platforms that transcend naturally occurring configurations of matter. Yet achieving comparable atomic control within a solid and at scale remains a foundational challenge, one that could revolutionize the design of artificial matter. Here, I demonstrate atomic engineering of artificial matter inside a scanning transmission electron microscope. By developing strategies to position and move the electron beam with few-picometer accuracy, deterministic control over atomic motion in both space and time is achieved. Full automation of the microscope enables the creation of three-dimensional defect superlattices in many-nanometer thick CrSBr with user-defined lattice spacing and symmetry, spanning tens of thousands of engineered sites over fields of view exceeding one hundred nanometers, all generated in under an hour. Our results establish atomic engineering in the electron microscope as a practical reality, opening unprecedented opportunities to create quantum defects and quantum phases with tunable charge and spin interactions, and to control host-lattice excitations by arranging atoms in patterns that are commensurate or incommensurate with the underlying crystal over mesoscopic, and potentially micro- or macroscopic, length scales.

TT 12.6 Mon 17:45 HSZ/0003

Interlayer electrodynamics of CDWs in van der Waals materials and heterostructures — Achyut Tiwari, Renjith Mathew Roy, Maxim Wenzel, Christian Prange, Bruno Gompf, and •Martin Dressel — 1. Physikalisches Institut, Universität Stuttgart

Layered transition metal dichalcogenides such as 1T-TaS_2, 2H-TaS_2 and their natural heterostructure $4H_b$-TaS_2 provide a platform for studying interlayer coupling, orbital hybridization, and charge transfer that determine collective electronic phenomena, such as unconventional superconductivity and strong electronic correlations. Temperature-dependent infrared measurements of the in-plane and out-of-plane optical response of 1T-TaS_2 across its CDW-driven metal-insulator transition are combined with DFT calculations. We find that a quasi-1D instability that induces interlayer dimerization is responsible for the MI-transition. Furthermore, spectroscopic ellipsometry combined with an anisotropic Bruggeman effective medium approximation reveals that metallic domains evolve in a strongly anisotropic way and often extend along the out-of-plane direction as the transition proceeds.

When 1T-TaS_2 is stacked between 1H-TaS_2, forming a natural heterostructure of $4H_b$-TaS_2, charge transfer occurs between the layers, that can be tuned with temperature, and which is related to the CDW in 1T-TaS_2 layer. We conclude that the phase transition in 1T-TaS_2 is inherently three dimensional, despite its layered structure, and that interlayer coupling is essential for its electronic structure and phase behavior both individually and in heterostructures.

TT 12.7 Mon 18:00 HSZ/0003

Enhancing Plasmonic Superconductivity in Layered Materials via Dynamical Coulomb Engineering — •Yann in 't Veld[1], Mikhail I. Katsnelson[2,3], Andrew J. Millis[4,5], and Malte Rösner[2,6] — [1]I. Institute of Theoretical Physics, Universität Hamburg, Hamburg, Germany — [2]Institute for Molecules and Materials, Radboud University, Nijmegen, the Netherlands — [3]Constructor Knowledge Institute, Constructor University, Bremen, Germany — [4]Center for Computational Quantum Physics, Flatiron Institute, New York, United States of America — [5]Department of Physics, Columbia University, New York, United States of America — [6]Faculty of Physics, Bielefeld University, Bielefeld, Germany

Conventional Coulomb engineering, through controlled manipulation of the environment, offers an effective route to tune the correlation properties of atomically thin van der Waals materials via static screening. Here we present tunable *dynamical* screening as a method for precisely tailoring bosonic modes to optimize many-body properties. We show that "bosonic engineering" of plasmon modes can be used to enhance plasmon-induced superconducting critical temperatures of layered superconductors in metallic environments by up to an order of magnitude, due to the formation of interlayer hybridized plasmon modes with enhanced superconducting pairing strength. We determine optimal properties of the screening environment to maximize critical temperatures. We show how bosonic engineering can aid the search for experimental verification of plasmon mediated superconductivity.

TT 13: Correlated Electrons: Method Development I

Time: Monday 15:00–18:30 Location: HSZ/0101

TT 13.1 Mon 15:00 HSZ/0101

Real-Frequency Dynamical Mean-Field Theory Without Broadening Inside the Self-Consistency Cycle — •Aleksandrs Zacinskis[1], Frank T. Ebel[2], Sina Shokri[1], Lukas Hellman[1], Fabian B. Kugler[3], Karsten Held[2], and Maurits W. Haverkort[1] — [1]Institute for Theoretical Physics, Heidelberg University — [2]Institute of Solid State Physics, TU Wien — [3]Institute for Theoretical Physics, University of Cologne

Dynamical mean-field theory has become one of the central frameworks for studying strongly correlated electron systems. Real-frequency implementations offer a major advantage by providing direct access to spectral properties without the need for analytic continuation. Most current real-frequency implementations work slightly off the real axis and evaluate $G(\omega+i\Gamma)$ instead of $G(\omega)$, which introduces an artificial broadening and can lead to systematic errors. We present a strictly real-frequency method with zero broadening inside the self-consistency cycle, addressing both the Dyson equation and the "improved estimator" self-energy [PRB 105, 245132]. Our formulation allows the self-energy to be extracted directly from the continued-fraction representation of the impurity Green's function, as obtained from Krylov bases in Lanczos methods, Wilson chains in NRG, or Kernel Polynomial methods. This method completely removes the need for artificial broadening and is applicable to all real-frequency impurity solvers. We compare the zero-broadening self-energy to its finite-broadening counterpart obtained with Exact Diagonalization solver, demonstrating the impact of broadening on accuracy and various quantities.

TT 13.2 Mon 15:15 HSZ/0101

Bath parameterization and multi-orbital physics in cluster DMFT — •Diego Florez-Ablan[1], Carlos Mejuto-Zaera[2], and Massimo Capone[1] — [1]International School for Advanced Studies (SISSA), Via Bonomea 265, 34136 Trieste, Italy — [2]Univ Toulouse, CNRS, Laboratoire de Physique Théorique, Toulouse, France.

Quantum embedding methods such as cluster dynamical mean-field theory (CDMFT) require accurate and reliable impurity solvers and a controlled treatment of the bath in order to be predictive for correlated materials. Building on an efficient selected configuration interaction impurity solver, a systematic analysis of bath discretization effects is presented for one- and two-orbital Hubbard models within Hamiltonian-based CDMFT, focusing on the impact of bath size and parameterization on the zero-temperature Mott transition and on possible tendencies towards symmetry-broken solutions. The study shows that, while large baths yield relatively robust results for the single-band half-filled Hubbard model, small baths can display a non-negligible dependence on parameterization, and that in the two-orbital case some quantitative sensitivity to bath parametrization persists.

Building on this benchmark, the same CDMFT machinery is applied to investigate the Hund metal regime of the two-band Hubbard model, which is relevant for the description infinite-layer nickelates, with the goal of assessing the effects of short-range spatial fluctuations on Hund-driven correlations and how they affect the stability of the Hunds metal phase in the presence of a crystal-field splitting.

TT 13.3 Mon 15:30 HSZ/0101

Uncovering correlated topological phases via a cluster-diagrammatic approach — •Félix Fossati and Evgeny Stepanov — CPHT, CNRS, École polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France

Topological phases exhibit remarkable properties, including protected conducting edge states and robustness against local perturbations. Most studies of topological phenomena have focused on the non-interacting limit, where complete topological classification can be done using a single-particle band structure. While topological properties are known to be robust against weak interactions and disorder, a fundamental question remains: can electronic correlations themselves induce topological phases starting from a trivial non-interacting system? In this work, we address this question by extending the diagrammatic D-TRILEX method to a two-site cluster DMFT reference system. This approach therefore enables capturing short-range correlations non-perturbatively, while treating long-range correlations diagrammatically beyond the cluster DMFT level. We apply our method to the one-dimensional Hubbard model and demonstrate that, by tuning the strength of the non-local Coulomb interaction, our approach captures the formation of both the bond-order-wave (BOW) and the charge-density-wave (CDW) states. We show that the BOW phase can be mapped onto the Su-Schrieffer-Heeger model, while the combined CDW+BOW state corresponds to a Rice-Mele model. The non-trivial topological character of these interaction-induced phases is confirmed by the presence of localised edge states.

TT 13.4 Mon 15:45 HSZ/0101

Cluster extension of the DMF^{2}RG and application to the $2d$ Hubbard model — •Marcel Krämer[1,2,3], Michael Meixner[3], Kilian Fraboulet[3], Demetrio Vilardi[3], Pietro Bonetti[4], Nils Wentzell[5], Alessandro Toschi[2], and Sabine Andergassen[1,2] — [1]Institute of Information Systems Engineering, TU Wien, Vienna, Austria — [2]Institute for Solid State Physics, TU Wien, Vienna, Austria — [3]Max Planck Institute for Solid State Research, Stuttgart, Germany — [4]Department of Physics, Harvard University, Cambdrige, USA — [5]Center for Computational Quantum Physics, Flatiron Institute, New York, USA

The DMF^{2}RG has been introduced to overcome the weak-coupling limitation of the fermionic functional renormalization group (fRG). This approach builds on the idea of exploiting the dynamical mean-field theory (DMFT) as starting point for the fRG flow, thus capturing local non-perturbative correlations via DMFT together with perturbative non-local correlations generated during the flow. We show how non-local non-perturbative correlations can be incorporated in the DMF^{2}RG scheme by employing solutions of non-local extensions of DMFT as a starting point of the flow. The one-loop fRG flow equations are formulated within the single-boson exchange decomposition (SBE), which classifies diagrams contributing to the two-particle vertex in terms of interaction reducibility and has been proven to be a powerful bosonization scheme. We illustrate the ability of this approach to capture non-local non-perturbative correlations in the $2d$ Hubbard model and summarize latest methodological advances.

TT 13.5 Mon 16:00 HSZ/0101

Exact t_{2g}^n super-exchange Hamiltonians for complex orbital ordering — •Amit Chauhan, Xue-Jing Zhang, and Eva Pavarini — Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany

We present a general approach for studying complex orbital ordering in t_{2g}^n correlated systems. The first step consists in building exact super-exchange (SE) Hamiltonians [1-4], projected onto irreducible tensor components. The technique we adopt is suitable both for analytic and efficient numerical calculations. Next, we obtain the total energy- which includes SE, spin-orbit and crystal-field contributions- via a variational Ansatz for the many-body wavefunction. The total energy is then optimized in the chosen parametric space to find the spin and orbitally ordered ground state. Finally, SE theory is combined with DFT+DMFT calculations via an order parameter decomposition scheme. Results for paradigmatic cases are presented.

[1] X.-J. Zhang, E. Koch, E. Pavarini, PRB **105**, 115104 (2022).
[2] X.-J. Zhang, E. Koch, E. Pavarini, PRB **102**, 035113 (2020).
[3] X.-J. Zhang, E. Koch, E. Pavarini, PRB **106**, 115110 (2022).
[4] A. Chauhan, X.-J. Zhang, E. Pavarini (in preparation).

TT 13.6 Mon 16:15 HSZ/0101

Dimer Hubbard operators and their applications — •Jie Xiong and Silke Biermann — CPhT, Ecole Polytechnique, Palaiseau, France

Hubbard operators, introduced in the 1960s as projectors between atomic many-body eigenstates [1], serve as quasiparticle operators that naturally represent the lower and upper Hubbard bands. They also provide one of the earliest systematic approaches for calculating Green's functions in the Hubbard model. Extending this approach, we construct quasiparticle operators for the dimer Hubbard model and propose a general framework for analyzing quasiparticle operators in interacting many-body systems with periodic boundary conditions. As an application, we derive the equations of motion for the dimer Hubbard operators and compute Green's functions for finite benchmark models. Our findings suggest broad prospects for extending the quasiparticle-operator construction to larger correlated systems and exploring its potential applications in topological phases.

[1] J. Hubbard, Proc. R. Soc. Lond. A 276, 238 (1963).

15 min. break

TT 13.7 Mon 16:45 HSZ/0101

Non-perturbative effects of short-range spatial correlations at the two-particle level — •Michael Meixner[1], Matthias Reitner[2], Thomas Schäfer[1,3], and Alessandro Toschi[2] — [1]Max-Planck-Institute for Solid-State Research, Stuttgart, Germany — [2]TU Wien, Vienna, Austria — [3]University of Trieste, Trieste, Italy

Non-local correlations have a strong impact on the electronic dynamics of the square lattice Hubbard model. Specifically, the Mott metal-insulator transition (MIT) occurs at lower interactions when including spatial correlations to the local model via cellular dynamical mean field theory (CDMFT). We present the Bethe-Salpeter equation (BSE) of the charge response and corresponding Ward identities applicable to the CDMFT. The scheme is employed to study the impact of real space bosonic correlations between the impurity sites onto the lattice thermodynamic derivatives such as the charge response. Firstly, we report the occurrence of the break down of self-consistent perturbation theory in the charge channel by observation of the divergence of the irreducible vertex. This is, we find, a precursor of the thermodynamic instability of CDMFT and the corresponding suppression of the charge response at the metal-insulator transition. Secondly, for both phenomena, we underline the essential role of next-neighbour spin correlations.

TT 13.8 Mon 17:00 HSZ/0101

Promising properties of Ghost Gutzwiller Ansatz: from Mott insulators to correlated antiferromagnets — •Antonio Maria Tagliente[1], Michele Fabrizio[1], and Carlos Mejuto-Zaera[2] — [1]International School for Advanced Studies (SISSA) — [2]Laboratoire de Physique Théorique, CNRS, Université de Toulouse, UPS

The ghost Gutzwiller wavefunction is a recently proposed variational Ansatz that generalizes the traditional Gutzwiller wavefunction. It consists of a Slater determinant defined in an enlarged Hilbert space that is variationally projected into the physical one. This wavefunction is therefore naturally capable of describing Hubbard bands and coexisting quasiparticle peaks.

Here, we present several results obtained through this wavefunction treated with the so-called Gutzwiller approximation.

We begin by showing that the wavefunction can describe genuine paramagnetic Mott insulators, whose finite spin susceptibility has remained elusive using other methods. A metal lead in contact with such a Mott insulator can directly reveal the spinon excitations responsible for the paramagnetic behavior, which emerge at the interface as a heavy-fermion band.

We finally demonstrate that the ghost Gutzwiller wavefunction can stabilize a correlated antiferromagnet with spin-unpolarized Hubbard bands but polarized spinons. This solution contains much more entanglement than the conventional dynamical mean-field one, and might be more representative of an actual correlated antiferromagnet in finite dimensions.

TT 13.9 Mon 17:15 HSZ/0101

Fluctuating field theory description of collective instabilities in the doped Hubbard model — •Erik Linnér[1,2], Laura Torchia[1], Silke Biermann[2,3,4], and Massimo Capone[1,5] — [1]International School for Advanced Studies (SISSA), Trieste, Italy — [2]CPHT, CNRS, École Polytechnique, Institut Polytechnique de Paris, Palaiseau, France — [3]Collège de France, Paris, France — [4]European Theoretical Spectroscopy Facility, Palaiseau, France — [5]CNR-IOM, Istituto Officina dei Materiali, Consiglio Nazionale delle Ricerche, Trieste, Italy

Fluctuating field theory is a recently developed method for the description of competing collective fluctuations in correlated electron systems, able to account for spin, charge, and superconducting instabilities. On the basis of a variational principle, the method allows to explicitly account for the leading collective modes and their interplay, with access to electronic and spectroscopic properties. Extending its prior application to the Hubbard model at half-filling, we investigate its description of the doped Hubbard model, accounting for various spin instabilities. Interestingly, unlike for Néel ordering which dominates near half-filling, we show that the phase structure of the fluctuating fields for collective instabilities with arbitrary ordering vector **Q** become important. Within the method, the incommensurate spin ordering driven by doping is associated with a phase structure expressing the modulation of the ordering relative the underlying lattice geometry. Thus, we observe the method, despite its weak-coupling rot, gives an efficient tool to investigate the phase diagram beyond mean-field theory.

TT 13.10 Mon 17:30 HSZ/0101

Competing instabilities for models with non-local and retarded interactions: a functional renormalization group perspective — •Kilian Fraboulet[1,2,3], Aiman Al-Eryani[4], Marcel Gievers[5], Sarah Heinzelmann[3], Friedrich Krien[5], and Sabine Andergassen[2,5] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]Institute of Information Systems Engineering, TU Wien, 1040 Vienna, Austria — [3]Institute for Theoretical Physics and Center for Quantum Science, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen, Germany — [4]Institute for Theoretical Physics III, Ruhr-Universität Bochum, 44801 Bochum, Germany — [5]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria

The functional renormalization group is an established approach to study competing orders in many-electron systems in an unbiased manner, notably with a bosonization technique called single-boson exchange formalism. The resulting fRG approach, referred to as single-boson exchange fRG, is used to analyze competing orders in the 2D extended Hubbard model, especially the growth of the charge-density wave instability when the nearest-neighbor Coulomb repulsion increases. Finally, I will show how one can, using the single-boson exchange fRG, efficiently design a temperature flow (where the temperature is used as flow parameter) for models involving retarded interactions with electron-phonon couplings, such as the Hubbard-Holstein model.

TT 13.11 Mon 17:45 HSZ/0101

Finite-difference parquet method and the strong-coupling pseudogap — Jae-Mo Lihm[1,2], Dominik Kiese[3], Seung-Sup B. Lee[2], and •Fabian B. Kugler[4,3] — [1]Université Catholique de Louvain, Louvain-la-Neuve, Belgium — [2]Seoul National University, Seoul, Korea — [3]Flatiron Institute, New York, USA — [4]University of Cologne, Cologne, Germany

We present the finite-difference parquet method [1], a two-particle diagrammatic approach with nonperturbative input. It takes the fully irreducible two-particle vertex from a reference solution while requiring only its full vertex explicitly. Using dynamical mean-field theory (DMFT) as a reference, this yields a reformulation of the parquet dynamical vertex approximation circumventing ill-behaved two-particle irreducible vertices. We use this method to investigate the pseudogap phase of the underdoped Hubard model. Our numerical results are consistent with diagrammatic Monte Carlo simulations and shed new light on the microscopic mechanism of the strong-coupling pseudogap: With dominant short-ranged antiferromagnetic spin fluctuations, we find an enhanced electron-paramagnon scattering amplitude crucial for the pseudogap opening. The form of this enhancement, reflected in the real part of the Hedin vertex, requires strong local correlations from DMFT as well as nonlocal correlations in multiple two-particle channels from solving the parquet equations.

[1] https://arxiv.org/abs/2505.20116

TT 13.12 Mon 18:00 HSZ/0101

Strong-coupling functional renormalization group: non-Fermi liquid physics in the infinite-U Hubbard model — Jonas Arnold, Peter Kopietz, and •Andreas Rückriegel — Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Straße 1, 60438 Frankfurt, Germany

Exact functional renormalization group (FRG) flow equations for quantum systems can be derived directly within an operator formalism without using functional integrals. This simple insight allows us to apply unbiased FRG methods directly to strongly correlated electron systems with projected Hilbert spaces. Here, we use this approach to compute the electronic spectral function of the Hubbard model at infinite on-site repulsion where many-body states involving doubly occupied lattice sites are eliminated from the physical Hilbert space. For a square lattice with nearest-neighbor hopping we find that the finite-temperature electronic spectrum evolves from a Fermi liquid at low densities to an incoherent non-Fermi liquid at larger densities. Both at high and low densities, the volume of the Fermi surface is not constrained by Luttinger's theorem.

TT 13.13 Mon 18:15 HSZ/0101

Nagaoka kinetic ferromagnetism in the infinite-U Hubbard model — •Jonas Arnold, Peter Kopietz, and Andreas Rückriegel — Institut für Theoretische Physik, Universität Frankfurt, Max-von-Laue Straße 1, 60438 Frankfurt, Germany

We present a study of the infinite-U Hubbard model using an extension of the functional renormalization group (FRG) that works directly with non-canonical fermionic operators. Thus the projected Hilbert space is incorporated exactly, yielding an unbiased diagrammatic method that works in the thermodynamic limit, suitable to capture the long range physics of the strongly correlated electrons. We discuss the magnetic phase diagram for the full range of hole doping. Upon increasing the density, we identify a paramagnetic ground-state, followed by an antiferromagnetic stripe order and finally Nangaoka's kinetic ferromagnetism at high densities. The dynamical susceptibilities reveal the evolution of a paramagnon band into a diffusive continuum with increasing electron density.

TT 14: Superconductivity: Properties and Electronic Structure

Time: Monday 15:00–18:15 Location: HSZ/0103

TT 14.1 Mon 15:00 HSZ/0103

Tuning the superconducting dome in granular aluminum thin films — Aniruddha Deshpande, Jan Pusskeiler, Christian Prange, Uwe Rogge, Martin Dressel, and •Marc Scheffler — 1. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany

The peculiar superconducting properties of granular aluminum, which consists of nanometer-sized aluminum grains separated by aluminum oxide, are attractive for applications in quantum circuitry, and they are interesting from a fundamental materials physics view. The phase diagram of granular aluminum as a function of normal-state resistivity features a superconducting dome with a maximum critical temperature T_c well above the T_c = 1.2 K of pure aluminum. We show how the maximum of this superconducting dome grows if the substrate temperature during deposition is lowered from 300 K to cooling with liquid nitrogen (150 and 100 K) and liquid helium (25 K). The highest T_c that we observe is 3.27 K [1]. These results highlight that granular aluminum is a model system for complex phase diagrams of superconductors and demonstrate its potential in the context of high kinetic inductance applications, where materials properties can be carefully tuned by optimized thin-film growth [2]. This is augmented by our observation of comparably sharp superconducting transitions of high-resistivity samples grown at cryogenic temperatures and by a thickness dependence even for films substantially thicker than the grain size [1].

[1] A. Deshpande *et al.*, J. Appl. Phys. **137** (2025) 013902
[2] A. Deshpande *et al.*, Physica C **634** (2025) 1354709

TT 14.2 Mon 15:15 HSZ/0103

Two facets of kinetic inductance in Corbino reflectometry on disordered and granular superconductors — •Jan Pusskeiler[1], Martin Dressel[1], Thomas Valentin[2], Ameya Nambisan[2], Simon Geisert[2], Ioan Pop[1,2], Christoph Strunk[3], Dennis Rieger[4], and Marc Scheffler[1] — [1]1. Physikalisches Institut, Universität Stuttgart — [2]Physikalisches Institut and IQMT, KIT — [3]Institut für Experimentelle und Angewandte Physik, Universität Regensburg — [4]Qinu GmbH, Karlsruhe

Kinetic inductance L_{kin} manifests as a linear-in-frequency contribution to the reactance, which determines the low-temperature electrodynamics of superconducting microwave circuitry. We directly probe this inductive response from MHz- to GHz-frequencies, $\mathrm{Im}(Z) = \omega \cdot L_{kin}$, by broadband microwave reflectometry on superconducting granular aluminum and titanium nitride in the Corbino geometry. Furthermore, we identify an unconventional collective mode with a phase velocity governed by L_{kin}. We observe an acoustic dispersion relation for

up to 10 harmonics, which enables us to obtain the kinetic inductance independently for both phenomena observed in one spectrum.

We report low-temperature kinetic inductances ranging from 20 pH/□ to 2 nH/□ for granular aluminum and up to 6.2 nH/□ for titanium nitride thin films, with critical temperatures T_c ranging from 1 K to 3 K. We calculate the low-temperature superfluid stiffness J_0 and observe its suppression with increased normal-state resistivity ρ_n. For both materials in regimes with large ρ_n, we find that J_0 converges to T_c, consistent with a phase-driven superconducting transition.

TT 14.3 Mon 15:30 HSZ/0103

Strange metals studied by EELS and RIXS — •Jörg Fink — IFW-Dresden, Dresden, Germany

Strange metal behavior, which occurs above the dome of unconventional superconductivity is characterized by a linear temperature dependence of the resistivity. This signals a breakdown of the quasiparticle concept used in normal Fermi liquids. In the phenomenological marginal Fermi liquid (MFL) theory the behavior is related to a continuum of low-energy electronic excitations. Holographic theories have predicted that this continuum causes an overdamping of plasmon excitations. On the other hand, our EELS and RIXS experiments reveal well pronounced optical and acoustic plasmons in cuprates and ruthenates. The contradiction can be explained by an energy-dependent effective mass related to a strong coupling of the charge carriers to an oscillator at about 0.4 eV also detected in ARPES experiments. Moreover, this energy is used as a cutoff energy in the MFL theory. The oscillator energy is well below the plasmon energies which leads to resilient quasiparticles at high energy. Possibly, the oscillator is related to a coupling of the charge carriers to spin fluctuations.

TT 14.4 Mon 15:45 HSZ/0103

ARPES and RIXS combined in the recently designed "TOF-PAX-RIXS" spectrometer — •Chafic Fawaz[1], Tom Lacmann[1], Olena Tkach[2], Sergii Chernov[3], Luis Filsinger[1], Yaryna Lytvynenko[2], Jan Schunck[4], Olena Fedchenko[2], Siegmar Roth[1], Harshit Agarwal[2], Markus Scholz[3], Jayjit Dey[3], Kai Rossnagel[5], Martin Beye[4], Mortiz Hoesch[3], Gerd Schönhense[2], Hans-Joachim Elmers[2], and Matthieu Le Tacon[1] — [1]Karlsruher Institut für Technologie (KIT), Germany — [2]Johannes Gutenberg Universität Mainz, Germany — [3]Deutsches Elektronen-Synchrotron DESY, Germany — [4]Stockholm University, Sweden — [5]Christian-Albrechts-Universität zu Kiel (CAU), Germany

The TOFPAXRIXS instrument, recently commissioned on the P04 beamline at DESY, offers a compact design that uniquely combines Angle-Resolved Photoemission Spectroscopy (ARPES) with a Time-of-Flight (ToF) detector and Resonant Inelastic X-ray Scattering (RIXS) using the Photoelectron spectrometry for Analysis of X-rays (PAX) approach [1]. This enables direct correlation between electronic properties measured by ARPES and collective excitations probed by RIXS, an essential step toward understanding electronic order in quantum materials, including unconventional superconductors, antiferromagnets, and van der Waals heterostructures.

In this talk, I will briefly introduce the ToF-PAX-RIXS concept and show first results combining ARPES and RIXS on the same sample.

[1] G. L. Dakovski et al., J Synchrotron Rad. 24 (2017) 1180

TT 14.5 Mon 16:00 HSZ/0103

On-site two-hole Coulomb energy in CuO and La_2CuO_4 from coincidence electron spectroscopy — •Danilo Kühn[1], Swarnshikha Sinha[1,2], Fredrik O. L. Johansson[3], Katarzyna Siewirska[1], Antonello Tebano[4], Nils Mårtensson[3], Andreas Lindblad[3], Daniele Di Castro[4], and Alexander Föhlisch[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [2]Universität Potsdam, Potsdam, Germany — [3]Uppsala University, Uppsala, Sweden — [4]Universitá di Roma Tor Vergata, Roma, Italy

The high temperature superconductivity in layered cuprates is likely driven by strong electron correlations, though not fully understood. Here, Auger photoelectron coincidence spectroscopy (APECS) data of undoped La_2CuO_4 and CuO from the COESCA station at the BESSY II storage ring will be shown [1]. O 1s/KVV and Cu 2p/ LVV coincidence measurements allow to disentangle the various structures in the Auger spectra and give detailed information of site specific multi-hole valence states. The Auger spectra are analysed with Cini-Sawatzky and atomic multiplet models, in order to extract electronic parameters such as on-site Coulomb energy in O 2p and Cu 3d orbitals. Dynamics of the core excited states and delocalization of the multi-hole states are investigated. Our unique setup with ARTOF 2 time-of-flight spectrometers in combination with the tailored photon-pulse structure of a soft x-ray undulator beam line enables APECS with unprecedented information rate.

[1] D. Kühn et al., Nat. Commun. 16, 9748 (2025)

TT 14.6 Mon 16:15 HSZ/0103

Signatures of the Fermi surface reconstruction of a doped Mott insulator in a slab geometry — •Gregorio Staffieri and Michele Fabrizio — International School for Advanced Studies (SISSA), Via Bonomea 265, I-34136 Trieste, Italy

In the underdoped regime of high-T_c superconductors, the Fermi surface consists of small pockets coexisting with a pseudogap at the antinodal points, while in the overdoped regime it becomes large and electron-like. Evidence for this doping-driven reconstruction has been found in the two-dimensional single-band Hubbard model using various numerical methods.

We study the reconstruction of the Fermi surface in a hole-doped Mott insulator with slab geometry using the Dynamical Cluster Approximation (DCA). We show that enhanced correlations at the surface lead to a strong layer dependence of the Fermi surface: hole-like pockets appear in the superficial layers and gradually evolve into a single electron-like surface in the innermost layers. We also investigate Friedel oscillations induced by the surface as a function of hole doping and identify clear signatures of the reconstruction in their periodicity. In addition, we introduce a computationally tractable quantity that diagnoses the same variation through a concurrent breakdown of Luttinger's theorem. Together, these observables provide reliable indicators of Fermi surface topology without requiring momentum-space periodization.

15 min. break

TT 14.7 Mon 16:45 HSZ/0103

How to activate and detect the Higgs mode in superconductors — •Dirk Manske — Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany

Higgs Spectroscopy is a new and emergent field [1-3] that allows to classify and determine the superconducting order parameter by means of ultra-fast optical spectroscopy. There are two established ways to activate the Higgs mode in superconductors, namely a single-cycle *quench* or an adiabatic, multicycle *drive* pulse. In the talk I will review and report on the latest progress on Higgs spectroscopy, in particular on the role of the third-harmonic-generation (THG) [4-6,9] and the possible IR-activation of the Higgs mode by impurities or external dc current [7,8]. Finally, I discuss recent results on Non-Equilibrium Anti-Stokes Raman Scattering (NEARS) [10,11], where the Higgs mode, for the first time, has been observed directly.

[1] L. Schwarz, D. Manske et al., Nat. Commun. 2020
[2] L. Schwarz and D. Manske, Phys. Rev. B 2020
[3] H. Chu, S. Kaiser, D. Manske et al., Nat. Commun. 2020
[4] L. Schwarz, R. Haenel, and D. Manske, Phys. Rev. B 2021
[5] H. Chu, S. Kaiser, D. Manske et al., Nature Commun. 2023
[6] M.-J. Kim, S. Kaiser, D. Manske et al., Sci. Adv. 2024
[7] M. Puviani, L. Schwarz, X.-X. Zhang, S. Kaiser, and D. Manske, Phys. Rev. B 2020
[8] R. Haenel, P. Froese, D. Manske, and L. Schwarz, Phys. Rev. B 104, 2021
[9] L.Schwarz, B. Fauseweh, and D. Manske, Phys. Rev. B 2020
[10] T. Glier, D. Manske et al., Nature Comm. 2025
[11] M. Puviani, R. Haenel, and D. Manske, Phys. Rev. 2023

TT 14.8 Mon 17:00 HSZ/0103

Probing Charge Density Wave in Superconductors via Phase-resolved Higgs Spectroscopy — •Liwen Feng[1], Igor Ilyakov[2], Jan-Christoph Deinert[2], Hao Chu[3], and Stefan Kaiser[1] — [1]TUD Dresden University of Technology, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [3]Shanghai Jiao Tong University, China

Superconductivity (SC) and charge density wave (CDW) orders often coexist in high-Tc superconductors, and their interplay is essential for understanding these correlated systems. Using high-field terahertz radiation, we coherently drive collective modes and investigate third-harmonic generation (THG) in superconductors exhibiting both CDW amplitude fluctuations and Higgs oscillations. In 2H-$NbSe_2$ and hole-doped $La_{2-x}Sr_xCuO_4$, we identify a clear Fano interference between CDW fluctuations and Higgs oscillations [1, 2]. In contrast, electron-doped $La_{2-x}Ce_xCuO_4$ shows distinct coupling behavior, revealing not only a weak Higgs-CDW interaction but also signatures of an intrinsic, field-depinned CDW [3]. These results establish THz phase-resolved Higgs spectroscopy as a powerful method for probing CDW dynamics and intertwined orders in superconductors.

[1] H. Chu et al., Nat Commun. 14 (2023) 1343
[2] L. Feng et al., Phys Rev B 108 (2023) L100504
[3] L. Feng et al., arXiv:2504.11947 (2025)

TT 14.9 Mon 17:15 HSZ/0103

Probing the intermediate state of the type-I topological superconductor SnAs using Muon Spin Spectroscopy — •Shashank Srivastava[1], Omkar Kulkarni[1], Arushi Arushi[1], Deepak Singh[2], Adrian D. Hillier[2], and Ravi Prakash Singh[1] — [1]Indian Institute of Science Education and Research, Bhopal 462066, India — [2]ISIS Facility, STFC Rutherford Appleton Laboratory, Didcot OX11 0QX, United Kingdom

The possibility of topological superconductivity in a type-I superconductor embraces exotic physics. The topological semimetal SnAs shows superconductivity below 3.6 K, but there is ambiguity in the nature of superconductivity. Some reports claim type-I superconductivity in SnAs, but recent studies contradict it. We have resolved this enigma using a thorough microscopic analysis of the superconducting ground state.

In this work, we report the muon spin rotation/relaxation (μSR) study of the possible topological superconductor SnAs. The zero-field (ZF) μSR data reveal that this system is a time-reversal-invariant superconductor. The systematic transverse field (TF) μSR measurements unveil the type-I superconductivity and the intermediate state using the superconducting phase diagram for SnAs. Moreover, ab initio calculations of band structure and phonons were performed, which correlate with the basic experimental characterization. Our study opens a platform for understanding the underlying physics behind the origin of topological superconductivity in type-I superconductors.

TT 14.10 Mon 17:30 HSZ/0103

Layer-selective Cooper pairing in an alternately stacked transition metal dichalcogenide — Haojie Guo[1], •Sandra Sajan[1], Irián Sánchez-Ramírez[1], Tarushi Agarwal[2], Alejandro Blanco Peces[1], Chandan Patra[2], Maia G. Vergniory[1], Rafael M. Fernandes[3], Ravi Prakash Singh[2], Fernando de Juan[1], Maria N. Gastiasoro[1], and Miguel M. Ugeda[1] — [1]Donostia International Physics Center, Paseo Manuel de Lardizábal 4, 20018 San Sebastián, Spain — [2]Department of Physics, Indian Institute of Science Education and Research Bhopal, 462066 Bhopal, India — [3]Department of Physics, The Grainger College of Engineering, University of Illinois Urbana-Champaign, Urbana, Illinois 61801, USA

Multigap superconductivity occurs when different superconducting gaps form on separate Fermi surfaces. In the layered material 4Hb-TaSSe, made of alternating trigonal (H) and octahedral (T) polymorph layers, we demonstrate the presence of two weakly coupled and spatially separated superconducting condensates. Using quasiparticle tunneling and Andreev reflection spectroscopy on each polymorph layer, we identify two gaps that differ in magnitude and internal structure. Their responses to temperature and magnetic field also differ: each gap opens at a distinct temperature and shows opposite resilience to magnetic fields, enabling selective external tuning of each condensate. A theoretical model supported by ab-initio calculations reproduces these features and accounts for the unusually high critical field in the T-layer, highlighting TMD polymorphs as tunable multigap superconductors.

TT 14.11 Mon 17:45 HSZ/0103

Probing hidden vortices and geometrical effect via surface-projected quasiparticle states — •Ruijun Xi and Hao Zheng — Tsung-Dao Lee Institute, Shanghai Jiao Tong University, Shanghai, China

Vortices host quasiparticle excitations such as Caroli-de Gennes-Matricon (CdGM) or Majorana states. Understanding how these states are modulated by various geometrical structures is essential for both fundamental superconductivity research and quantum device design. Yet, this relationship remains challenging to elucidate. Here, using a scanning tunneling microscope equipped with a dilution refrigerator, we clearly resolve coherent quasiparticle states from lateral vortices buried beneath the surface of $NbSe_2$ under in-plane magnetic fields. Our combined spectroscopic visualization and model calculation uncover a depth-dependent quantum coupling behavior between vortices and the superconductor surface: shallow vortices (depth of ~ 1.5 coherence lengths) exhibit anomalous split quasiparticle states accompanied by a pseudogap, while deeper vortices (> 4 coherence lengths) restore the conventional CdGM characteristics. Our findings establish a rescaling law of vortex bound states under geometrical effect and identify a critical length scale relevant for superconducting devices aimed to utilize intrinsic vortex quasiparticles.

TT 14.12 Mon 18:00 HSZ/0103

Crystal Structure Effects on Vortex Dynamics in Superconducting MgB_2 Films — •Clemens Schmid[1], Corentin Pfaff[2], Theo Courtois[2], Anton Pokusinskyi[3], Alexander Kasatkin[4], Karine Dumesnil[2], Stephane Mangin[2], Thomas Hauet[2], and Oleksandr Dobrovolskiy[3] — [1]Faculty of Physics and Vienna Doctoral School in Physics, University of Vienna, Austria — [2]Institute Jean Lamour, Université de Lorraine-CNRS, Vandoeuvre-lès-Nancy, France — [3]Cryogenic Quantum Electronics, EMG and LENA, Technische Universität Braunschweig, Germany — [4]G. V. Kurdyumov Institute for Metal Physics, NAS Ukraine, Kyiv, Ukraine

MgB_2 offers one of the highest critical temperatures among non-cuprate superconductors. However, its dynamic phase diagram at high vortex velocities remains unexplored, and the film structure and interface quality are expected to affect the current-driven resistive transition. Here, we investigate two different structures incorporating MgB_2 thin films sputtered on sapphire (Al_2O_3) substrates. The difference between the films is in the inclusion of an additional MgO layer between the substrate and MgB_2, resulting in a single crystal structure, as opposed to an MgO-free textured one. We find that the activation energy for vortex motion is a factor of two higher for the single-crystal film. Current-voltage measurements reveal multiple jumps, suggesting that the transition to the normal state is driven by the formation of normal domains. Additionally, a lower instability current in the textured film suggests less efficient heat removal, which agrees with the results of an HRTEM inspection of the film-substrate interface.

TT 15: Topology: Majorana Physics

Time: Monday 15:00–18:30 Location: HSZ/0105

TT 15.1 Mon 15:00 HSZ/0105

Negative hybridization: a potential cure for braiding with imperfect Majorana modes — Cole Peeters, Themba Hodge, and •Stephan Rachel — School of Physics, University of Melbourne, Australia

Majorana zero modes, the elementary building blocks for the quantum bits of topological quantum computers, are known to suffer from hybridization when they get too close to each other. In that case, their wavefunctions start to overlap and the energy of the Majorana zero modes is pushed to finite energies. This breaking of the ground-state degeneracy leads to an accumulation of error during a braid–the fundamental process which encodes topological quantum gates. Here we show that, in certain situations, the energy splitting of the Majorana wavefunctions can become *negative* which can be utilized to reduce the average hybridization energy of the total braid. We discuss two instructive examples where *negative hybridization* improves the braiding performance to the point where imperfect Majorana modes have their non-Abelian statistics restored, resulting in successfully operated quantum gates. The upshot is that negative hybridization as an intrinsic property of Majorana modes has the potential to bring a Majorana-based quantum computer closer to reality.

TT 15.2 Mon 15:15 HSZ/0105

Distinguishing Majorana bound states from accidental zero-energy modes with a microwave cavity — Sarath Prem[1], •Olesia Dmytruk[2], and Mircea Trif[1] — [1]International Research Centre MagTop, Institute of Physics, Polish Academy of Sciences, PL-02668 Warsaw, Poland — [2]CPHT, CNRS, Ecole polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France

Detecting Majorana bound states (MBSs) in hybrid nanowires is challenging as their transport measurement signatures can be mimicked by trivial zero-energy Andreev bound states (ABSs) or zero-energy quasi-Majorana bound states (QMBSs). We propose an alternative approach that relies on microwave absorption visibility that is extracted from parity-dependent cavity-nanowire susceptibility measurements. We study a one-dimensional Rashba spin-orbit nanowire with an s-wave superconductor-covered proximitized region and an uncovered quantum dot region subjected to a magnetic field with spatially varying capacitive coupling to a single-mode cavity. True MBSs yield a visibility extremum only when both Majorana modes at superconducting edges simultaneously couple to the cavity exhibiting their nonlocal characteristics. In contrast, the zero-energy ABSs or QMBSs show a visibility extremum even when the cavity couples only locally to part of the nanowire. Owing to the recent experiments on poor man's Majoranas, we show that the visibility retains the nonlocal detection features.

[1] S. Prem, O. Dmytruk, and M. Trif, arXiv:2509.13194

TT 15.3 Mon 15:30 HSZ/0105

Scaling up a quantum dot Kitaev chain — Chun-Xiao Liu, Sebastian Miles, Alberto Bordin, Sebastiaan ten Haaf, Greg Mazur, Mert Bozkurt, and •Michael Wimmer — QuTech and Kavli institute of nanoscience, TU Delft, The Netherlands

Superconducting quantum dot devices can be used to implement a Kitaev chain, and tuned reliably into a topological phase. Recent experiments have succesfully implemented two- and three-site Kitaev chains [1,2]. In this talk, I discuss challenges of scaling up to longer chains and how to overcome them. To this end,

I will show that the relative phase between sites in a quantum dot Kitaev chain can be adjusted by electrostatic means only. Finally, I will compare our theory to recent experiments.
[1] T. Dvir *et al.*, Nature **614** (2023) 445
[2] S.L.D. ten Haaf *et al.*, Nature **641** (2025) 890

TT 15.4 Mon 15:45 HSZ/0105

Experiments on hybrid topological insulator superconductor nanostructures — •Jakob Schluck, Ella Nikodem, and Yoichi Ando — Institute of Physics II, University of Cologne

Hybrid structures of topological insulators and conventional s-wave superconductors are predicted to generate topological superconductivity, which can host Majorana zero modes [1]. These quasiparticle excitations display non-Abelian exchange statistics and hold great potential for quantum computation [2]. Recently, we studied for the first time the phase-tunable density of states in topological insulator Josephson junctions via tunneling measurements [3]. The periodic gap closing and reopening can be interpreted as a signature of a topological phase transition. Furthermore, we established a new platform for experiments on topological superconductivity, the topological nano-SQUID [4]. By contacting top and bottom surface of the topological insulator simultaneously, we realize a scenario, where an in-plane magnetic field is sufficient to reliably reach the topological regime. In my talk, I will focus on the ongoing experimental efforts building on these achievements.
[1] L. Fu and C. L. Kane, Phys. Rev. Lett. 100 (2008) 096407
[2] C. Nayak et al., Rev. Mod. Phys. 80 (2008) 1083
[3] J. Schluck et al., arXiv:2406.08265v2
[4] E. Nikodem et al., arXiv:2412.07993v3

TT 15.5 Mon 16:00 HSZ/0105

Characterization of side-contacted topological-insulator-nanowire junctions — •Ella Nikodem, Jakob Schluck, and Yoichi Ando — II. Physikalisches Institut, Universität zu Köln

Superconducting hybrid devices based on topological insulator (TI) nanowires are a promising platform for realizing topological superconductivity and hosting Majorana zero modes (MZMs). We report our recent efforts to realize high-quality Josephson junctions based on etched BiSbTeSe2 nanowires laterally sandwiched with superconducting Nb. This device architecture enables full surface proximitization and forms an intrinsic columnar nano-SQUID, in which the top and bottom surfaces act as parallel SNS junctions. Upon threading a magnetic flux, we observe two key phenomena: (1) robust SQUID-like oscillations of the critical current with the periodicity of the superconducting flux quantum, confirming surface-dominated supercurrent [1]; and (2) a large gate- and field-tunable Josephson diode effect [2]. Conceptually, this device geometry allows for individual tuning of the phase difference of the top and bottom junctions, enabling the creation of a discrete vortex at the end of the nanowire that hosts a MZM [3]. This is substantiated by theoretical considerations based on both a phenomenological approach and full 3D tight-binding simulations. Preliminary tunnel spectroscopy results further pave the way towards detecting Majorana bound states in this platform.
[1] E. Nikodem et al., https://arxiv.org/abs/2412.07993
[2] E. Nikodem et al., Sci. Adv. 11 (2025) eadw4898
[3] L. Fu and C. Kane, Phys. Rev. Lett. 100 (2008) 096407

TT 15.6 Mon 16:15 HSZ/0105

Towards microwave measurements of topological insulator nano-SQUID devices — •Jorge Esteban Bolio, Lucas Marten Janssen, Ella Nikodem, Jakob Schluck, Christian Dickel, and Yoichi Ando — Physics Institute II, University of Cologne, Zülpicher Str. 77, 50937 Köln, Germany

A topological insulator (TI) nanowire side contacted by superconducting leads gives rise to a TI nano-SQUID formed by the two parallel S-N-S Josephson junctions of the top and bottom surface. This platform is expected to exhibit a robust topological phase. While DC measurements in this platform have been performed [1,2], microwave measurements can also illuminate the junction quality and open a path for fast and robust detection of Majorana zero-modes (MZMs) [3]. We describe the integration of the TI nano-SQUID into a 3D transmon setup, and report our progress in the development of a dual nano-SQUID device where the overlap between two MZMs could be gate controlled.
[1] Nikodem et al. arXiv:2412.07993 (2024)
[2] Nikodem et al. Sci. Adv. 11 (2025) eadw4898
[3] E. Ginossar & E. Grosfeld, Nat. Commun. 5 (2014) 4772

TT 15.7 Mon 16:30 HSZ/0105

Poor man's Majorana bound states in quantum dot based Kitaev chain coupled to a photonic cavity — •Francesco Buonemani[1], Alvaro Gomez-Leon[2], Marco Schiro[3], and Olesia Dmytruk[1] — [1]CPHT, CNRS, Ecole polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France — [2]Institute of Fundamental Physics IFF-CSIC, Calle Serrano 113b, 28006 Madrid, Spain — [3]JEIP, UAR 3573 CNRS, College de France, PSL Research University, 11, place Marcelin Berthelot, 75231 Paris Cedex 05, France

Majorana bound states (MBSs) in topological superconductors, given their robustness against external perturbations, are the ideal building blocks for quantum computation. In light of this, poor man's Majorana bound states (PMMBSs), isolated zero-energy bound states, promise to engineer Majorana bound states in a highly tunable setup consisting of a chain of quantum dots that are connected via superconductors.

We analyze the interaction between the minimal microscopic dot chain with proximity-induced superconductivity for PMMBSs and a single mode photonic cavity. We showed how the coupling to the light in the microscopic model leads to a different phenomenology compared to the case where the coupling was introduced in the two-site Kitaev chain model. Thus, we demonstrated that even starting from the microscopic quantum dot model coupled to photons, it is possible to control the sweet spot condition, for the emergence of PMMBSs, through the cavity parameters.

15 min. break

TT 15.8 Mon 17:00 HSZ/0105

Proximity-induced superconducting states in high Chern number quantum anomalous Hall heterostructures — Alejandro S. Gómez[1,2], Rafael A. Molina[3], Pablo Burset[1,2,4], and •Yuriko Baba[2,3] — [1]Universidad Autónoma de Madrid, Madrid, Spain — [2]IFIMAC-UAM, Madrid, Spain — [3]Instituto de Estructura de la Materia IEM-CSIC, Madrid, Spain — [4]Instituto Nicolás Cabrera-UAM, Madrid, Spain

Multilayer stackings of magnetically doped and undoped topological insulators can host multiple chiral channels forming a high Chern number quantum anomalous Hall (QAH) state [1]. This topological state does not require an external magnetic field. Therefore, a single channel QAH proximized by an s-wave superconductor has been proposed as a promising platform to achieve topological superconductivity and chiral Majorana modes [2,3]. In this work, we generalize these proposals to the case of heterostructures with multiple chiral states proximitized by a superconductor. We theoretically study the topological phases of the bulk system and the appearance of zero-energy states due to the bulk-boundary correspondence in the band inversion regime. Finally, we discuss the nature and topological protection of the zero-energy states against disorder and finite-size confinement effects.
[1] Y.F. Zhao et al. Nature 588 (2020) 419
[2] X.L. Qi, T.L. Hughes, S.C. Zhang Phys. Rev. B 82 (2010) 184516
[3] A. Udayet al., Nat. Phys. 20 (2024) 1589

TT 15.9 Mon 17:15 HSZ/0105

Braiding of Majorana wave packets at surfaces of noncentrosymmetric superconductors — •Georg Heedt[1], Clara Johanna Lapp[1,2], Julia Monika Link[1,2], and Carsten Timm[1,2] — [1]TU Dresden, 01062 Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, 01062 Dresden, Germany

Broken inversion symmetry in noncentrosymmetric superconductors causes singlet-triplet mixing of Cooper pairs. If the triplet pairing is sufficiently strong flat zero-energy Majorana surface bands are expected. We describe such a system in terms of a finite concentration of localized Majorana wave packets, which may be promising for quantum computation. Moving Majorana wave packets along closed paths leads to braiding of Majorana modes. We determine the non-Abelian phase associated with this braiding. To that end, we construct an exact time-dependent many-particle Hamiltonian that describes the desired motion and show that the phase can efficiently be evaluated in an effective single-particle picture.

TT 15.10 Mon 17:30 HSZ/0105

Phase dynamics and parity effects in quantum spin Hall Josephson junctions with coupled edges — •Cajetan Heinz[1], Patrik Recher[1,2], and Fernando Dominguez[3] — [1]Technische Universität Braunschweig, D-38106 Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology, D-38106 Braunschweig, Germany — [3]Universität Würzburg, D-97074 Würzburg, Germany

We investigate a novel backscattering mechanism in quantum spin Hall N'SNSN' Josephson junctions in the presence of time-reversal symmetry. This extended geometry allows for the interplay between two types of Andreev bound states (ABS): the usual phase-dependent ABS localized at the edges of the central SNS junction *and* phase-independent ABS localized at the edges of the N'S regions. Crucially, the latter arise at discrete energies E_n and mediate a backscattering process between opposite edges of the SNS junction, opening gaps whenever both types of ABS are at resonance. In this scenario, the 4π-periodic ABS decouples from the rest of the 2π-periodic spectrum. Using the parameters extracted from the microscopic calculation, we construct an RSJ model that incorporates the 4π-periodic ABS, the remaining 2π-periodic part of the spectrum and the quasi-particle continuum. Here, two types of parity changes can arise: transitions between the 4π- and 2π-periodic ABS, and parity leakage from the 2π-periodic ABS into the continuum. Our results show different dynamical regimes depending on the rate of non-adiabatic transitions, ranging from Shapiro steps

at integer multiples of $\hbar\omega_{ac}/2e$, over non-integer steps, to steps only at even integers, with ω_{ac} as the external ac driving frequency.

TT 15.11 Mon 17:45 HSZ/0105

Manipulating the topological spin of Majoranas — •Stijn de Wit[1], Emre Duman[2], Mert Bozkurt[3], Alexander Brinkman[1], and Inanc Adagideli[1,2] — [1]MESA+ Institute for Nanotechnology, University of Twente, The Netherlands — [2]Faculty of Engineering and Natural Sciences, Sabanci University, Istanbul, Turkey — [3]QuTech, Delft University of Technology, Delft 2600 GA, The Netherlands

The non-Abelian exchange statistics of Majorana zero modes make them interesting for both technological applications and fundamental research. Unlike their non-Abelian counterpart, the Abelian contribution is often neglected in the discussion of Majorana braiding. We consider Majoranas bound to vortices in topological superconductors. Here, the Abelian exchange phase originates from the Majoranas so-called topological spin, and it is interpreted as an Aharonov-Casher phase arising from a vortex encircling an e/4 charge. In this work, we show how this fractional charge and hence the topological spin of Majoranas can be manipulated, introducing an additional knob for braiding operations in topological quantum computing. Final, we propose a vortex interference experiment to probe the presence of this fractional e/4 charge.

TT 15.12 Mon 18:00 HSZ/0105

Ab Initio Exploration of Material Platforms for Majorana Zero Modes in Magnetic Chains on Superconductors — •András Lászlóffy[1,2], Bendegúz Nyári[3], Levente Rózsa[2], László Szunyogh[3], and Balázs Újfalussy[2] — [1]Pázmány Péter Catholic University, Budapest, Hungary — [2]HUN-REN Wigner Research Centre for Physics, Budapest, Hungary — [3]Budapest University of Technology and Economics, Budapest, Hungary

In magnetic chains on superconductors, Shiba bands are formed within the superconducting gap. Spin-orbit coupling or a spin-spiral configuration can lead to the hybridization of Shiba bands which can open a topologically non-trivial gap around the Fermi energy. To have a quantitative and realistic description of these systems, we solve the Kohn-Sham-Dirac Bogoliubov-de Gennes equations within the Korringa-Kohn-Rostoker multiple scattering theory. Elementary superconducting surfaces rarely support the appearance of a topological superconducting state, since either the superconducting gap or the spin-orbit coupling strength is small.[1] By adding a non-magnetic overlayer between the superconductor and the chain, we explore the topological properties of a large variety of systems in terms of varying the type of magnetic atoms in the chain and its crystallographic direction. We demonstrate that the formation of a spin spiral state has a larger impact on the robustness of the topologically non-trivial band structure than the enhanced spin-orbit coupling.

[1] Nyári et. al., PRB 112 (2025) 115414

TT 15.13 Mon 18:15 HSZ/0105

Ab initio band structure of magnetic chains on superconductors — •Bendegúz Nyári[1,3], András Lászlóffy[2], Balázs Újfalussy[2], László Szunyogh[3], and Levente Rózsa[2,3] — [1]HUN-REN-BME Condensed Matter Research Group — [2]HUN-REN Wigner Research Centre for Physics — [3]Budapest University of Technolofy and Economics

The detection of band topology and the reliability of Majorana Zero Mode (MZM) observations based only on real space quantities is a long standing problem. Due to the bulk edge correspondence the appearance of MZMs in a finite chain is related to the properties of the band structure, or more precisely the topological invariant, however these quantities can not be measured directly. In this work I present an ab initio approach which provides direct access to the band structure of magnetic chains on superconductors. The method relies on a 1D embedding scheme and includes the effect of the infinite host to the chain. The method was applied to Mn chains on Nb(110) and Ta(110) where the topological properties and symmetry aspects of the band structure were studied together showing the coexistence of trivial and non-trivial bands in the band structure [1].

[1] B. Nyári et al., Phys. Rev. B 112 (2025) 115414

TT 16: 2D Materials beyond graphene: Growth, structure and substrate interaction (joint session O/HL/TT)

Time: Monday 15:00–17:45 Location: HSZ/0204

TT 16.1 Mon 15:00 HSZ/0204

A virtual super-moiré: $MnBr_2$ on graphene on Ir(110) — Affan Safeer[1], Oktay Güleryüz[1], Nicolae Atodiresei[2], •Thomas Michely[1], and Jeison Fischer[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich, Germany

$MnBr_2$ on Gr/Ir(110) constitutes a three lattice system, giving rise to a super-moiré pattern – a moiré of moirés. The super-moiré of Gr/$MnBr_2$/Ir(110) is unique, as it involves a virtual moiré of $MnBr_2$ with the Ir(110) surface lattice – two lattices not in contact with each other. Using a careful Fourier analysis of the bias dependence of scanning tunneling microscope topographs, scanning tunneling spectroscopy, the known properties of Gr/Ir(110), and the results of ab initio calculations, the origin of the virtual moiré is uncovered and related to the inhomogeneous binding of Gr to Ir(110). Comparative experiments with $MnBr_2$ on Gr/Ir(111) show similar growth and structure as on Gr/Ir(110), but highlight the unique properties of the $MnBr_2$/Gr/Ir(110) super-moiré.

TT 16.2 Mon 15:15 HSZ/0204

Magnetism of monolayers of $FeCl_2$ and $FeBr_2$ Epitaxially Grown on Bi_2Se_3 — •Sebastien E. Hadjadj[1], Weibin Li[2], Pierluigi Gargiani[2], Cinthia Piamonteze[3], Oleksandr Stetsovych[4], Pavel Jelínek[4], Maxim Ilyn[1], and Celia Rogero[1] — [1]Materials Physics Center(MPC - CFM), Donostia, Spain — [2]ALBA Synchrotron Light Source, Barcelona, Spain — [3]Paul Scherrer Institut, Villigen, Switzerland — [4]FZU - Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic

Two-dimensional transition metal dihalides exhibit novel magnetic and electronic properties. By combining 2D magnetic semiconductors with topological insulators (TIs) novel quantum and spintronic phenomena can be investigated. Here, we report the uniform and epitaxial growth of monolayer $FeCl_2$ and $FeBr_2$ on the TI Bi_2Se_3. Structural and electronic characterization via LEED, STM, and STS measurements revealed a material-specific moiré pattern resulting from lattice mismatch, as well as a position-independent bandgap of 4 eV. Synchrotron-radiation-based XAS and XMCD measurements confirm robust ferromagnetic order down to the monolayer limit, with an intrinsic reduction of the effective spin magnetic moment by 40-50%. These magnetic vdW heterostructures provide a platform for investigating magnetic proximity effects and moiré-induced modifications of topological surface states. [1] S. E. Hadjadj et al., Chem. Mater., 35, 23, 9847*9856,(2023) [2] S. Kerschbaumer et al., Adv. Science, e08262,(2025)

TT 16.3 Mon 15:30 HSZ/0204

Rise and fall of 1T-TaS_2: Epitaxial growth of monolayer TaS_2 on Au(111) — •Lars Buss[1], Cathy Sulaiman[1], Raquel Sánchez-Barquilla[1], Iulia Cojocariu[2], Marcin Szpytma[3], Tevfik Onur Menteş[2], Andrea Locatelli[2], Jens Falta[4], and Jan Ingo Flege[1] — [1]Applied Physics and Semiconductor Spectroscopy, BTU Cottbus-Senftenberg, Cottbus, Germany — [2]Elettra-Sincrotrone Trieste S.C.p.A, Basovizza, Trieste, Italy — [3]Faculty of Physics and Applied Computer Science, AGH University of Krakow, Poland — [4]Institute of Solid State Physics, University of Bremen, Germany

Two-dimensional TaS_2 has attracted extensive research interest due to its ability to exhibit electron correlation effects, including charge density waves (CDWs). In particular, 1T-TaS_2 is of interest as it shows a CDW at room temperature. However, when grown on metal substrates, only 2H-TaS_2 has been reported. To elucidate the reasons for the apparent lack of 1T-TaS_2 growth in the literature, we have investigated the growth of TaS_2 on Au(111) employing *in situ* low-energy electron microscopy (LEEM) and micro-diffraction (μLEED) as well as X-ray photoemission electron microscopy (XPEEM) [1]. We show that at elevated temperatures TaS_2 nucleates and grows in the metastable 1T-TaS_2 phase, which transforms into the stable 2H-TaS_2 phase via a temperature-activated process and then continues to grow at a considerably lower rate. Furthermore, we observe CDW-like ordering in 1T-TaS_2/Au(111), though it is suppressed in 2H-TaS_2/Au(111).

[1] L. Buß et al. Phys. Rev. Materials **9**, 074006 (2025).

TT 16.4 Mon 15:45 HSZ/0204

Band-Like Transport and its Modulation by Nitrogen Doping in Transferable Semi-Conducting 2D-imine Covalent Organic Framework — •Vijay Bahadur Yadav, Diksha Srivastava, Satya Veer Singh, Itu Pandey, Manabendra Chandra, and Thiruvancheril G. Gopakumar — Indian Institute of Technology Kanpur

Two-dimensional (2D) imine-based covalent organic frameworks (COFs) are promising semiconductors for thin-film electronics and sensing due to their extended in-plane π-conjugation, enabling efficient charge transport. Here, we investigate two highly crystalline 2D imine COF films synthesised via quasi-equilibrium Schiff base condensation. By selecting molecular precursors, we tuned the nitrogen content, producing COFs with ten and six nitrogen atoms per unit cell (10N-COF and 6N-COF). The films are chemically stable in organic solvents and water, mechanically robust, and transferable onto various substrates,

allowing fabrication over areas of tens of square centimeters. Electrical measurements using silver electrode arrays show linear current*voltage behaviour, indicating band-like transport, with consistent responses across multiple regions. The conductivity of 10N-COF is ~36 times higher than that of 6N-COF. Density functional theory calculations reveal similar band gaps but enhanced band dispersion near the Fermi level in 10N-COF, improving charge carrier mobility. Nitrogen incorporation thus effectively tunes charge transport in 2D COFs.

TT 16.5 Mon 16:00 HSZ/0204

Co_2S_2: a new 2D material and its phase transitions — •Abdallah Karaka, Max Wolfertz, Affan Safeer, Guangyao Miao, Wouter Jolie, Thomas Michely, and Jeison Fischer — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Cologne, Germany

Using molecular beam epitaxy under ultra high vacuum conditions, 2D materials can be synthesized under conditions far from equilibrium for which no bulk parent compound exists.

Co_2S_2-2D is such an example. Using scanning tunneling microscopy and low energy electron diffraction we characterize this new single-layer 2D material crystallizing in the CuI structure (space group: $P\bar{3}m1$ trigonal), when grown on graphene on Ir(111) using molecular beam epitaxy. We found it can be synthesized phase pure upon low temperature growth and moderate annealing with a lattice constant of 3.66 ± 0.05 Å and a height of 6.2 Å. Beyond the single-layer limit it transforms into a new hexagonal crystal structure with a distinctly different lattice parameter of 3.52 ± 0.05 Å and a height of 11.7 Å. This transition typically occurs between 650 and 750 K, although the exact temperature depends on the annealing conditions. The phase transition is accompanied by the emergence of a 2x2 superstructure in the high temperature phase.

TT 16.6 Mon 16:15 HSZ/0204

Tailored growth of 2D alloy transition metal dichalcogenides with tunable optical and electrical properties using liquid precursors — •Md Tarik Hossain[1], Axel Printschler[1], Nhat Lam Duong[1], Julian Picker[1], Rahul Sharma[1], Christof Neumann[1], Mona Sedighi[2], Johannes Biskupek[2], Muhammad Sufyan Ramzan[1], Caterina Cocchi[1], Ute Kaiser[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Jena, Germany — [2]University of Ulm, Ulm, Germany

Doping or alloying of two-dimensional (2D) transition metal dichalcogenides (TMDs) provides a promising route to tune the optical, magnetic, and electronic properties. Here, we present a liquid-precursor-based chemical vapor deposition (CVD) for the controlled growth of large-area monolayer $(V_xW_zMo_{1-x-y})S_2$ alloys with tunable optical and electrical properties. Comprehensive characterization using atomic force microscopy, transmission electron microscopy, Raman spectroscopy, photoluminescence (PL) spectroscopy, and ab initio calculations confirms the structural and optical quality. Notably, PL shows a noticeable defect exciton peak at room temperature in the V-doped monolayer. Furthermore, by adjusting the composition, we modulate the carrier type of these monolayers from n-type to p-type or even make the monolayers metallic for high vanadium concentrations, which is deduced from electrical transport measurements and density functional theory calculations. This work demonstrates high potential of liquid-precursor CVD as a platform for the tailored growth of complex 2D TMD alloys for next-generation optoelectronic devices.

TT 16.7 Mon 16:30 HSZ/0204

CVD growth and characterization of WSe_2 monolayers on Au(111) and their conversion to Janus SeWS — •Julian Picker[1], Jonas Brandhoff[2], Maximilian Schaal[2], Felix Otto[2], Christof Neumann[1], Torsten Fritz[2], and Andrey Turchanin[1] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena, Germany — [2]Institute of Solid State Physics, Friedrich Schiller University Jena, Germany

Transition metal dichalcogenides (TMDs) exhibit distinctive optical and electronic properties in the two-dimensional monolayer limit. Recently, Janus TMDs have attracted significant attention because their asymmetric chalcogen composition breaks the out-of-plane symmetry and enables properties not attainable in conventional TMDs. In this work, we initially investigate the structural and electronic characteristics of WSe_2 monolayers grown on Au(111) via ambient-pressure chemical vapor deposition (CVD). Surface-sensitive techniques - including scanning tunneling microscopy (STM), low-energy electron diffraction (LEED), X-ray photoelectron spectroscopy (XPS), and angle-resolved photoelectron spectroscopy (ARPES) - were employed to characterize the properties of these monolayers. Subsequently, the WSe_2 monolayers were transformed into Janus SeWS monolayers through selective chalcogen replacement at the WSe_2/Au interface. A comparative analysis reveals the structural and electronic differences between the two systems.

TT 16.8 Mon 16:45 HSZ/0204

Controlling polymorphism in the growth of 2D manganese sulfide on graphene via substrate interaction — •Max Wolfertz, Abdallah Karaka, Nicolas Georgopoulos, Oktay Güleryüz, Affan Safeer, Thomas Michely, and Jeison Fischer — II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Cologne, Germany

We investigate the epitaxial growth of single-layer manganese sulfide on graphene/Ir substrates grown via molecular beam epitaxy. Morphology, crystal structure and electronic properties are examined using scanning tunneling microscopy and - spectroscopy and low energy electron diffraction. While bulk MnS exists in the three polymorphs, α-(rock-salt structure), β-(zincblende structure), and γ-MnS (wurtzite structure), its structure in a single-layer is unknown, as fabrication using exfoliation methods cannot be applied. We find that when grown by molecular beam epitaxy on Gr/Ir substrates manganese sulfide grows in two competing phases: manganese sulfide in trigonal CuI-structure (space group P-3m1) and MnS in thin platelets of a cubic rock-salt structure (space group Fm-3m). Their in-plane lattice parameters are 4.16 Å, and 3.63 Å respectively. We show that the substrate exerts a strong influence on the phase selected. While the growth on Gr/Ir(111) results in a large share of cubic MnS, the Gr/Ir(110) substrate favors the formation of single layer trigonal manganese sulfide. Also, the use of seeding methods for avoiding loss of Mn into the bulk Ir crystals is discussed.

TT 16.9 Mon 17:00 HSZ/0204

Low Temperature MOCVD Growth of two-dimensional InSe and InSe/WS2 Heterostructures — •Robin Guenkel, Nils Langlotz, Matvei Kislitsyn, Juergen Belz, and Kerstin Volz — mar.quest|Marburg Center for Quantum Materials and Sustainable Technologies, Philipps University Marburg, Germany

Two-dimensional van der Waals heterostructures offer powerful opportunities for engineered optoelectronic functionality, particularly when type-II band alignment enables efficient charge separation and interlayer transitions. InSe and WS* are especially promising in this regard because their band structures allow for the formation of a type-II interface at the Γ point, which avoids momentum mismatch. This is an essential requirement for robust radiative processes in 2D stacks. This talk presents a low-temperature metal-organic chemical vapor deposition (MOCVD) approach for synthesizing high-quality InSe and vertically integrated InSe/WS2 heterostructures. Using DTBSe and TMIn at 350 °C, we synthesize homogeneous, single-phase InSe films on 2-inch sapphire substrates and extend the process to directly grow on monolayer WS2. Atomic force microscopy, Raman spectroscopy, and energy-dispersive X-ray spectroscopy provide insight into the morphology, crystallinity, and composition of the films, offering a detailed understanding of the growth behavior and the influence of the substrate surface chemistry.

TT 16.10 Mon 17:15 HSZ/0204

Synthesis of Vertically Stacked 2D-hBN/Borophene Heterostructures on Ir(111) via Intrinsic Segregation — •Marko Kriegel, Karim Omambac, Smruti Mohanty, Birk Finke, Frank-J. Meyer zu Heringdorf, and Michael Horn-von Hoegen — University Duisburg-Essen and Center for Nanointegration Duisburg-Essen (CENIDE), Lotharstr. 1, 47057 Duisburg, Germany

Research efforts on 2D materials increasingly target complex architectures built from high-quality heterostructures. A key challenge remains the reliable and scalable in-situ fabrication of such systems. In this work, we use high-resolution spot-profile analysis LEED (SPA-LEED) and -microscopy (LEEM) to investigate a synthesis route for an hBN/borophene heterostructure on Ir(111) based on *intrinsic segregation*. At elevated temperatures, boron dissolves into the Ir subsurface region during exposure to the borazine precursor $B_3N_3H_6$ in a CVD process [1], thereby creating a boron reservoir. Increasing the precursor pressure drives the chemical balance toward formation of a complete hBN layer across the Ir surface [2]. Upon cooldown, the decreasing boron solubility induces segregation, resulting in the growth of a continuous borophene layer beneath the hBN overlayer. This one-step CVD approach establishes a promising, scalable pathway for the controlled synthesis of high-quality 2D heterostructures.

[1] K. Omambac et al., ACS Nano **15** (2021) 7421
[2] K. Omambac et al., ACS Nano **17** (2023) 17946

TT 16.11 Mon 17:30 HSZ/0204

MBE growth and characterization of high-quality monolayer MoS2 on stepped Au surface — •Sayan Debnath, Ram Prakash Pandeya, Konstantin Shchukin, Patrik Staudenmayer, and Alexander Grüneis — Optoelektronische Materialien Institut für Festkörperelektronik, TU Wien, 1040 Wien, Austria

In the present work, we investigate the growth of sub-monolayer MoS2 on Au(788) and Au(111), using molecular beam epitaxy. Sample growth quality is characterized using low-energy electron diffraction, X-ray photoemission spectroscopy, and scanning electron microscopy. Furthermore, a comparative study of the electronic properties was performed by studying the band structure using angle-resolved photoemission spectroscopy (ARPES), and the vibrational properties were measured by angle-resolved polarized Raman (ARPR) spectroscopy.

Our study reveals superior crystalline quality, with fewer S deficiencies, and better azimuthal order of MoS2 grown on the stepped Au(788) substrate compared to the Au(111). In the case of ARPES, we observed more resolved band dispersion on MoS2/Au (788), confirmed by probing the spin-orbit splitting at the Brillouin zone boundary (K point). On the other hand, ARPR of the first Raman mode E2g on MoS2/Au (788) deviates from the symmetry of freestanding MoS2, suggesting the effect of the stepped surface on the vibrational properties. We discuss the role of increased catalytic activity at step edges in promoting the growth of high-quality TMDCs, such as MoS2 and WS2, on stepped surfaces.

TT 17: Quantum Manybody Systems (joint session QI/TT)

Time: Monday 15:00–18:30 Location: BEY/0245

Invited Talk TT 17.1 Mon 15:00 BEY/0245

Reducing Noise, Complexity, and Optimization Barriers in Quantum Simulations of Strongly Correlated Systems — •Werner Dobrautz — Center for Advanced Systems Understanding (CASUS), Görlitz, Germany — Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany — Center for Scalable Data Analytics and Artificial Intelligence (ScaDS.AI) Dresden/Leipzig, Dresden, Germany — Technical University Dresden, Dresden, Germany

Near-term quantum hardware poses severe constraints for quantum chemistry and quantum many-body simulations due to noise, limited coherence, and challenging optimization landscapes. We present a unifying set of algorithmic strategies to address these bottlenecks, combining transcorrelated Hamiltonians, spin-adapted representations, and advanced variational optimization techniques. By embedding electronic correlations directly into the Hamiltonian, transcorrelated methods yield compact, noise-resilient quantum circuits and improved convergence for both molecular systems and lattice models. Spin-adapted formulations further reduce Hilbert space complexity and enable efficient simulations of correlated spin systems. To enhance robustness and trainability, we introduce multireference error mitigation strategies and qBang, a momentum-aware variational optimization scheme that effectively navigates flat and ill-conditioned energy landscapes. Together, these approaches establish a scalable and hardware-aware framework for accurate quantum simulations of strongly correlated systems on current and near-term quantum devices.

TT 17.2 Mon 15:30 BEY/0245

Hybrid superconducting devices — •Anamaria Ghihor[1], Yejin Lee[1], Haolin Jin[1], Markus König[1], Andreas Leithe-Jasper[1], Roemer Hinlopen[1,2], Carsten Putzke[2], Philip Moll[2], Uri Vool[1], and Eteri Svanidze[1] — [1]MPI CPfS - Nothnitzer Str. 40, Dresden, Germany — [2]MPI MPSD - Luruper Chaussee 149, Hamburg, Germany

Superconducting resonators are highly tunable, low-loss coherent macroscopic devices, making them ideal for quantum technology and sensing applications. Recently, these resonators have been paired with van der Waals (vdW) materials to explore their microwave losses, dielectric properties and kinetic inductance. However, creating a hybrid device that only integrates a superconducting resonator with a vdW flake limits the range of materials that can be used. To overcome this limitation, we fabricate a lamella using a focused ion beam (FIB), effectively replicating the flake. This approach offers the added benefit of precise dimensional control, something that is difficult to achieve with exfoliated flakes. The lamella can then be attached in situ to the resonator using a micro-manipulator. In this talk we will show preliminary hybrid devices with lamella developed from conventional and unconventional superconductors.This approach greatly expands the range of materials that can be explored and enables detailed studies of their superfluid density.

TT 17.3 Mon 15:45 BEY/0245

Hybrid Monte Carlo enhanced by exact diagonalization: simulating interacting Hubbard systems — •Martina Gisti[1], Finn Temmen[2], Thomas Luu[1], David Luitz[2], and Johann Ostmeyer[3] — [1]Institute of Physics, University of Bonn, Nußallee 12, 53115 Bonn — [2]Forschungszentrum Jülich GmbH Wilhelm-Johnen-Straße 52428 Jülich — [3]Helmholtz Institute for Radiation and Nuclear Physics, University of Bonn

We present a hybrid simulation framework that integrates the hybrid Monte Carlo method with exact diagonalization techniques to study Hubbard chains coupled through many-body interactions. Within a path integral formulation, thermal expectation values are expressed and evaluated exactly along the chains. We study the impact of the hybrid method on persistent challenges in the application of stochastic simulations, such as the sign problem and ergodicity violations. The approach mitigates the sign problem that hampers conventional simulations, providing a feasible path for studying strongly correlated quantum systems beyond one dimension.

TT 17.4 Mon 16:00 BEY/0245

Topological properties of coupled superconducting chains in the presence of interactions — •Frederick Del Pozo — aboratoire Kastler Brossel, Sorbonne Universite, CNRS, ENS-PSL Research University, Coll'ege de France; 4 Place Jussieu, 75005 Paris, France

We investigate the topological and critical properties of coupled and interacting superconducting wires.

As a prototype of superconductors with topological order, the Kitaev chain model is a perfect testing ground for novel theoretical and numerical tools, including the density-matrix-renormalization-group (DMRG) algorithm and bipartite entanglement entropy.

In the following talk we report on the results of several recent works, which have lead to a deeper understanding of the topological and critical properties of coupled and interacting Kitaev chains, also in the presence of real-space disorder. We reveal that the usual topological invariant, defined in the absence of interactions, remains a sensible marker for the topology when two wires are brought into close proximity of each other where interaction effects and inter-wire hopping processes become relevant. We also reveal the appearance of a many-body entangled ground state, and interaction reinforced critical region in the wires' phase diagram.

Our results highlight the rich physics present in quasi one-dimensional quantum systems, and motivates the further research into properties relevant for applications in superconducting qubits and topological quantum computation protocols.

TT 17.5 Mon 16:15 BEY/0245

Quantum Assisted Ghost Gutzwiller Ansatz — •PV Sriluckshmy, Francois Jamet, and Fedor Simkovic — IQM Quantum Computers, Georg-Brauchle-Ring 23-25, 80992 Munich, Germany

The ghost Gutzwiller ansatz (gGut) technique was shown to achieve accuracy comparable to dynamical mean-field theory at a much lower computational cost. However, gGut is limited by the bottleneck of computing the density matrix. We develop a hybrid quantum-classical gGut technique that computes ground state properties of embedding Hamiltonians on a quantum computer using the quantum-selected configuration interaction (QSCI) algorithm. We find that the ground states of interest become sufficiently sparse as the number of ghost orbitals increases. We investigate QSCI's performance using local unitary cluster Jastrow (LUCJ) ansatz with circuit cutting on IQM's quantum hardware for up to 24 qubits. Our converged gGut calculations correctly capture the metal-to-insulator phase transition in the Fermi-Hubbard model. This was achieved using quantum samples to build a basis with as little as 1% of the total CI states.

30min. break

TT 17.6 Mon 17:00 BEY/0245

Measurement-Based Quantum Computation in Symmetry-Enriched Topological Phases — •Paul Herringer[1,2,3], Vir B. Bulchandani[4,5], Younes Javanmard[1], David T. Stephen[6,7], and Robert Raussendorf[1,3] — [1]Leibniz Universität Hannover, Hannover, Germany — [2]University of British Columbia, Vancouver, Canada — [3]Stewart Blusson Quantum Matter Institute, Vancouver, Canada — [4]Rice University, Houston, USA — [5]National University of Singapore, Singapore — [6]University of Colorado Boulder, Boulder, USA — [7]California Institute of Technology, Pasadena, USA

We present the first examples of topological phases of matter with uniform power for measurement-based quantum computation. This is possible thanks to a new framework for analyzing the computational properties of phases of matter that is more general than previous constructions, which were limited to short-range entangled phases in one dimension. We show that ground states of the toric code in an anisotropic magnetic field yield a natural, albeit non-computationally-universal, application of our framework. We then present a new model with topological order whose ground states are universal resources for MBQC. Both topological models are enriched by subsystem symmetries, and these symmetries protect their computational power. Our framework greatly expands the range of physical models that can be analyzed from the computational perspective.

TT 17.7 Mon 17:15 BEY/0245

Many-body localization in the Sherrington-Kirkpatrick model — •Gergo Dénes[1], Balázs Hetényi[1], Márton Kormos[1], Angelo Valli[1], Pascu Moca[1,2], and Gergely Zaránd[1] — [1]Department of Theoretical Physics, Institute of Physics, Budapest University of Technology and Economics, Muegyetem rkp. 3., H-1111 Budapest, Hungary — [2]Department of Physics, University of Oradea, Str. Universitatii nr. 1 Oradea, 410087, Romania

The Sherrington-Kirkpatrick (SK) model has been extensively studied for more than 50 years [1]. In the context of optimization problems, it represents one of the most difficult paradigmatic optimization problems, the MAXCUT problem. Its quantum extension, the transverse field SK model (TFSK model) is therefore a paradigmatic model for the Quantum Adiabatic Optimization Approach (QAOA).

We performed extensive finite-size numerical simulations of the TFSK model at different transverse field strengths to extract various many-body localization (MBL) indicators, such as inverse participation ratio, Shannon entropy, and level spacing ratio. Our numerical and analytical analysis suggest the presence of an MBL transition as a function of the transverse field at certain energy densities, different from the spin-glass transition, and in contrast to the findings of Ref. [2]. In the MBL phase, states do not seem to be exponentially localized, rather, our data suggest the presence of power-law MBL.

[1] M. Mezard, G. Parisi, M. A. Virasoro Spin Glass Theory and Beyond, ISBN: 978-9971-5-0116-7 (1986).

[2] S. Mukherjee, S. Nag, A. Garg, Phys. Rev. B 97, 144202 (2018).

TT 17.8 Mon 17:30 BEY/0245

Typical entanglement entropy of anyon chains — Yale Yauk[1,2], •Alexander Hahn[1,3,2], and Lucas Hackl[4,5] — [1]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Straße 1, D-85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstraße 4, D-80799 Munich, Germany — [3]Technical University of Munich, TUM School of Natural Sciences, Physics Department, D-85748 Garching, Germany — [4]School of Mathematics and Statistics, The University of Melbourne, Parkville, VIC 3010, Australia — [5]School of Physics, The University of Melbourne, Parkville, VIC 3010, Australia

Random-state entanglement serves as a key probe of quantum chaos, thermalization, and information scrambling, but its behavior in topologically ordered systems remains unclear. Here we study the statistical properties of bipartite entanglement in one-dimensional anyon chains, where the Hilbert space is constrained by the fusion rules. In such systems, the conventional trace must be replaced by the quantum trace, requiring a consistent redefinition of density matrices and entanglement measures that incorporates topological data. We compute the average bipartite entanglement entropy and its variance for both open and periodic boundary conditions. The resulting average anyonic entanglement entropy reproduces the Page curve exactly, revealing that topological constraints modify the normalization but not the universal form of typical entanglement. Despite topological charge conservation, the average entanglement shows no symmetry-related correction of the kind that appears in systems with Lie group symmetries.

TT 17.9 Mon 17:45 BEY/0245

Thermal Entanglement and Out-of-Equilibrium Thermodynamics in 1D Bosonic Systems — •Julia Mathe, Nicky Kai Hong Li, Pharnam Bakhshinezhad, and Giuseppe Vitagliano — TU Wien, Atominstitut, Stadionallee 2, 1020 Vienna, Austria

We investigate entanglement in- and out-of equilibirum in harmonic chains, with direct relevance to low-energy descriptions of paradigmatic models, like 1D Bose-Einstein condensates. Working in a regime where all states are Gaussian, we employ the logarithmic negativity and the covariance matrix criterion (CMC) as known entanglement quantifiers. For thermal states, we extensively characterize entanglement and its scaling behaviour, including in the massless (critical) limit. We extract the optimal entanglement witness coming from the CMC and uncover a simple mode-resolved structure underlying the entanglement-to-separability transition. At finite temperature, the optimal witnesses are diagonal in the normal-mode basis, allowing to characterize entanglement from a few normal mode uncertainties, which are physically related to static susceptibilities. We then investigate out-of-equilibrium dynamics arising from a time-dependent coupling and analyze entanglement growth, suppression, and transport. Based on this, we construct a full Gaussian framework for studying entanglement in thermodynamic cycles. Our results give a unified and physically intuitive picture of how entanglement emerges and evolves in 1D Gaussian many-body systems and show that thermal separability and entanglement are mainly governed by the low-energy (infrared) sector that also underlies the continuum field-theory description.

TT 17.10 Mon 18:00 BEY/0245

Symmetry-preserving warm starts for variational ground state preparation — •Ivana Miháliková — Matej Bel University, Národná ulica 12, Banská Bystrica, 97401, Slovakia — Institute of Physics, Slovak Academy of Sciences, Bratislava 84511, Slovakia

Enforcing physical symmetries can dramatically simplify ground-state preparation in the variational quantum eigensolver (VQE). This work considers a 12-spin all-to-all neutrino-inspired model and a 4×3 Heisenberg lattice. In both systems, simple product states are projected onto symmetry subspaces with fixed total spin J and J_z (and, for the Heisenberg lattice, translation and mirror symmetries), then refined using swap-based entangling layers that generate only symmetry-compatible correlations. The resulting warm starts lie well within previously established worst-case upper bounds on the energy error normalized by system size and interaction-graph degree, showing that symmetry-aware initialization can substantially outperform generic guarantees. For the Heisenberg lattice, the symmetry-preserving construction reduces the relevant search space from 4096 basis states to just 9 symmetry-compatible states and increases the effective spectral gap from about 7 to about 28 energy units. Within a VQE setting this yields a smoother optimization landscape and faster convergence with shallow circuits. In practice, the neutrino-inspired model reaches $\sim$ 98.8% fidelity within the $J = 0$ subspace, and the Heisenberg lattice exceeds 98.0% fidelity once translation and mirror symmetries are enforced.

TT 17.11 Mon 18:15 BEY/0245

An emerging generator of rotations for a 1- or many-particle Hofstadter problem on a lattice pierced by magnetic field — •Arabi Seshappan[1,2], Tangi Morvan[2], Alberto Nardin[2], and Leonardo Mazza[2] — [1]Department of Physics, University of California, Merced, CA 95343, USA — [2]Université Paris-Saclay, CNRS, LPTMS, 91405, Orsay, France

Topological quantum computation is an exciting direction for development of fault-tolerant qubits—a quintessential example being manipulation of excitations in fractional quantum Hall (FQH) systems. As recent cold-atom and photonic experiments have realized few-particle FQH states in small lattices, and theoretical results have shown spectra of specific lattice sizes to exhibit exactly flat-bands in momentum space, we have theoretically studied similar FQH lattices for 1- and many-particle bosonic cases. Our construction is that of a two-dimensional (2D) square lattice, with nearest-neighbor hopping, pierced by a perpendicular, uniform magnetic field. We vary the magnetic field such that, for lattice edge length L, the flux per plaquette ranges between $\alpha = 1/L$ and $\alpha = 1/4$, and analyze the resultant spectra. We have found that, for low energy levels, measurements of density are an excellent proxy for defining a gauge-invariant generator of rotations (GIGR) and can make order in the spectra. This removes any need for assumption of circular droplet invariance, and provides a useful characterization technique for cold-atom experiments.

TT 18: Focus Session: Relaxation Timescales in Open Quantum Systems (joint session TT/DY)

In the quantum year 2025 many applications of quantum systems are revisited for their actual physical implementability. Realizing that no quantum system is truly isolated from its environment highlights the need for a thorough understanding of the coupling between an open system and its environment. While many standard treatments lead to Lindblad equations, the underlying approximations are not always applicable and require detailed case-by-case studies. This theoretical focus session provides a platform discussing modern developments in the field in the regime of strongly interacting or driven open systems and their impact on relaxation timescales. We aim to enhance attention and trigger also experimental activity in the field of system-environment interactions and the induced relaxation timescales.

Coordinators: Gernot Schaller (Helmholtz-Zentrum Dresden-Rossendorf), Nikodem Szpak (Universität Duisburg-Essen)

Time: Monday 15:00–18:00 Location: CHE/0089

Topical Talk TT 18.1 Mon 15:00 CHE/0089

Markovian and non-Markovian approaches to quantum relaxation — •Heinz-Peter Breuer — Institute of Physics, University of Freiburg, Hermann-Herder-Straße 3, D-79104 Freiburg, Germany

Relaxation and decoherence processes in open quantum systems are often approximated by means of a Markovian evolution in which the open system irretrievably loses information to its surroundings, expressing the memoryless nature of the dynamics. However, strongly coupled open systems often exhibit a pronounced non-Markovian behavior distinguished by a flow of information from the environment back to the open system. This information backflow implies the presence of memory effects and represents the key feature of non-Markovian quantum dynamics. In the talk we will discuss fundamental physical concepts used to characterize and quantify non-Markovian relaxation dynamics in open systems, and present some applications to irreversibility and entropy production in nonequilibrium quantum thermodynamics.

Topical Talk TT 18.2 Mon 15:30 CHE/0089

Asymptotic relaxation in quantum Markovian dynamics — •Susana Huelga — Institute of Theoretical Physics, Ulm University, Germany

We investigate the long-time dynamics of generic time-dependent GKLS master equations and provide sufficient conditions such that the dynamics is asymptotically independent of the initial state. These conditions represent a natural extension of the Spohn-Frigerio theorem to the case of a time-dependent generator. To illustrate our results, we analyze a specific master equation for driven systems and connect our conditions to the microscopic Hamiltonian of system and environment. The case of a 3-level system is also treated in detail. A brief mention of the non-Markovian case is included, with specific focus on time-local master equations which are asymptotically in Lindblad form. These findings pave the way for the development of a more general theory of relaxation beyond the Markovian case.

Topical Talk TT 18.3 Mon 16:00 CHE/0089

Floquet engineering of open quantum Systems — •André Eckardt — Institut für Physik und Astronomie, TU Berlin, Berlin

In recent years, we have seen tremendous progress in the control of quantum systems by means of time-periodic driving. This includes the realization of effective time-independent Hamiltonians with interesting properties, such as artificial magnetic fields coupling to the motion of charge neutral particles in quantum simulators (e.g. of ultracold atoms in optical lattice or photons in superconducting circuits). Also phenomena without equilibrium counterpart, like chiral edge modes connecting Bloch bands with zero Chern number, have been investigated. Another paradigm for the control of quantum systems is reservoir engineering. Here a system is coupled to a controlled environment that is designed to either cool the system or to stabilize a non-equilibrium steady state of interest. I will report on recent theoretical work, where we combine both approaches in open Floquet systems. One motivation is to use dissipation in order to counteract unwanted heating, as it necessarily occurs in Floquet engineered systems, e,.g. for the preparation of Floquet engineered topological states of matter. The other motivation is the stabilization of interesting non-equilibrium steady states beyond the strict constraints of thermal equilibrium. Here I will discuss driving-induced non-equilibrium Bose condensation in high-temperature environments. Finally, I will also briefly address challenges arising when simulating open many-body quantum systems out of equilibrium and ideas how to tackle them.

15 min. break

Topical Talk TT 18.4 Mon 16:45 CHE/0089

Nonequilibrium thermodynamics of time-dependent quantum transport — •Janine Splettstoesser — Chalmers University of Technology, Gothenburg, Sweden

Quantum transport induced by time-dependent driving fields is not only of interest when considering the conductor's charge response. On the contrary, in recent years there has been strong interest in the thermodynamics and energetic properties of quantum conductors. By applying time-dependent driving fields to a conductor cyclic quantum heat engines can be implemented and quantum properties can be used to rapidly load and discharge so-called quantum batteries.

In this presentation, I will first show how different time-scales in the response of a quantum dot impact the (energy) decay of a quantum dot brought out of equilibrium. This is visible both in the relative entropy, where Coulomb interaction results in an anomalous decay referred to as Mpemba effect [1], as well as in the geometric properties of a slowly driven cyclic engine [2]. I will then show how the precision of time-dependently driven engines is bounded by the produced or dissipated power [3].

[1] J. Graf, J. Splettstoesser, J. Monsel, J. Phys.: Condens. Matter 37, 195302 (2025)
[2] J. Monsel, J. Schulenborg, Th. Baquet, J. Splettstoesser, Phys. Rev. B 106, 035405 (2022)
[3] L. Tesser, J. Balduque, J. Splettstoesser, arXiv:2509.07583 (2025)

Topical Talk TT 18.5 Mon 17:15 CHE/0089

Connecting time-nonlocal and time-local quantum master equations — •Maarten Wegewijs — Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany — Institute for Theory of Statistical Physics, RWTH Aachen, 52056 Aachen, Germany

A perhaps puzzling feature of open-system dynamics is that it admits both a retarded description via a *time-nonlocal* memory-kernel $\mathscr{K}$ and an *equivalent* time-convolutionless description by a *time-local* generator $\mathscr{G}$. This leads to a split in approaches to the problem of time scales in open quantum systems.

In this talk I discuss an elegant fixed-point relation $\mathscr{G} = \tilde{\mathscr{K}}(\mathscr{G})$ that connects these two approaches directly, without first solving the respective quantum master equations for the dynamics ultimately of interest. As applications, I connect the distinct results (!) obtained when expanding in the same perturbation parameter and relate distinct time-scales (!) obtained by approximations approaching the same, exact stationary state. The fixed-point relation is also explicitly related to quantum Markovianity as defined by completely-positive divisibility of the dynamics (Huelga, Rivas, Plenio): What generates the retardation of the memory kernel turns out to be precisely what defines the Markovian divisibility of the dynamics. Exact solutions of simple models of electron transport (resonant level) and atomic-decay (dissipative Jaynes-Cummings) illustate these findings.

[1] SciPost Phys. 7, 012 (2019)
[2] Phys. Rev. X 11, 021041 (2021)
[3] Phys. Rev. B 104, 155407 (2021)
[4] SciPost Phys. 12, 121 (2022)
[5] J. Chem. Phys. 161 (2024)

TT 18.6 Mon 17:45 CHE/0089

Coupling–energy driven pumping through quantum dots: The role of coherences — •Lukas Litzba[1], Gernot Schaller[2], Jürgen König[1], and Nikodem Szpak[1] — [1]Universität Duisburg-Essen, Duisburg, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

We study the impact of off–resonant tunneling and coherences on the electron transport through quantum dots. We focus on two electron pump setups where first–order tunneling processes are suppressed and the pumping mechanism is exclusively driven by modulations of the coupling energy. For calculations we use an exact solution for a non–Coulomb interacting situation. The first setup is driven by a coupling and decoupling procedure of the quantum dot and the environment and the second setup by measurement–induced effects resembling the anti–Zeno effect. We show that both electron pumps are based on decoherence operations and modulations of the coupling energy and there is quantitative and qualitative agreement between them. Furthermore, we show that non–Markovian effects can increase the performance of the devices and are signatures for the importance of coherences in electron transport.

TT 19: Focus Session: New Routes to Localization and Quantum Non-Ergodicity II (joint session TT/DY)

Time: Monday 15:00–17:30 Location: CHE/0091

TT 19.1 Mon 15:00 CHE/0091

Localized obstructed pairs with zero superfluid stiffness from doping an antiferromagnetic insulator — •Tamaghna Hazra[1], Nishchhal Verma[2], and Jörg Schmalian[1] — [1]Institüt für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]Department of Physics, Columbia University

Doping a Mott antiferromagnet is widely expected to yield mobile Cooper pairs whose kinetic energy sets the superfluid stiffness. We show instead that, when doped charges propagate on the line graph of a lattice with strong antiferromagnetic exchange, they bind into *obstructed* Cooper pairs, which are compact localized bosons that possess *zero* superfluid stiffness at leading order in the strong-coupling expansion. The pair-hopping Hamiltonian generates an exactly flat bosonic band whose compact localized states dominate the low-energy Hilbert space, yielding a ground-state manifold with extensive degeneracy and a phase stiffness that vanishes anomalously as the *third* inverse power of the pairing strength in the strong-coupling limit. At quarter filling, the frustrated dynamics maps onto a quantum dimer model at the Rokhsar-Kivelson point, realizing a d-wave resonating-valence-bond spin liquid with topological ground-state degeneracy and deconfined holon excitations. Our results establish a mechanism for interaction-driven localization without disorder, in which strong magnetically-mediated pairing produces Cooper pairs whose kinetic energy collapses to zero, revealing a distinct failure mode of unconventional superconductivity in strongly-correlated materials.

TT 19.2 Mon 15:15 CHE/0091

Disorder-free localization from mass-imbalanced fractionalization — •Shi Feng, Johannes Knolle, and Michael Knap — Technical University of Munich, Garching, Germany

We report disorder-free localization of Majorana fermions over intermediate timescales in an emergent gapless non-integrable Z_2 quantum liquid. A large density of heavy visons induced by an external magnetic field provides coherent disorder that localizes the light fermions while preserving translation symmetry. Compelling evidence of the localization within intermediate time scale is provided by the time evolution of the local energy density, which shows negligible spreading after a local quench on its ground state; and a vanishing energy current response despite the gapless energy spectrum. These results demonstrate that the disorder-free localization can also occur near equilibrium at low energy, and offer an explanation to the thermal paradox in recent experiments where a linear specific heat coexists with vanishing thermal transport in frustrated Mott insulators with disorder-free gapless quantum magnets.

TT 19.3 Mon 15:30 CHE/0091

Fock space fragmentation in quenches of disordered interacting fermions — •Ishita Modak[1], Rajesh Narayanan[2], Ferdinand Evers[3], and Soumya Bera[1] — [1]Department of Physics, Indian Institute of Technology Bombay, Mumbai, India. — [2]Department of Physics, Indian Institute of Technology Madras, Chennai, India — [3]Institute of Theoretical Physics and Halle-Berlin-Regensburg Cluster of Excellence CCE, University of Regensburg, Regensburg, Germany

Hilbert space fragmentation primarily originates from specific kinematic constraints or emergent conservation laws in many-body systems with translation invariance. It leads to non-ergodic dynamics and breakdown of the eigenstate thermalization hypothesis. We demonstrate that also in disordered systems (e.g. random-field XXZ model), fragmentation appears as a natural concept offering fresh perspectives on many-body delocalization (MBdL). We split the Fock-space into potential-energy shells, which contain the accessible phase space for the relaxation of a quenched initial state. In this construction, dynamical observables reflect properties of the shell geometry, e.g., the drastic sample-to-sample fluctuations observed in the weak disorder regime, $W < W_c$, represent fluctuations of the shell-mass. Upon crossing over to strong disorder, $W > W_c$, the potential-energy shell decays into fragments; we argue that, unlike percolation, fragmentation is a strong-coupling scenario with turn-around flow: $W_c(L)$ diverges with increasing system size. We conjecture that the slowing down of the relaxation dynamics reported in traditional MBdL studies is a manifestation of Fock-space fragmentation introduced here.

TT 19.4 Mon 15:45 CHE/0091

Non-ergodic one-magnon magnetization dynamics of the Kagome lattice antiferromagnet — Henrik Schlüter, •Jannis Eckseler, and Jürgen Schnack — Bielefeld University

The present view of modern physics on non-equilibrium dynamics is that generic systems equilibrate or thermalize under rather general conditions, even closed systems under unitary time evolution. The investigation of exceptions thus not only appears attractive, in view of quantum computing where thermalization is a threat it also seems to be necessary. Here, we present aspects of the one-magnon dynamics on the Kagome lattice antiferromagnet as an example of a non-equilibrating dynamics due to flat bands. Similar to the one-dimensional delta chain localized eigenstates also called localized magnons lead to disorder-free localization and prevent the system from thermalization [1].

[1] H. Schlüter, J. Schnack and J. Eckseler, Zeitschrift für Naturforschung A (2025) doi:10.1515/zna-2025-0249

TT 19.5 Mon 16:00 CHE/0091

Cooling dynamics of a disorder-free localized Kitaev model — •Arkadeep Mitra, Francesco Piazza, and Markus Heyl — Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

The Kitaev spin-1/2 model on a 2D honeycomb lattice has a Z_2 gauge symmetry that translates to an effective picture of free Majorana fermions on a background static charge field. This yields a ground state that realizes a quantum spin liquid (QSL) with fractional excitations. At high temperatures, however, it has recently been observed to enter a disorder-free localized phase, so that any experimental cooling of a Kitaev material has to cross this localized and associated phase transition. Motivated from this, we study theoretically the cooling dynamics upon coupling the Kitaev model to phonons with a symmetry breaking interaction. We envisage that signatures obtained from this dynamics could act as probes for QSL.

15 min. break

TT 19.6 Mon 16:30 CHE/0091

Scrambling signature of scars — •Thomas Michel[1], Mathias Steinhuber[2], Juan Diego Urbina[2], and Peter Schlagheck[1] — [1]Université de Liège, Liège, Belgique — [2]Universität Regensburg, Regensburg, Germany

We study signatures of scrambling, such as out-of-time-ordered correlators, that are associated with weakly unstable periodic orbits in a mixed or chaotic classical phase space, fulfilling Heller's criterion [1] for the existence of scars. As verified within generic dynamical systems like the kicked rotor and the driven pendulum, evaluating scrambling observables for coherent states centred in phase space about such periodic orbits gives rise to characteristic scar features both in the short and long time regimes, the latter amounting to a significant amendment of the characteristic growth exponent with respect to the generic semiclassical prediction [2,3]. Extensions to many-body scars in Bose-Hubbard rings [4] are discussed.

[1] E. J. Heller, Phys. Rev. Lett. 53, 1515 (1984).
[2] J. Rammensee, J.-D. Urbina, and K. Richter, Phys. Rev. Lett. 121, 124101 (2018).
[3] T. R. Michel, J. Diego Urbina, and P. Schlagheck, J. Phys. A: Math. Theor. 58, 275303 (2025).
[4] Q. Hummel, K. Richter, and P. Schlagheck, Phys. Rev. Lett. 130, 250402 (2023).

TT 19.7 Mon 16:45 CHE/0091

Many-Body Cages - Flat bands on the state graph — •Tom Ben-Ami[1,2], Markus Heyl[1], and Roderich Moessner[2] — [1]University of Augsburg, D-86135 Augsburg, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, Dresden 01187, Germany

We identify the many-body counterpart of flat bands, which we term many-body caging, as a general mechanism for non-equilibrium phenomena such as a novel type of glassy eigenspectrum order and many-body Rabi oscillations in the time domain. We focus on constrained systems of great current interest in the context of Rydberg atoms and synthetic or emergent gauge theories. We find that their state graphs host motifs which produce flat bands in the many-body spectrum at a particular set of universal energies. Basis states in Fock space exhibit Edwards-Anderson type order in the absence of quenched disorder, with an intricate, possibly fractal, distribution over Fock space. This is reflected in a distinctive structure of a non-vanishing post-quench long-time Loschmidt echo, an experimentally accessible quantity. In general, phenomena familiar from single-particle flat bands manifest themselves in characteristic many-body incarnations, such as a reentrant 'Anderson' delocalisation, offering a rich ensemble of experimental signatures in the abovementioned quantum simulators. The variety of single-particle flat band types suggests an analogous typology–and concomitant phenomenological richness to be explored–of their many-body counterparts.

TT 19.8 Mon 17:00 CHE/0091

Dynamics in the presence of local symmetry-breaking impurities — •Yahui Li[1,2], Pablo Sala[3,4], Frank Pollmann[1,2], Sanjay Moudgalya[1,2], and Olexei Motrunich[3,4] — [1]Technical University of Munich, Germany — [2]Munich Center for Quantum Science and Technology, Germany — [3]California Institute of Technology, USA — [4]Walter Burke Institute for Theoretical Physics, USA

Continuous symmetries lead to universal slow relaxation of correlation functions in quantum many-body systems. In this talk, I will show how local symmetry-breaking impurities affect the dynamics of these correlation functions using Brownian quantum circuits. While explicitly breaking the symmetry is generally expected to lead to eventual restoration of full ergodicity, we find that approximately conserved quantities that survive under such circumstances can still induce slow relaxation. This can be understood using a super-Hamiltonian formulation, where low-lying excitations determine the late-time dynamics. We show that in one dimension, symmetry-breaking impurities modify diffusive and subdiffusive behaviors associated with U(1) and dipole conservation at late times, e.g., by increasing power-law decay exponents of the decay of autocorrelation functions. On the other hand, for an impurity that disrupts strong Hilbert space fragmentation, it leads to prethermal plateaus in autocorrelation functions. Overall, our approach systematically characterizes how symmetry-breaking impurities affect relaxation dynamics in symmetric systems.

TT 19.9 Mon 17:15 CHE/0091

Late time dynamics of quantum entanglement — •Felix Dusel[1,2], Frank Pollmann[1,2,3], Tobias Micklitz[4], and Alexander Altland[5] — [1]Department of Physics, Technical University of Munich, 85748 Garching, Germany — [2]Munich Quantum Valley, 80807 Munich, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Schellingstraße 4, 80799 Munich, Germany — [4]Centro Brasileiro de Pesquisas Físicas, Rua Xavier Sigaud 150, 22290-180 Rio de Janeiro, Rio de Janeiro, Brazil — [5]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Straße 77, 50937 Cologne, Germany

We study entanglement spreading in quantum circuits composed of local qudits with large Hilbert space dimension, and single-particle dynamics relaxing slower than the characteristic timescale for entangling of neighboring qudits.

TT 20: 2D Materials II – Electronic and Transport Properties (joint session HL/TT)

Time: Monday 15:00–16:30 Location: POT/0081

TT 20.1 Mon 15:00 POT/0081

Ballistic electrostatic graphene superlattices using He ion-milled etching masks — •Rebecca Hoffmann[1], Giulia Piccinini[1], Julien Barrier[1], David Barcons Ruiz[1], Hanan Herzig Sheinfux[1], Takashi Taniguchi[2], Kenji Watanabe[3], Adrian Bachtold[1,4], and Frank H.L. Koppens[1,4] — [1]ICFO-Institut de Ciencies Fotoniques, Castelldefels, Spain. — [2]International Center for Materials Nanoarchitectonics, NIMS, Tsukuba, Japan — [3]Research Center for Functional Materials, NIMS, Tsukuba, Japan — [4]ICREA-Institució Catalana de Recerca i Estudis Avançats, Barcelona, Spain

An electrostatic superlattice is created by applying a periodic electrostatic potential to a material using patterned gates or dielectrics, leading to tunable band structure reconstruction. This approach enables free design of the superlattice geometry and lattice period. While high mobility has been observed, signatures of ballistic transport (e.g. negative resistance in cross geometry, transverse magnetic focusing) remain to be reported. Here, we present a nanofabrication technique combining Helium ion milling of etching masks with damage-free etching of graphite gates [1]. Using these gates in a graphene heterostructure creates an electrostatic superlattice which preserves graphene's high mobility. We report superlattice features. The high electronic quality is confirmed by transverse magnetic focusing and device-size limited mean free path.

[1]D. Barcons Ruiz, et al., Nat. Commun. 13, 6926 (2022)

TT 20.2 Mon 15:15 POT/0081

Tomographic flow regime in the 2D Corbino disk geometry — •Grigorii Starkov — Institute for Theoretical Physics and Astrophysics, University of Würzburg, D-97074 Würzburg, Germany

2D materials offer a unique test ground to study electron transport regimes dominated by the electron-electron collisions. This makes them the perfect platform to observe the electron hydrodynamic flows.

Not so long ago, it has been realized that precisely in 2D, the electron collisions constrained due to Pauli blocking result in the appearance of the long lived collective modes with odd angular character. The corresponding novel transport regime has been dubbed "tomographic".

In the recent experiment [2], magnetoresistance in Corbino-shaped graphene devices was used to disentangle different contributions to the electron transport and to determine viscosity. The obtained temperature-dependence thereof has been linked to the tomographic flow. However, the analysis is based on the bulk expressions for the conductivity and does not treat boundary corrections in detail. At the same time, boundary layers have been shown to be anomalously large in the tomographic flow regime [3].

To take into account the boundary effects, I analyze the magnetoresistance in the 2D Corbino disk geometry across different regimes, using the linearized Boltzmann equation.

[1] P. Ledwith et al, Phys. Rev. Lett. 123, 116601 (2019) [2] Y. Zeng et al, arXiv:2407.05026 (2025) [3] N. Ben-Schachar, J. Hoffmann, arXiv:2503.14431 (2025)

TT 20.3 Mon 15:30 POT/0081

Pulsed-gate spectroscopy of the electron-hole block- ade in bilayer graphene double quantum dots — •Lars Mester[1,2], Hubert Dulisch[1,2], Katrin Hecker[1,2], Konstantinos Kontogeorgiou[3], Samuel Möller[1,2], Leon Stecher[1], Kenji Watanabe[4], Takashi Taniguchi[5], Fabian Hassler[3], Christian Volk[1,2], and Christoph Stampfer[1,2] — [1]JARA-FIT and 2nd Institute of Physics, RWTH Aachen University, Aachen, Germany — [2]PGI-9, Forschungszentrum Jülich, Jülich, Germany — [3]JARA- Institute for Quantum Information, RWTH Aachen University, Aachen, Germany — [4]Research Center for Functional Materials, Na- tional Institute for Materials Science, Namiki, Japan — [5]International Center for Materials Nanoarchitectonics, National Institute for Materials Science, Namiki, Japan

Pauli blockade is an established read-out mechanism for quantum-dot (QD) spin qubits. Using bilayer graphene (BLG) as a platform offers advantages such as a tunable valley degree of freedom. Recently, a strong spin-valley blockade was demonstrated in an electron-hole BLG double quantum dot (DQD) using time-averaged transport measurements. Here, we employ pulsed-gate spectroscopy by pulsing between the (0e, 0h) and (1e, 1h) charge configurations. Comparison with sim- ulations allows us to identify unconventional higher-order tunneling as the dominant blockade-lifting mechanism, with timescales governed by QD-lead coupling and the number of accessible states. Our results provide direct access to blockade-lifting dynamics in a BLG DQD, offering relavant insights for the development of future BLG-based qubits.

TT 20.4 Mon 15:45 POT/0081

Temperature Dependent Electrical Transport in Thin $SnSe_2$ — •Lars Thole[1], Aarti Lakhara[2], Preeti A. Bhobe[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany — [2]Department of Physics, Indian Institute of Technology Indore, Khandwa Road, Indore, Simrol, 453552, India

The two-dimensional material $SnSe_2$ shows special temperature dependent behavior [1], which has not been understood to its full capacity as of now.

We fabricated thin samples of $SnSe_2$ and investigated its electrical transport behavior in regards to its temperature dependence [2]. These samples show a metal-insulator transition with a metallic state for higher temperatures. The low-temperature transport regime is dominated by variable-range hopping. Additionally, the influence of defect states in these samples is investigated by looking at the thickness dependence for different samples [3].

[1] C. Guo, et al., Appl. Phys. Lett. 109, 203104 (2016).
[2] A. Lakhara, L. Thole, R. J. Haug, and P. Bhobe. arXiv: 2507.14536 (2025).
[3] A. Lakhara, L. Thole, R. J. Haug, and P. Bhobe. Phys. Rev. B 112, 235401 (2025).

TT 20.5 Mon 16:00 POT/0081

Polarization resolved Electron Spin Resonance in two-dimensional electron systems — •Daniiar Khudaiberdiev[1], Alexey Shuvaev[1], Michail Glazov[2], Anton Shchepetilnikov[3], Viacheslav Muravev[3], Christian Reichl[4], Werner Wegscheider[4], and Andrei Pimenov[1] — [1]Institute of Solid State Physics, Technische Universität Wien, 1040 Vienna, Austria — [2]St. Petersburg, Russia — [3]Chernogolovka, Russia — [4]Laboratory for Solid State Physics, ETH Zurich, CH-8093 Zurich, Switzerland

Electron spin resonance (ESR) has long served as a powerful probe of g-factor anisotropy, spin-orbit interactions, hyperfine coupling, and collective many-body spin phenomena in two-dimensional electron systems (2DESs). Most prior studies detect ESR in the photoresistance of Hall bars, where the excitation-field distribution and polarization are distorted, complicating the analysis of the excitation conditions.

In contrast, we report polarization-resolved ESR in sub-THz transmission using a quasi-optical setup and large-area samples that ensure high polarization purity. First we study the 2DES hosted in a 4.5-nm AlAs quantum well with a single isotropic valley. The selection rules indicate that Dresselhaus spin-orbit coupling mediates the electric-dipole-active spin absorption. Further we examine systems with more complex spectra such as wide AlAs wells with an active

pseudospin, HgTe and InAs quantum wells with low effective mass and strong spin-orbit coupling enhancing the effects.

TT 20.6 Mon 16:15 POT/0081

First-Principles Investigation of Electronic Transport in 2D GaSe: Backward Diodes, p-i-n FETs, and Double-Gate MOSFETs — •Dogukan Hazar Ozbey and Engin Durgun — UNAM - National Nanotechnology Research Center and Institute of Materials Science and Nanotechnology, Bilkent University, Ankara, Turkey

In this study, we present a comprehensive first-principles investigation of charge transport in monolayer GaSe nanodevices by combining density functional theory with the nonequilibrium Green's function (DFT + NEGF) formalism. Three representative architectures, namely p–n junctions, p–i–n field-effect transistors (FETs), and double-gate MOSFETs, are systematically analyzed. Our calculations reveal that GaSe p–n junctions display an unconventional backward diode response, in which reverse currents within the ±1 V window exceed forward currents owing to tunneling-assisted transport, as evidenced by the projected local density of states. When configured as p–i–n FETs, electrostatic gating allows selective control over tunneling conduction. Moderate gate biases suppress the reverse current, whereas stronger gating reactivates and amplifies it. Finally, double-gate GaSe MOSFETs with channel lengths of approximately 5 nm exhibit competitive figures of merit that meet or surpass the ITRS-2028 high-performance benchmarks, achieving an on/off ratio of 1.2×10^4, intrinsic delay time of 0.24 ps, and power–delay product of only 0.06 fJ·μm^{-1}. Our results highlight GaSe as a single 2D semiconductor capable of integrating backward-diode behavior with high-speed transistor operation.

TT 21: Electron Theory of Magnetism and Correlations (joint session MA/TT)

Time: Monday 15:00–18:00 Location: POT/0151

TT 21.1 Mon 15:00 POT/0151

Origin of pressure-induced anomalies in the nodal-line ferrimagnet $Mn_3Si_2Te_6$ — Varun Venkatasubramanian[1], Makoto Shimizu[2], •Daniel Guterding[3], and Harald O. Jeschke[1] — [1]Research Institute for Interdisciplinary Science, Okayama University, Okayama, Japan — [2]Department of Physics, Graduate School of Science, Kyoto University, Kyoto, Japan — [3]Technische Hochschule Brandenburg, Brandenburg an der Havel, Germany

The nodal-line ferrimagnet $Mn_3Si_2Te_6$ exhibits a pressure-induced insulator-to-metal transition (IMT), which coincides with pronounced anomalies in its magnetic ordering temperature and anomalous Hall conductivity. We employ density functional theory (DFT) in combination with classical Monte Carlo simulations to elucidate the origin of these effects. Pressure-dependent Heisenberg Hamiltonians extracted from DFT reveal a strong evolution of exchange couplings across the structural transition from the trigonal to the monoclinic phase, producing a dome-shaped variation of the ferrimagnetic ordering temperature in quantitative agreement with experiment. While our simulations capture the pressure-driven IMT and magnetic evolution, the anomalous Hall response cannot be fully explained by intrinsic Berry curvature effects, indicating additional extrinsic contributions.

[1] V. Venkatasubramanian, M. Shimizu, D. Guterding, and H. O. Jeschke, *Origin of pressure-induced anomalies in the nodal-line ferrimagnet $Mn_3Si_2Te_6$*, arXiv:2509.18238

TT 21.2 Mon 15:15 POT/0151

Near Room-Temperature Ferromagnetism and Insulator-Metal Transition in van der Waals Material $CrGeTe_3$ — Daniel Guterding[1], Jihaan Ebad-Allah[2], Gili Scharf[3], Han-Xiang Xu[4], Makoto Shimizu[5], Junya Otsuki[6], Alon Ron[3], Christine Kuntscher[2], and •Harald O. Jeschke[6] — [1]Technische Hochschule Brandenburg, Brandenburg an der Havel, Germany — [2]Augsburg University, Augsburg, Germany — [3]Tel Aviv University, Tel Aviv, Israel — [4]Chinese Academy of Sciences, Beijing, China — [5]Kyoto University, Kyoto, Japan — [6]Research Institute for Interdisciplinary Science, Okayama University, Okayama, Japan

We investigate how pressure tunes the electronic and magnetic properties of the van der Waals ferromagnet $CrGeTe_3$, a promising material for near room-temperature applications. Using DFT+DMFT, we trace the transition from semiconducting to metallic ferromagnet [1]. Optical conductivity reveals a mid-infrared feature, signalling orbital-selective correlations, while a double-exchange mechanism stabilizes high-temperature ferromagnetism [2]. The anomalous Hall effect shows extrinsic behaviour beyond pure Berry curvature effects [3]. These results highlight the interplay of magnetism and electronic correlations in achieving tunable ferromagnetism in $CrGeTe_3$, suggesting that pressure and charge carrier doping offer promising routes to control magnetism and transport in layered materials.

[1] H.-X. Xu *et al.*, Phys. Rev. B **108**, 125142 (2023)
[2] J. Ebad-Allah *et al.*, Phys. Rev. B **111**, L140402 (2025)
[3] G. Scharf *et al.*, Phys. Rev. Res. **7**, 013127 (2025)

TT 21.3 Mon 15:30 POT/0151

Ground State of the Topological Insulator Candidate Eu_2AuGe_3 — •Vinicius Estevo Silva Frehse[1], Aleksandr Sukhanov[1], Artem Korshunov[2], Eugen Weschke[3], Aly Abdeldaim[4], Priscila Rosa[5], and Marein Rahn[1] — [1]Universität Augsburg, Augsburg, Germany — [2]Donostia International Physics Center, San Sebastián, Spain — [3]Helmholz Zentrum Berlin, Berlin, Germany — [4]Diamond Light Source, Didcot, UK — [5]Los Alamos National Laboratory, Los Alamos, USA

Eu_2AuGe_3 is an unusual rare earth germanide in which quasi-trigonal europium sheets are interleaved with Au-Ge honeycomb layers, where high-throughput calculations indicate potential for topological band inversions. Bulk and transport data have revealed a series of (re-)ordering transitions upon cooling, as well as metamagnetic transitions at low temperature. Recently, we identified a broad transition around T_{CDW} = 130 K as the continuous freezing-out of a buckling mode of the honeycomb layers.

Here, we present preliminary evidence from neutron and resonant elastic X-ray scattering, which hints at helical magnetic order below T_N = 11 K. Unexpectedly for the nominally spin-only divalent europium, the magnetic order also appears to be accompanied by a modulated orbital order parameter. This phase is preceded by a transition at 23 K, where we observe a subtle doubling of the *ab*-plane, possibly related to the charge density wave formed during T_{CDW}.

TT 21.4 Mon 15:45 POT/0151

Electronic structure, magnetic and optical properties of antiferromagnetic 3*d*-oxides from a Wannier-localized optimally-tuned screened range-separated hybrid functional — •Alexander Shick[1,2], Guy Ohad[2], Jeffrey Neaton[3,4], and Leeor Kronik[2] — [1]FZU-Institute of Physics, Czech Academy of Sciences, Prague, Czech Republic — [2]Weizmann Institute of Science, Rehovoth, Israel — [3]University of California, Berkeley, USA — [4]Lawrence Berkeley National Laboratory, Berkeley, USA

We apply the recently developed Wannier-localized, optimally tuned, screened range-separated hybrid (WOT-SRSH) functional to prototypical bulk antiferromagnetic insulators — MnO, NiO, and hematite (Fe_2O_3). Comparison to calculations based on well-established functionals, namely PBE0, and HSE06, as well as to self-consistent quasiparticle GW and dynamic mean field theory calculations, and to experiment, shows that the WOT-SRSH functional provides a good quantitative description of band gaps, spin magnetic moments, photoemission, and optical absorption spectra. This establishes WOT-SRSH as a uniform, non-empirical framework for band theory of electronic, magnetic, and optical properties of magnetic insulators.

TT 21.5 Mon 16:00 POT/0151

Spectroscopic evidence of Kondo resonance in 3*d* van der Waals ferromagnets — •Deepali Sharma[1,2], Neeraj Bhatt[1], Asif Ali[1], Rajeswari Roy Chowdhury[1], Chandan Patra[1], Ravi Prakash Singh[1], and Ravi Shankar Singh[1] — [1]IISER Bhopal, Bhopal, India — [2]TU Dortmund, Dortmund, Germany

Two-dimensional van der Waals (vdW) ferromagnets drive the advancement in spintronic applications and enable the exploration of exotic magnetism in low-dimensional systems. The entanglement of the dual–localized and itinerant–nature of electrons lies at the heart of the correlated electron systems giving rise to exotic ground state properties such as complex magnetism, heavy fermionic behavior, Kondo lattice formation, etc. Through temperature-dependent electronic structure of vdW ferromagnets, Co substituted Fe_3GeTe_2, probed using high-resolution photoemission spectroscopy and density functional theory combined with dynamical mean field theory (DFT + DMFT), we provide direct evidence of the emergence of Kondo resonance peak driven by complex interplay between localized and itinerant electrons. Further, in overall agreement with the experimental electronic structure and magnetic properties, DFT + DMFT also reveals non-Stoner magnetism. The findings provide a way forward to the understanding of complex interplay between electronic structure, exotic magnetism, and heavy fermionic behavior leading to the Kondo scenario in 3*d* vdW ferromagnets.

TT 21.6 Mon 16:15 POT/0151

T-linear and quadratic transport across the Cuprate and Nickelate phase diagram : pseudogap, strange-metal and Fermi-liquid — •Dongwook Kim[1], Motoharu Kitatani[2], Juraj Krsnik[3], and Karsten Held[4] — [1]Wiedner Hauptstraße 8-10, 1040 Wien — [2]3-2-1 Koto, Kamigori-cho, Ako-gun, Hyogo 678-1297, Japan — [3]Trg Republike Hrvatske 14. HR-10000 Zagreb Croatia — [4]Wiedner Hauptstraße 8-10, 1040 Wien

We investigate DC resistivity and nodal quasiparticle (QP) scattering in hole-doped cuprates-nickelate type superconductors by ladder dynamical vertex approximation (LDΓA). In the pseudogap regime of doping δ = 0.1-0.175, we observe a crossover from T-linear to T^2 resistivity at low T. For dopings δ = 0.2-0.25, the resistivity remains fully T-linear down to the lowest temperatures, indicating strange-metal behavior associated with a nearby quantum critical point (QCP). At higher doping of δ = 0.3 the T^2 recovery reappears, signaling exit from the quantum-critical regime. The nodal QP scattering rate and the first-Matsubara-frequency rule analysis independently confirm the same FL*NFL crossover, providing consistent support for the T-dependent transport obtained within LDΓA

15 min break

TT 21.7 Mon 16:45 POT/0151

Toward ab-initio simulation for resonant inelastic X-ray scattering in strongly correlated materials — •Yun Yen[1,2], Matthias Krack[2], and Michael Schüler[2,3] — [1]Institute for Theoretical Physics, Bremen Center for Computational Materials Science, University of Bremen, Bremen, Germany — [2]PSI Center for Scientific Computing, Theory and Data, Villigen PSI, Switzerland — [3]Department of Physics, University of Fribourg, Fribourg, Switzerland

X-ray absorption spectroscopy (XAS) and resonant inelastic X-ray scattering (RIXS) can be used to study low-energy excitations in complex materials, which are challenging to interpret due to strong correlations during the photoexcitation processes. We aim to develop ab-initio methods for XAS and RIXS, by constructing Anderson impurity models using Wannier-based tight-binding parameters and constrained random phase approximation. The spectrums are then computed via exact diagonalization and Krylov subspace methods. We will show a benchmark on spin spiral materials, where the d-d excitation intensity dependence can be related to the onset of magnetic order with the support of our methods.

TT 21.8 Mon 17:00 POT/0151

Magnetic Persistence in PrAlGe via RIXS and XAS modeling — •Juan Felipe Pulgarin Mosquera[1,2], Yun Yen[3], Tianlun Yu[4], Yeong-Ah Soh[4], Thorsten Schmitt[4], and Michael Schueler[1,2] — [1]PSI Center for Scientific Computing, Theory and Data, Villigen PSI, Switzerland — [2]University of Fribourg, Department of Physics, University of Fribourg, Fribourg , Switzerland — [3]Institute for Theoretical Physics and Bremen Center for Computational Materials Science, University of Bremen, Bremen, Germany — [4]PSI Center for Photon Sciences, Villigen-PSI, Switzerland

The interplay between topological electronic states and magnetism is in the spotlight of condensed matter for potential applications. PrAlGe is a prime candidate in this context, with several works reporting it as a magnetic Weyl semimetal. However, the microscopic relationship between the magnetic ordering, anomalous Hall effect and local spectroscopic signatures remains an open question. We study this phenomenon based on a combination of X-ray spectroscopy and first-principle calculations. We present our ab-initio approach to computing X-ray absorption spectroscopy and resonant inelastic X-ray scattering based on accurate Anderson Impurity model derived from density-functional theory with Hubbard corrections. This comparison is crucial for understanding the experimental finding that the ferromagnetic transition occurs at $T_c \sim 16$ K, significantly lower than the temperature scale at which the AHE and circular dichroism vanish $T_{AHE} \sim 35$ K). The survival of circular dichroism above T_c serves as a local probe for the persistence of local magnetic moments.

TT 21.9 Mon 17:15 POT/0151

Ab initio spin Hamiltonians and magnetism of Ce and Yb triangular-lattice compounds — Leonid V. Pourovskii[1,2], •Rafael D. Soares[3], and Alexander Wietek[3] — [1]CPHT, CNRS, École polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France — [2]Collège de France, Université PSL, 11 place Marcelin Berthelot, 75005 Paris, France — [3]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38, 01187 Dresden, Germany

We calculate the crystal-field splitting, ground-state Kramers doublet and intersite exchange interactions within the ground-state doublet manifold for a representative set of Ce and Yb triangular-lattice compounds. These include the putative quantum spin liquids (QSL) $RbCeO_2$ and $YbZn_2GaO_5$ and the antiferromagnets $KCeO_2$ and $KCeS_2$. The calculated nearest-neighbor (NN) couplings are antiferromagnetic and exhibit noticeable anisotropy. The next-nearest-neighbor (NNN) couplings are ferromagnetic in the Ce systems and dominated by classical dipole–dipole interactions in the Yb case. Solving the resulting effective spin-1/2 models by exact diagonalization up to N = 36 sites, we predict ordered magnetic ground states for all systems, including the two QSL candidates. We explore the phase space of an anisotropic NN + isotropic NNN triangular-lattice model finding that a significant antiferromagnetic NNN coupling is required to stabilize QSL phases, while the NN exchange anisotropy is detrimental to them. Our findings highlight a possibly important role of deviations from the perfect triangular model in real materials.

TT 21.10 Mon 17:30 POT/0151

Transition metal dihalides: from band structure to magnetic properties — •Alexander Yaresko[1], Sebastien Hadjadj[2], and Maxim Ilyn[2] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Centro de Física de Materiales, Donostia-San Sebastián, Spain

Transition metal dihalides TX_2 (T=Fe, Ni, X=Cl, Br) have recently attracted attention because of successful growth of monolayer-thick TX_2 films on various substrates, such as Au or $NbSe_2$, allowing to study 2D magnetism. We compare results of band structure calculations for bulk and monolayer FeX_2 and NiX_2. By mapping the total energies calculated for helical spin structures with various q to the Heisenberg model we show that the change of magnetic order within a layer from ferro- in $NiCl_2$ to helimagnetic in $NiBr_2$ can be explained by the increased strength of antiferromagnetic (AF) 3-rd neighbor exchange interaction J_3 which competes with FM nearest neighbor J_1. We found that inter-layer coupling J_{2c} stabilizes FM order within a layer. Thus, one can expect stronger tendency to a helimagnetic state in a NiX_2 monolayer.

In contrast to NiX_2, J_1 estimated from LDA+U spin-spiral calculations for FeX_2 is weak but shows substantial dependence on the strength of the Coulomb repulsion U. In agreement with experimental findings, calculations including spin-orbit coupling result in appreciable easy axis anisotropy with Fe magnetic moments normal to layers.

We also discuss various microscopic contributions to intra- and inter-layer exchange interactions.

TT 21.11 Mon 17:45 POT/0151

Coexistence of charge order and antiferromagnetism in three-dimensional Hubbard-Holstein model: A study (exploring phases) at and away from half-filling — •Sandip Halder and Moshe Schechter — Ben-Gurion University of the Negev, Beer-Sheva, Israel

The physics of correlated electron systems has long been explored through the Hubbard model and its extensions, including models with long-range hopping. Likewise, phenomena arising from electron-phonon coupling- such as charge order and superconductivity- have been extensively studied within the Holstein model, though largely in lower dimensions. In transition-metal oxides, however, both electron correlations (U) and electron-phonon coupling (V) coexist intrinsically, motivating a comprehensive study of the Hubbard-Holstein model in three dimensions.

Using an exact diagonalization-based semi-classical Monte Carlo (s-MC) method, we investigate the intriguing properties of this model. At half-filling, the system undergoes a first-order transition between a charge-ordered (CO) phase and an antiferromagnetic (AF) phase as U and V are varied. In the AF regime, near the phase boundary, hole doping drives the system from the AF state (n=1) to a CO state (n=0.5), and eventually to a disordered phase at low densities. Notably, a robust coexistence of AF and CO emerges around x=0.35 (n=0.65), with T_{CO} exceeding T_N, consistent with experiments on $La_{2-x}Sr_xNiO_4$. The study provides new insight into correlated materials and guiding future experimental explorations.

TT 22: Superconductivity – Poster I

Time: Monday 18:00–20:00 Location: P1

TT 22.1 Mon 18:00 P1

Sextets in four-terminal Josephson junctions — •Miriam R. Ebert[1], David C. Ohnmacht[1], Wolfgang Belzig[1], and Juan C. Cuevas[2,3] — [1]Fachbereich Physik, Universität Konstanz, D-78457 Konstanz, Germany — [2]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, 28049 Madrid, Spain — [3]Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049 Madrid, Spain

Multiterminal superconducting junctions have revitalized the investigation of the Josephson effect. One of the most interesting aspects of these hybrid systems is the occurrence of multi-Cooper pair tunneling processes that have no analog in two-terminal devices. Such correlated tunneling events are also intimately connected to the Andreev bound states (ABSs) supported by these structures. Josephson junctions with four superconducting terminals have attracted special attention because they are predicted to support ABSs with nontrivial topological properties. Here, we present a theoretical study of sextets, which are correlated tunneling processes involving three Cooper pairs and four different superconducting terminals [1]. We investigate how sextets can be identified from the analysis of the current-phase relation and show how sextets are connected to the hybridization of ABSs. Furthermore, we discuss their existence in recent experiments on four-terminal devices realized in hybrid Al/InAs heterostructures [2].

[1] M. R. Ebert et al., Phys. Rev. B 112, 195430 (2025)
[2] T. Antonelli et al., Phys. Rev. X 15, 031066 (2025)

TT 22.2 Mon 18:00 P1

Superconducting proximity effect in non-collinear anti-ferromagnets — •Anshuman Padhi[1], Prajwal Rigvedi Madhusudan Rao[1], Ajin Joy[2], Ajesh K Gopi[1], Jiho Yoon[1], Jaechun Jeon[1], Banabir Pal[1], and Stuart S. P. Parkin[1] — [1]Max Planck Institute of Microstructure Physics, 06120, Halle (Saale), Germany — [2]Indian Institute of Science, 560012, Bengaluru, India

Triplet Cooper-pair generation in superconducting hybrids is typically achieved using multilayer ferromagnetic structures with non-collinear magnetization, but such systems restrict material flexibility and can introduce vortex-related artefacts. Non-collinear antiferromagnets (NCAFMs) provide a promising alternative: their intrinsic spin textures and residual uncompensated moments can support long-range superconducting correlations without complex magnetic stacking. Here, we interface superconducting thin films (thickness lesser than the coherence length) with two magnetic phases of a Mn-based antiperovskite and track how their critical temperature evolves under magnetic fields of various orientations. The symmetry and spin configuration of the NCAFMs are expected to modify the Andreev spectrum at the interface and thereby affect the robustness of the superconducting condensate, a common indicator of triplet pairing. We further attempt to study the interface using tunneling spectroscopy and explore possible signatures of spin-dependent Andreev states.

TT 22.3 Mon 18:00 P1

RF-Driven Josephson Dynamics in an STM-Defined Pb-NbS_2 Junction — •Ajla Karic, Rian Ligthart, Alexander LaFleur, Kevin Hauser, Benjamin Froelich, and Fabian D. Natterer — Department of Physics, University of Zurich, Winterthurerstrasse 190, CH-8057, Switzerland

We use a scanning tunneling microscope to form an ultrasmall Josephson junction between a Pb tip and an NbS_2 sample at 1.5 K and investigate how its electromagnetic environment shapes the Josephson response. We apply radio-frequency (RF) driving up to 40 GHz and track the evolution of dI/dV spectra as a function of RF amplitude. The measurements reveal pronounced photon-assisted tunneling features and a strong modulation, suppression, and reemergence of the zero-bias Josephson peak, consistent with a phase-diffusive regime dominated by environmental fluctuations. In ongoing work, we increase the effective junction capacitance to directly probe how controlled changes in the junction capacitance modify the Josephson dynamics. Understanding these environmental effects is essential for identifying the conditions under which STM-based Josephson junctions can be pushed toward more coherent operation relevant for qubit applications.

TT 22.4 Mon 18:00 P1

prediction of SJTM observables in putative PDW state in cuprates — •Monikana Gope, Shaswat Chaturvedi, and Peayush Choubey — Department of Physics, Indian Institute of Technology Roorkee, Roorkee-247667, Uttarakhand, India

The coexistence of competing electronic phases, such as pair-density wave (PDW) and charge-density wave (CDW), in high-temperature superconductors remains unresolved. These phases originate from distinct mechanisms, exhibit spatial modulations, and influence superconductivity differently. Scanning Josephson Tunnelling Microscopy (SJTM) enables atomic-scale probing of these modulations by measuring Josephson and quasiparticle tunnelling currents between a superconducting tip and a superconducting sample, thus serving as a direct local probe of the superconducting gap order parameter. Using this technique, we aim to distinguish PDW signatures from other competing orders in cuprates. Starting with the tJ model, which captures strong electron correlations and the interplay between electron hopping, exchange interactions, and strong correlation effects in cuprate superconductors, we stabilise a metastable PDW phase under specific doping and fixed-temperature conditions. We then compute the critical current for a superconducting s-wave tip in both PDW and PDW + dSC states, finding distinct modulations in Ic and abs(Ic). Finally, we employ a Wannier-function-based continuum approach to calculate the critical current and predict characteristic SJTM signatures of the PDW state.

TT 22.5 Mon 18:00 P1

Theory of ESR-STM in superconducting hybrids — •Marcel Polák and Björn Trauzettel — Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany

The electron spin resonance scanning tunneling microscopy (ESR-STM) is a technique that has emerged in the last few years and is a focus of both experimental and theoretical studies. It combines tunneling with an external rf field to probe magnetic adatoms with high resolution in energy and space. Such tunneling problems can be studied in the presence of superconducting electrodes. This leads to the presence of Yu-Shiba-Rusinov states, Andreev reflection and Shapiro steps. We employ the Green's function approach, to study the effect of an external rf driving on the tunneling current in superconducting hybrids in the presence of driven spins.

TT 22.6 Mon 18:00 P1

Schrieffer-Wolff-transformation approach to Josephson junctions: quasiparticle effects and Josephson harmonics — •Ádám Bácsi[1,2], Teodor Iličin[3,4], and Rok Žitko[3] — [1]Széchenyi István University, Győr, Hungary — [2]MTA-BME Lendület "Momentum" Open Quantum Systems Research Group, Institute of Physics, Budapest University of Technology and Economics, Budapest, Hungary — [3]Jožef Stefan Institute, Ljubljana, Slovenia — [4]University of Ljubljana, Ljubljana, Slovenia

We use the Schrieffer-Wolff transformation (SWT) to analyze Josephson junctions between superconducting leads described by the charge-conserving BCS theory. Starting from the single-electron tunneling terms, we directly recover the conventional effective Hamiltonian proportional to $\cos\phi$, with an operator-valued phase bias ϕ. The SWT approach has the advantage that it can be systematically extended to more complex scenarios. We show that if a Bogoliubov quasiparticle is present its motion couples to that of Cooper pairs, introducing correlated dynamics that reshape the energy spectrum of the junction. Furthermore, higher-order terms in the SWT naturally describe Josephson harmonics, whose amplitudes are directly related to the microscopic properties of the superconducting leads and the junction. We derive expressions that could facilitate tuning the ratio between the different harmonics in a controlled way.

TT 22.7 Mon 18:00 P1

Towards new precision measurements of the AC Josephson effect — •Sandip Saha[1], Oliver Kieler[1], Ralf Behr[1], Jörn Beyer[2], Johannes Kohlmann[1], and Mark Bieler[1] — [1]Physikalisch-Technische Bundesanstalt (PTB), Bundesallee 100, 38116 Braunschweig, Germany — [2]Physikalisch-Technische Bundesanstalt (PTB), Abbestraße 2-12, 10587 Berlin, Germany

The AC Josephson effect is used today to realise the unit volt since it establishes a perfect relationship between voltage and frequency just based upon the magnetic flux quantum $\phi_0 = \frac{h}{2e}$. Around four decades ago, the universality of the Josephson effect was studied and experimentally verified with an uncertainty of 3 parts in 10^{19} [1]. Considering the recent progress in superconducting quantum technology and metrology, we believe that re-evaluating this uncertainty could shed new light on the precision of the AC Josephson effect. We plan to use two independent Josephson junction arrays comprising several thousand Josephson junctions, being driven by a microwave generator to synthesize DC voltages. To detect small voltage differences between these two arrays, which will be connected in a superconducting loop, a state-of-the-art DC SQUID will be inductively coupled and used as an extremely sensitive null detector. At the conference, we will explain the principle behind our experimental setup, provide a detailed introduction of the involved quantum devices, which will be fabricated using the established Nb thin film technology at PTB, and present a roadmap for the upcoming measurements.

[1] https://doi.org/10.1103/PhysRevLett.58.1165

TT 22.8 Mon 18:00 P1

Coulomb blockade in ultrasmall step-edge junctions made of granular aluminum — •Sergey Lotkhov and Lukas Grünhaupt — Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig

We developed a fabrication routine and implemented a Coulomb blockade transistor with two step-edge junctions made of granular aluminum (grAl) super-

conductive film. Our process neither involves widely-used shadow-evaporated overlaps, nor the surface oxidation of aluminum for creating the tunnel barriers. This technique enables multijunction single-charge circuitry free of stray replicas. At low temperatures, the transistor exhibited a typical periodic structure of Coulomb diamonds adjacent to the superconducting voltage gap of grAl, both varying under experimental conditions. The gap was found to depend weakly on the transversal magnetic field up to at least 2 Tesla, which we explain by the microstructure of the superconductive grAl film. Furthermore, the charging effects persisted unaffected across the superconducting transistion of grAl, thus supporting a simple, single-electron tunneling picture of the Coulomb effects observed.

TT 22.9 Mon 18:00 P1

Towards next-generation Josephson arbitrary waveform synthesizers — •Nishtha Chaudhry, Oliver Kieler, Abdulrahman Widaa, Michael Haas, Omar M. Aladdin, and Johannes Kohlmann — Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

With the rapid emergence of new quantum technologies, there is a crucial need for cryogenic microwave generation and detection systems that eliminate additional noise and improve signal quality. We put forward the Josephson Arbitrary Waveform synthesizer (JAWS) as a drive-signal source for these quantum devices for ultrabroadband operation at cryogenic temperatures. The JAWS consists of a pulse-driven series array of Niobium-based SNS Josephson junctions. JAWS delivers ultra-precise, quantum-accurate quantized arbitrary waveforms with exceptional spectral purity of up to -125 dBc and extremely low noise or voltage drift. In this conference presentation, we will introduce the current effort at PTB in which we are extending the operation of previously established JAWS circuits to temperatures as low as 1 K by exploring different substrate options and optimizing parameters of the Josephson junctions. The JAWS chips will be able to provide four different signal channels from DC to GHz and can also be placed close to the quantum chips at cryogenic temperatures.

TT 22.10 Mon 18:00 P1

Impedance-matched Josephson Parametric Amplifiers — •Amitesh Gupta — Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

Frequency-multiplexed microwave readout of superconducting qubits is greatly benefited by low-noise and wide-band amplification. Over the past decade, Josephson junction based amplifiers, like the impedance-matched Josephson parametric amplifiers (JPAs), have become one of the solutions, offering quantum-limited noise performance along with bandwidth of a few hundreds of MHz. We present a streamlined way to design a matching network for JPAs using quarter-wave and half-wave transmission lines. It relies on eliminating the complex part of the impedance of the JPA*s dc-SQUID, and matching the input to the negative resistance arising from pumping the JPA. We present harmonic balance simulations of our designs, and show first experimental results of the devices fabricated using Nb-trilayer technology.

TT 22.11 Mon 18:00 P1

Charge Sensitive Superconducting Transmon Qubits for Infrared Radiation Detection — •Jonathan Huschle[1], Markus Griedel[1,2], Hannes Rotzinger[1,2], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut (PHI), Karlsruhe Institute for Technology — [2]Institute for Quantum Materials and Technologies (IQMT), Karlsruhe Institute for Technology

In superconductors, the absorption of photons with energies exceeding the energy gap breaks Cooper pairs. This increases the population of quasiparticles, enhances noise, and introduces additional dissipation at microwave frequencies. The coherence of superconducting qubits is particularly sensitive to these effects and can thus serve as probes of quasiparticle dynamics. To enhance the sensitivity, we use a charge susceptible transmon qubit to investigate charge noise. In combination with a controllable infrared radiation source, we study the impact on both the charge noise and the coherence time of the modified transmon qubit. We present the qubit design and report on our measurement results at millikelvin temperatures.

TT 22.12 Mon 18:00 P1

Tuneup Protocol for Superconducting Qubits — •Paul Kugler[1], Nicolas Gosling[1], Masum Uddin[2], Asen Georgiev[3], Li-Wei Chang[3], Shroya Vaidya[2], Hiresh Jadoenathmissier[4], Mahmut Çetin[4], Philipp Lenhard[1], Nicolas Zapata[1], Lukas Scheller[5], Robert Gartmann[5], Wang N. Wong[2], Manognya Acharya[2], Tobias Lindström[2], Mark Bieler[3], Sebastian de Graaf[2], Lukas Grünhaupt[3], and Ioan Pop[1,6,7] — [1]IQMT, KIT, Karslruhe — [2]NPL, Teddington, United Kingdom — [3]PTB, Braunschweig — [4]Orange Quantum Systems, Delft, The Netherlands — [5]IPE, KIT, Karlsruhe — [6]PHI, KIT, Karlsruhe — [7]PI1, Stuttgart University, Stuttgart

We present a standardized, control-platform-agnostic procedure for tuning up superconducting qubits, developed to ensure consistency and reproducibility across laboratories and to enable metrological studies of qubit performance. A central component of the protocol is the calibration of a high-fidelity QND readout, which forms the foundation for all subsequent qubit measurements. Building on this, we establish the control pulses required for reliable qubit manipulation, including calibrated π and $\pi/2$ pulses. After completing the pulse-calibration workflow, we validate the tuneup through randomized benchmarking and readout-induced leakage benchmarking, providing quantitative checks of both gate performance and measurement backaction. This unified procedure supports transparent comparison of results across different control stacks and contributes to building a consistent metrological framework for superconducting-qubit experiments.

TT 22.13 Mon 18:00 P1

Investigation of Parasitic Two-Level Systems in Merged-Element Transmon Qubits — •Etienne Daum, Benedikt Berlitz, Alexey V. Ustinov, and Jürgen Lisenfeld — Physikalisches Institut, Karlsruhe Institute of Technology, Wolfgang-Gaede-Straße 1, Karlsruhe, 76131, Baden-Württemberg, Germany

In conventional transmon qubits, decoherence is dominated by a large number of parasitic two-level systems (TLS) residing at the edges of its large area coplanar shunt capacitor and junction leads. Avoiding these defects by improvements in design, fabrication and materials proved to be a significant challenge that so far led to limited progress. The merged-element transmon qubit ("mergemon"), a recently proposed paradigm shift in transmon design, attempts to address these issues by engineering the Josephson junction to act as its own shunt capacitor. With its energy mostly confined within the junctions, efforts required to improve qubit coherence can be concentrated on the junction barrier, a potentially easier to control interface compared to exposed circuit areas. Incorporating an additional aluminium deposition and oxidation into the *in-situ* bandaged Niemeyer-Dolan technique, we were able to fabricate flux-tunable mergemon qubits achieving mean T_1 relaxation times of up to 130μs ($Q \approx 3.3 \times 10^6$). TLS spectroscopy under applied strain and electric fields, together with systematic design variations, revealed that even for mergemon qubits - despite their significantly reduced footprint and increased junction barrier volume - careful design considerations are still essential to avoid coherence limitations due to surface loss.

TT 22.14 Mon 18:00 P1

Superconducting quarton qubits with stacked Josephson junctions — •Alex Kreuzer[1], Hossam Tohamy[1], Thilo Krumrey[1], Jürgen Lisenfeld[1], Hannes Rotzinger[1,2], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut (PHI), Karlsruher Institut für Technologie (KIT) — [2]Institut für Quantenmaterialien und -technologien (IQMT), Karlsruher Institut für Technologie (KIT)

Realizing compact, low-loss inductive elements is a key challenge for scalable superconducting qubits. Although planar Josephson junction arrays offer large inductances, they also have a substantial footprint, which causes additional surface loss and increases the stray capacitance. We implement quarton flux qubits with a large positive anharmonicity using vertically stacked Josephson junctions, which offer compact inductance, low stray capacitance, and reduced surface participation.

We present DC transport characteristics of stacked junctions and microwave-loss measurements of quarton qubits. Qubit spectroscopy reveals numerous avoided crossings induced by two-level systems (TLS), suggesting the TLS in the array junctions as the dominant loss channel. We discuss how qubit coherence and the TLS density are influenced by stack geometry.

TT 22.15 Mon 18:00 P1

Building a Quantum Wheatstone Bridge — •Thilo Krumrey[1], Alex Kreuzer[1], Hossam Tohamy[1], Alan C. Santos[3], Hannes Rotzinger[1,2], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, Karlsruhe, Germany — [2]IQMT, Karlsruher Institut für Technologie, Karlsruhe, Germany — [3]Instituto de Física Fundamental (IFF), Consejo Superior de Investigaciones Científicas (CSIC), Madrid, Spain

Today's qubits, while still quite noisy, are sufficiently coherent for non-computing applications. We are exploring the possibility of using an arrangement of superconducting qubits to study the quantum version of the Wheatstone resistance bridge[1]. It would allow for comparative measurements of coupling energies using the interference of an excitation gradient across strongly coupled qubits. We propose an implementation of a quantum Wheatstone bridge using superconducting quantum circuits with quarton flux qubits. Here, the large positive anharmonicity and the tunability [2] of the operating frequency are beneficial for our application. We will discuss the current status on the qubits and resonators designs, simulation and fabrication results.

[1] K. Poulsen *et al.*, PRL **128**, 240401 (2022)
[2] F. Yan *et al.*, arXiv:2006.04130v1

TT 22.16 Mon 18:00 P1

Designing a W-band Josephson parametric amplifier. — •Jonas N. Kämmerer[1], Urs Strobel[1], Jakob Lenschen[1], Karapet Hambardzumyan[1], Sergei Masis[1], Jürgen Lisenfeld[1], Hannes Rotzinger[1,2], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut (PHI), Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany — [2]Institut für QuantenMaterialien und Technologien (IQMT), Karlsruher Institut für Technologie, 76344 Eggenstein-Leopoldshafen, Germany

Superconducting quantum circuits operating in the millimeter-wave regime are expected to offer several advantages that could impact the scalability of future quantum computing systems. These advantages include a reduced footprint, faster qubit manipulation, increased thermal resilience, and higher operating temperatures.

The realization of superconducting qubits in the millimeter-wave regime presents several challenges, one of which is an efficient readout chain. It should include a Josephson parametric amplifier (JPA), which is a nonlinear device that amplifies microwave signals with added noise approaching the quantum limit.

Here, we propose a tunable JPA design operating in the W-band at a frequency of about 100 GHz. Our approach employs a frequency-tunable DC-SQUID made using niobium-based Josephson junction technology. We present numerical simulations conducted to determine the optimal design and operating parameters for three- and four-wave mixing and also address the challenges to overcome in practical devices, such as pumping and coupling schemes.

TT 22.17 Mon 18:00 P1

Immersion Cooling of Transmon Qubits — •Vasilii Sevriuk[1], Amber Carreck[1], Daniel Doling[1], Zakaria Mohamed[1], Rais Shaikhaidarov[1], Lev Levitin[1], Petri Heikkinen[1], Tobias Lindstrom[2], Alexander Tzalenchuk[1,2], Sebastian de Graaf[2], Andrew Casey[1], and John Saunders[1] — [1]Royal Holloway University of London, UK — [2]National Physical Laboratory, UK

Superconducting qubits have become a standard platform both for developing new engineering approaches in quantum computation and for exploring fundamental questions in solid-state physics and quantum mechanics [1]. Despite this progress, achieving efficient thermalization of qubits remains an important challenge [2]. In this work, we present experimental results obtained by immersing a transmon qubit device into liquid helium and studying the temperature dependence of its key parameters. Our approach extends prior studies on immersion cooling of superconducting resonators [3].

[1] M. Devoret et al., arXiv:cond-mat/0411174
[2] D. Lvov et al., arXiv:2409.02784
[3] M. Lucas et al., Nat. Commun. 14, 3522 (2023)

TT 22.18 Mon 18:00 P1

Dual-tone spectroscopy of atomic tunneling systems in amorphous solids — •Anton Jarecka, Jan Blickberndt, Moritz Maur, Andreas Fleischmann, Andreas Reiser, and Christian Enss — Kirchhoff Institute for Physics, Heidelberg University

The performance of state-of-the-art superconducting quantum devices is limited by noise and decoherence effects, which are known to originate from atomic tunneling systems (TSs) residing in interfaces and dielectric layers. With the goal of further understanding the dielectric properties of such TSs, we investigate their non-equilibrium response by performing radio-frequency dual-tone spectroscopy using a probe and a pump field. For that purpose, we have developed a superconducting microstructured LC-resonator consisting of four identical interdigital capacitors (IDCs) arranged in a Wheatstone bridge setup and two meander inductances, giving rise to two resonance branches. A bulk glass serves as the IDC's dielectric, providing an ensemble of TSs. We use the setup to probe a dielectric volume shared by the two resonances. Therefore, the resonances address the same ensemble of TSs. By tuning the TS-pump field interaction so that the dominant TS Rabi frequencies match the frequency difference of the resonant branches, we can precisely control the dielectric loss of our sample. The measurements are qualitatively described within a framework based on the dressing of tunneling states induced by strong pump fields. Probing these dressed state transitions provides insights into the non-equilibrium dynamics and, consequently, the dielectric response of atomic TSs.

TT 22.19 Mon 18:00 P1

Landau-Zener transitions in ultra-cold glasses — •Jan Blickberndt, Christian Ständer, Anton Jarecka, Andreas Fleischmann, Andreas Reiser, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, Germany

Atomic tunneling systems (TSs) are inherent to disordered structures and therefore appear not only in amorphous solids, but also in oxide layers, tunneling barriers and interfaces of superconducting micro-structured devices, deteriorating their performance by introducing noise and decoherence. Understanding their nature is thus crucial to mitigate the adverse effects of TSs on quantum devices. In this work we investigate the non-equilibrium dynamics of a resonantly driven TS ensemble, which is influenced by slowly varying electric or mechanical bias fields by tuning the TSs energy splitting. To directly probe the TSs dielectric response, we developed a superconducting lumped element resonator microfabricated onto a bulk glass substrate, enabling controlled excitation and readout of the underlying TS population. By varying the sweep rate of the applied bias, we demonstrate rate-dependent control over the dielectric loss of the sample. Furthermore, when applying sufficiently large bias amplitudes we observe a dispersive red shift of the resonator frequency due to an excess saturation of low-energy TSs. Introducing noise bias fields leads to a measurable reduction of effective TS coherence times, demonstrating their sensitivity to spectral fluctuations in their environment. To complement our experiments, we developed a GPU-accelerated Monte Carlo simulation of the tunneling dynamics to validate and extend our findings.

TT 22.20 Mon 18:00 P1

Optimization of cross-type dc-SQUIDs for the readout of MMCs — Alexander Stoll, •Lukas Münch, Daniel Hengstler, Andreas Reifenberger, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, Germany

Readout chains of ultra-low-temperature detector systems often limit the achievable energy resolution. Even superconducting quantum interference devices (SQUIDs), the state-of-the-art sensors for cryogenic detectors such as metallic magnetic calorimeters (MMCs), typically dominate the white-noise regime. The energy sensitivity of a dc-SQUID $\epsilon \sim T\sqrt{LC}$ is mainly set by the inductance, intrinsic Josephson junction capacitance, and temperature. While the inductance is fixed for practical reasons, the capacitance can be reduced by moving from a window-type to a cross-type junction geometry. Furthermore, the operation temperature of the SQUIDs which typically decouples from the much lower mixing chamber temperature due to heat dissipation in the shunt resistors, can be lowered. Following an idea from Stephen Boyd and coworkers (to be published), we divide the cooling fins into multiple sectors across the shunt resistor to improve electronic heat dissipation. We describe the fabrication of cross-type dc-SQUIDs for MMC readout, emphasizing the role of CMP-based processing in achieving high wafer-scale yield and uniformity on three-inch wafers. Finally, we present their characterization and compare the noise performance to earlier dc-SQUID generations.

TT 22.21 Mon 18:00 P1

AuTi Magnetic Penetration Depth Thermometers for low temperature microcalorimeters — •Naemi Grun, Christian Enss, Andreas Fleischmann, Loredana Gastaldo, Daniel Hengstler, Florian Kaiser, Lukas Münch, Andreas Reifenberger, and Martin Schwendele — Kirchhoff Institute for Physics, University Heidelberg

Low temperature microcalorimeters reach high energy resolution in a wide energy range thanks to very sensitive thermometers. Magnetic penetration depth thermometers (MPTs) would represent a very interesting alternative with respect to commonly used metallic magnetic calorimeters (MMCs) and transition edge sensors (TESs). The working principle of MPTs is based on the Meissner-Ochsenfeld effect and the temperature dependence of the magnetic penetration depth. A temperature increase due to energy deposition in the absorber material translates into an increase in the magnetic penetration depth of the MPT, which can be read out by highly sensitive SQUID magnetometers. We are investigating AuTi bilayers as a possible MPT sensor material and are targetting a transition temperature below 100 mK. To avoid hysteretic effects, the sensor does not have a bulk geometry, but is deposited onto the readout coil in the geometry of separate stripes or dots. We discuss the properties of the AuTi bilayers and the results obtained with MPT prototypes based on different geometries.

TT 22.22 Mon 18:00 P1

Identification of Noise Sources in Superconducting Microstructures — •Krishnam Mimani, Daniel Hengstler, Matthew Herbst, David Mazibrada, Lukas Münch, Andreas Reifenberger, Markus Renger, Christian Ständer, Rui Yang, Andreas Fleischmann, Loredana Gastaldo, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University

Improving the performance of superconducting devices often means identifying and eliminating noise sources. Many noise sources are transferable across different device categories such as qubits, SQUIDs, and superconducting detectors due to the intrinsic nature of the micro-fabricated thin film materials. Our stand-alone device can analyze the specific noise contributions of these microfabricated thin films. The device consists of a Wheatstone-like bridge of four micro-fabricated superconducting inductors, two of which are filled with a sample material, and a pair of two-stage dc-SQUID read-out chains. We can use the method of cross-correlation, to suppress the noise of the read-out chains and derive the total noise contribution of our device, or drive the Wheatstone bridge with an ac-current to measure the complex ac-susceptibility of the sample material. Our experiments are performed at temperatures between $T = 20$ mK and $T = 800$ mK in the frequency range from $f = 100$ mHz to $f = 500$ kHz. We present the results of multiple measurements on thin films of SiO2, AuPd, Ag:Er, as well as Au:Er and perform a detailed comparison. We discuss our efforts to increase the frequency bandwidth for both our measurement modes, measuring towards noise levels of below $\sqrt{S_\Phi} = 10\,\mathrm{n}\Phi_0/\sqrt{\mathrm{Hz}}$.

TT 22.23 Mon 18:00 P1

Superconducting Resonators from Ultrathin NbN Films — •Hrishikesh Borah, Meenakshi Sharma, Haolin Jin, Yejin Lee, and Uri Vool — Max Planck Institute for Chemical Physics of Solids

We explore the transport and microwave response of ultrathin Niobium Nitride (NbN) of 3 nm thickness. Transport measurements confirm the 2D behavior of our system, consistent with the Berezinskii-Kosterlitz-Thouless transition. In such ultrathin limit, the inertia of the cooper pairs defined as kinetic inductance becomes dominant. Our films exhibit a high kinetic inductance of 300 pH/sq, which significantly impacts the response of superconducting microwave resonators patterned from the films. Moreover, temperature dependence measurements of the microwave response reveal that in low temperature regime, the superfluid density follows a power-law rather than the BCS prediction. Energy losses at low temperature are dominated by two-level system (TLS) defects while at higher temperatures, losses are caused by the breaking of Cooper pairs. This work investigates the ultrathin NbN regime for compact, high-impedance devices ideal for quantum circuits and sensitive detectors.

TT 22.24 Mon 18:00 P1

Chaotic Behavior of Josephson Diodes — •Vjeko Dimić[1], Simon Feyrer[1], Alexander Kirchner[1], Daniel Crawford[2], Davide Curcio[3], Giorgio Biasiol[3], Tero Heikkilä[2], Christoph Strunk[1], and Leandro Tosi[1,4] — [1]Institute of Experimental and Applied Physics, University of Regensburg, Germany — [2]Department of Physics and Nanoscience Center, University of Jyväskylä — [3]CNR-Istituto Officina dei Materiali Laboratorio TASC, Italy — [4]Centro Atomico Bariloche, Comision Nacional de Energia Atomica, Argentina

The behavior of nonlinear resonators is well described by the Duffing oscillator model. For sufficiently high driving powers, the response of the system has three solutions, two metastable, and one unstable, i.e., the system enters bifurcation regime. This also applies for nonlinear superconducting resonators where the nonlinearity stems from the nonlinear behavior of Josephson junctions. If instead we have a junction exhibiting the Josephson diode effect, the Duffing model acquires an additional term which results in reemergence of stable solutions for certain parameters. Here we present the design and measurement of two tunable $\lambda/4$ resonators fabricated out of a hybrid Al/InAs heterostructure. One resonator is terminated with a single Josephson junction, while the other is terminated with a SQUID. We perform microwave measurements of the resonators and observe the onset of the bifurcation regime in both devices, while the reemergence of stable solutions is observed in the SQUID device. We have also explored the dependence with in-plane magnetic field, in particular the range where superconducting diode effect has been observed.

TT 22.25 Mon 18:00 P1

Planar Broadband Superconducting Waveguide for Coherent Control of Rare-Earth Spin Ensembles — •Arjun Bhasker[1,2], Georg Mair[2,1], Léa Richard[2,1], Michael Stanger[1], Andreas Erb[2,1], Hans Huebl[2,1,3], and Nadezhda Kukharchyk[2,1,3] — [1]School of Natural Sciences, Technische Universität München, 85748 Garching, Germany — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology, 80799 München, Germany

Solid-state quantum memories based on rare-earth ions require highly homogeneous microwave fields to enable coherent control of large spin ensembles. While coplanar waveguides can be used for this purpose, they inherently produce non-uniform field distribution: The microwave field peaks at the center conductor, and the field direction varies substantially within the gaps, which leads to a variety of Rabi frequencies. To overcome this limitation, we introduce a new planar superconducting broadband transmission-line architecture implemented via a technique such as flip-chip bonding, designed to generate a highly uniform microwave field across the active region. In this approach, a $CaWO_4$ crystal doped with erbium ions has to be thinned producing a flat and uniform membrane to ensure proper impedance matching and optimal coupling to the microwave field. Such a design provides a promising platform for implementing rare-earth-based quantum memories with microwave superconducting quantum technologies.

TT 22.26 Mon 18:00 P1

High-quality superconducting broadband microwave structures for broadband electron spin resonance experiments — •Robert Pant[1,2], Georg Mair[1,2], Arjun Bhasker[1,2], Sebastian Dominguez-Calderon[1,2], Hans Huebl[1,2,3], and Nadezhda Kukharchyk[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]School of Natural Sciences, Technische Universität München, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology, 80799 München, Germany

Electron spin resonance (ESR) spectroscopy is a powerful tool when it comes to studying the internal structure of materials and characterizing spins of unpaired electrons within. Superconducting microwave resonators are widely employed for such studies allowing to achieve strong coupling to spin systems. However, a generally narrow frequency range of their operation limits the amount of simultaneously coupled spin states. Over-coupled resonating structures can provide a substantially broader spectrum of microwave frequencies for resonance absorptions, thus improving the measurement efficiency. In the following work, several promising configurations of superconducting coplanar waveguide resonators in the over-coupled regime are developed, including a $\lambda/2$ transmission-line resonator with implemented interdigital capacitors that ensure an increased coupling rate to spin ensembles in the low frequency range of 0–4 GHz.

TT 22.27 Mon 18:00 P1

Metallic-Magnetic Calorimeters for Efficient High Resolution X-ray Spectroscopy for Energies up to 150 keV — •Daniel Kreuzberger, Andreas Abeln, Hendrik Hadenfeldt, Daniel Hengstler, Andreas Reifenberger, Daniel Unger, Andreas Fleischmann, Loredana Gastaldo, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, Germany

Metallic Magnetic Calorimeters are cryogenic detectors for broadband x-ray spectroscopy with high energy resolution and small, well understood nonlinearity. They consist of a metallic particle absorber, typically made of gold and a paramagnetic temperature sensor made of an erbium doped noble metal host material. If a photon is absorbed, its energy is converted to heat, leading to a temperature change of the sensor material. This temperature rise changes the magnetization of the sensor material, which is read out by a sensitive SQUID magnetometer.

Experiments on highly charged ions and light muonic atoms have brought up the necessity to build densely packed arrays of MMCs with a high stopping power for photon energies up to 150 keV. This can be achieved with the presented new microfabrication-process for 120 μm thick absorbers made of electroplated gold. We also present fabrication results for the fast thermalization of the MMCs using the backside of the silicon substrate, which can be achieved by using DRIE processes, and filling these TSVs with copper. Finally we present characterization results for two different MMC arrays fabricated with those newly developed processes and results from most-recent beamtimes.

TT 22.28 Mon 18:00 P1

MMC-based photon and phonon detector for scintillating crystals at mK temperatures — •Ioana-Alexandra Nitu, Christian Enss, Andreas Fleischmann, Clara Marie Günther, Daniel Hengstler, Sebastian Hilscher, Ashish Jadhav, Cagla Mahanoglu, Andreas Reifenberger, and Loredana Gastaldo — Kirchhoff Institute for Physics, Heidelberg University

Scintillating bolometers operated at mK temperatures provide a means to probe for neutrinoless double beta decay ($0\nu\beta\beta$) and Dark Matter. The ratio of light to heat signals permits discrimination between heavy particles, for instance α particles, and lighter ones, like β or γ particles. The AMoRE collaboration uses separate photon and phonon detectors based on metallic magnetic calorimeter (MMC) technology to search for $0\nu\beta\beta$ in ^{100}Mo using $LiMoO_4$ crystals.

We present an integrated photon-phonon (P2) detector concept, where both detectors are microfabricated on the same 3-inch silicon substrate and thermally separated by etched trenches. Presently, the optimization of the photon and phonon detectors is done separately. The development of the photon detector has been completed and preliminary results validate fabrication procedures. A phonon detector prototype was designed and microfabricated using the same steps as the pre-existing photon detector. We present the fabrication steps to obtain the target mechanical and thermal properties and discuss preliminary results in comparison to the expected performance.

TT 22.29 Mon 18:00 P1

Time response of an MMC-based large-area photon detector operated at mK — •Sebastian Hilscher, Christian Enss, Andreas Fleischmann, Clara Marie Günther, Daniel Hengstler, Ashish Jadhav, Cagla Mahanoglu, Ioana-Alexandra Nitu, Andreas Reifenberger, Christian Ritter, Daniel Unger, and Loredana Gastalo — Kirchhoff Institute for Physics, Heidelberg, Germany

We present a large-area photon detector based on low temperature metallic magnetic calorimeters (MMCs), for which the silicon substrate acts as absorber. The detector is designed for measuring light emission in scintillating crystals, for instance in the AMoRE experiment. The visible photons emitted in the scintillating crystal are absorbed on a central silicon area isolated by through-silicon trenches from the rest of the substrate. Prototype devices have been produced and characterized at mK temperatures with focus on the time profile of temperature pulses. Very important for the optimization of the detector is modeling this time profile. Here, we present simulations of the phonon propagation and scattering inside the silicon absorber, with either specular or diffusive reflections at the surfaces. These simulations provide a time dependence of the fraction of energy reaching the MMC sensor. We compare the results obtained from measurement and simulation and discuss the implications of the photon detector for the AMoRE experiment.

TT 22.30 Mon 18:00 P1

Towards large-area 256-pixel MMC arrays for high resolution X-ray spectroscopy — •Andreas Abeln, Daniel Hengstler, Lucas Herbstritt, Daniel Kreuzberger, Andreas Reifenberger, Andreas Fleischmann, Loredana Gastaldo, and Christian Enss — Kirchhoff Institute for Physics, Heidelberg University

Metallic Magnetic Calorimeters (MMCs) are energy-dispersive cryogenic particle detectors. Operated at temperatures below 50 mK, they provide very good energy resolution, high quantum efficiency as well as high linearity over a large energy range. In many precision experiments in X-ray spectroscopy the photon flux is small, thus a large active detection area is desirable. Therefore, we develop arrays with increasing number of pixels.

In this contribution we present a detector setup featuring a novel dense-packed 16 × 16 pixel MMC array. The pixels provide a total active area of 4 mm × 4 mm and are equipped with 5 μm thick absorbers made of gold. This ensures a stopping power of at least 50 % for photon energies up to 20 keV. The expected energy resolution is 1.4 eV (FWHM) at an operating temperature of 20 mK. For the cost-effective read-out of the 128 detector channels we envisage the flux-ramp multiplexing technique. We present first results of the detector characterization obtained utilizing parallel 2-stage dc-SQUID read-out chains. We discuss the detector performance, focusing on the thermal behavior within the detector as well as to the thermal bath.

TT 22.31 Mon 18:00 P1

MOCCA: A molecule camera for the position and energy resolved detection of neutral molecule fragments — •N. Fiedler[1], A. Fleischmann[1], C. A. Jakob[2], D. Kreuzberger[1], A. Özkara[1], D. Hengstler[1], A. Reifenberger[1], L. Gastaldo[1], P. Martini[3], S. Rosén[3], H. Zettergren[3], O. Novotný[2], H. T. Schmidt[3], and C. Enss[1] — [1]Kirchhoff Institute for Physics, Heidelberg University — [2]Max Planck Institute for Nuclear Physics, Heidelberg — [3]Department of Physics, Stockholm University

The MOCCA detector is a high-resolution camera for neutral molecule fragments with kinetic energies in the keV range. It features several thousand pixels based on metallic magnetic calorimeters and is read out using SQUIDs. To reconstruct the kinematics of electron-ion and ion-ion reactions, MOCCA measures both the energy and the impact position of molecular fragments incident on the detector, even with multiple particles hitting the detector simultaneously. The latest fabricated version is currently being deployed at the Cryogenic Storage Ring (CSR) at the Max Planck Institute for Nuclear Physics in Heidelberg, where molecular ions are stored and prepared in their rotational and vibrational ground states, allowing detailed studies of electron-ion interactions. We present plans for integrating the 11.5k-pixel MOCCA-Quattro detector system into the Double ElectroStatic Ion Ring ExpEriment (DESIREE) at Stockholm University, which enables mutual neutralization of ions at extremely small relative velocities. This will significantly enhance studies of neutralization processes in complex molecules prepared in their quantum ground state.

TT 22.32 Mon 18:00 P1

Towards reproducible Transition Edge Sensors for rare event searches — •Kilian Heim[1], Godehard Angloher[1], Laci Andricek[2], Mukund Bharadwaj[1], Dieter Hauff[3], Bernd Liebig[2], Gerhard Liemann[2], Jelena Ninkovic[2], Karoline Schäffner[1,3], Kumrie Shera[1], Raimund Strauss[3], Philipp Wasser[3], and Lutz Ziegele[1] — [1]Max-Planck-Institut für Physik — [2]Max-Planck Halbleiterlabor — [3]Technische Universität München

One approach to the search for dark matter is the use of scintillating crystals, such as sodium iodide (NaI), operated at cryogenic temperatures, as implemented by the COSINUS experiment. The readout of the signal, generated upon a nuclear recoil in a NaI crystal, relies on tungsten based transition edge sensors (TESs). These sensors consist of thin (~200 nm) tungsten films that are operated in the transition between the normal and superconducting state.

The transition temperature of such thin tungsten films depends on a multitude of factors, including grain size, stress level, and film impurities. However, for COSINUS, and next-generation rare event searches, the ability to mass-produce sensors with a consistent transition temperature of ~15 mK is crucial. Achieving this necessitates a solid understanding of the factors influencing the transition temperature as well as a precise control of these parameters during the fabrication process.

This contribution presents the first steps taken towards the establishment of a reproducible TES fabrication process as well as future measures to achieve consistent transition temperatures.

TT 22.33 Mon 18:00 P1

In-situ thermometry of Holmium in $LiYF_4$ crystals with Erbium as a probe — •Julia Latour[1,2,3], Cesare Mattiroli[2], Matthias Althammer[3,1], Nadezhda Kukharchyk[3,1,4], and Henrik M. Rønnow[2] — [1]Technische Universität München — [2]École Polytechnique Fédérale de Lausanne — [3]Walther-Meißner-Institut für Tieftemperaturforschung — [4]Munich Center for Quantum Science and Technology

Measurements of sample temperatures in cryogenic environments are, in most cases, performed using resistance thermometers. Such measurements, however, do not allow for determining the actual temperature inside optical crystals, such as $LiYF_4$, due to thermal boundary resistance and thermal-conductivity mismatches between the sample, mounting plate, and sensor. These limitations can be overcome by employing an in-situ spin-temperature measurement technique based on the analysis of changes in the hyperfine energy-level populations of fast-thermalizing, highly coherent electron spin systems. In this work, we investigate mixed ensembles of Holmium and Erbium ions diluted in a $LiYF_4$ host for in-situ spin thermometry. To this end, we monitored the relative changes in the absorption spectra of $LiYF_4$ with 0.1% and 1% Ho doping and 0.005% Er co-doping in the magnetic fields of 0–5 T over the temperature range of 0.1–1 K. We compare the thermometry results for the lower- and higher-doped samples to estimate the impact of ion-ion interactions. Samples doped with only Holmium and Erbium are similarly probed to serve as temperature references.

TT 22.34 Mon 18:00 P1

Fast calibration and performance verification of RuO_2 chip thermometers down to 20 mK utilizing adiabatic demagnetization refrigeration in the PPMS. — •Jorginho Villar Guerrero, Philipp Gegenwart, Christian Heil, and Tim Treu — University Augsburg

Access to temperatures in the millikelvin (mK) range is essential for the research and development of quantum technologies. Calibrated low-temperature sensors are expensive and only available with long lead times. We focus on the fast calibration of cheap Ruthenium Oxide (RuO_2) thick-film resistor chips that are widely used in the automotive industry and are therefore readily available. Upon cooling to below 4 K, they show a pronounced rise of the resistance, which follows variable-range hopping and can be used for low-temperature thermometry down to 20 mK [1]. The thermometers feature a low mass and consequently a low specific heat. Their small size allows mounting them on small contact surfaces. For calibration and performance tests down to mK temperatures, we utilize adiabatic demagnetization of frustrated oxide quantum magnets in the Quantum Design Physical Property Measurement System [2]. We present a miniaturized thermometer calibration setup with reduced response time and minimal self-heating for use down to 20 mK. We report measurements against secondary thermometers with traceable calibration as well as verification with superconducting transitions of Rh-Ir alloy.

[1] R. W. Willekers et al., Cryogenics 30, Issue 4, 1990

[2] T. Treu et al., J. Phys. Condens. Matter 37, 013001 (2025)

TT 22.35 Mon 18:00 P1

Optimizing the Energy Resolution of Calorimetric Low Temperature Detectors (CLTDs) by Reducing Mechanical Vibrations of the Cryogenic Setup — •Elias Eisenschmidt[1,3], Hardy Weisweiler[1], Andre Schirmeisen[2,3], Jack-Andre Schmidt[2,3], and Saskia Kraft-Bermuth[1] — [1]Technische Hochschule Mittelhessen, D-35390 Giessen, Germany — [2]Justus-Liebig-Universität Giessen, D-35392 Giessen, Germay — [3]TransMIT GmbH, D-35392 Giessen, Germany

A CLTD consists of an absorber whose temperature can be measured with a thermometer. Due to the careful consideration of absorber*s heat capacity and thermal coupling, the temperature increase of the absorber due to the impact of a particle can be directly related to the energy of said particle [1],

One limit to the energy resolution is electronic noise which is partly due to vibrations. In this study, the required low temperature is reached using a Pulse Tube Cooler (PTC) for precooling and a pumped 4He pot on a second stage. The CLTD*s energy resolution is noticeably influenced by mechanical vibrations. In this work, measurements and FEM simulations of vibrations at different cold finger designs are correlated to the energy resolution of heavy ion CLTDs obtained from alpha particles.

[1] P. Egelhof and S. Kraft-Bermuth, Prog. Part. Nucl. Phys. 132, 104031 (2023) DOI:10.1016/j.ppnp.2023.104031.

TT 22.36 Mon 18:00 P1

Optimization of a Single-Stage GM-Type Cooler for Large Thermal Masses — Miriam Reif[3], •Jan Ole Sonnenberger[1,2], Bernd Schmidt[2,3], Jack-André Schmidt[2], and André Schirmeisen[2,3] — [1]Technische Hochschule Mittelhessen, Friedberg, Germany — [2]TransMIT GmbH, Giessen, Germany — [3]Instiute of Applied Physics, Justus-Liebig University, Giessen, Germany

The demands placed on cooling systems are constantly increasing, which is why they are becoming larger resulting in more overall mass, yet are still expected to cool as quickly as existing systems. Therefore, the systems must be optimized to cool larger masses.[1] A single-stage cooler is ideal for pre-cooling, which is why a single-stage GM-type PTS power cooler was tested as part of the investigation. The performance data of the system was recorded and analyzed under various operating conditions. Based on these measurements, a cooling curve was measured and optimized varying the operating frequency to determine the optimal operating point of the system.

Another another test was then carried out with an attached thermal load in the form of 42 kg of copper to investigate the cooling behavior under increased mass. Once the mass had cooled down without optimization, the cooling time was reduced by around 25% based on the data gained from the previous experi-

ments. These tests provide deeper insight into the performance and optimization of the single-stage GM-type power cooler.
[1] Snodgrass et al., Nat Commun 15, 3386 (2024)

TT 22.37 Mon 18:00 P1

Purification of liquid Helium with a heat flush purifier in a dry cryostat — •Franziska Hömke and for the DELight Collaboration — Kirchhoff-Institute for Physics, 69120 Heidelberg, INF 227, Germany

The Direct search Experiment for Light dark matter (DELight) aims to search for dark matter by probing elastic scattering interactions of light dark matter particles with helium atoms in liquid helium. The helium is cooled to low millikelvin temperatures within a ^{3}He/^{4}He dilution refrigerator. At these temperatures ^{4}He is in its superfluid phase, enabling a long mean free path for the phonons and rotons produced in the scattering events. However, ^{3}He impurities drastically limit the mean free path and hinder the ballistic propagation of the phonons and rotons. To achieve a sufficiently large mean free path, the ^{3}He concentration in the helium must be reduced by at least three orders of magnitude from the natural concentration.

A heat flush purifier makes use of the unique properties of superfluid ^{4}He to remove ^{3}He and other impurities via a temperature gradient. It can be operated in continuous flow and will be integrated into the helium filling circuit of the cell. In wet cryostats, these devices were able to achieve the desired ^{3}He concentration in ^{4}He within a single cycle, but no implementations in dry cryostats have yet been described.

This contribution presents the ongoing developments in the design and optimization of a heat flush purifier for the DELight cell.

TT 23: Correlated Electrons – Poster I

Time: Monday 18:00–20:00 Location: P1

TT 23.1 Mon 18:00 P1

High-field magnetization of clinoatacamite $Cu_2Cl(OH)_3$ — •David Röll[1], Leonie Stödter[2], Carolin Kastner[1], Sven Luther[3], Ralf Feyerherm[4], Dirk Menzel[1], Anja U. B. Wolter[5], Kirrily Rule[6], and Stefan Süllow[1] — [1]IPKM, TU Braunschweig — [2]FZ Jülich, JCNS at MLZ, Garching, Germany — [3]HLD-EMFL, HZDR, Dresden-Rossendorf, Germany — [4]HZB, Berlin, Germany — [5]Leibniz IFW Dresden, Dresden, Germany — [6]ANSTO, Lucas Heights, Australia

The mineral clinoatacamite $Cu_2Cl(OH)_3$ is closely related to the Kagome material herbertsmithite $ZnCu_3Cl_2(OH)_6$ and has been discussed as a geometrically frustrated magnet. Its Kagome structure of Cu^{2+} ions features antiferromagnetic in-plane coupling and weaker ferromagnetic interlayer exchange, giving rise to exotic quantum states at low temperatures and in applied magnetic fields. In recent years, we have extensively characterized the magnetic phase diagram up to 14 T, revealing multiple distinct magnetic phases.

Here, we present high-field magnetization measurements on a single-crystalline sample up to 52 T. The magnetization at 2.2 K increases with field but begins to saturate at about 15 T, reaching only a fraction of full magnetization and indicating that the system is not fully magnetized. This stands in clear contrast to previously published results, where the mineral is reported to be fully magnetized at around 35 T. Consequently, we expect the magnetization to rise again at fields beyond our current range, implying the possible presence of a magnetization plateau.

TT 23.2 Mon 18:00 P1

Anisotropic spin models on frustrated lattices: from spin liquids to supersolids — •Martin Ulaga[1], Jure Kokalj[2,3], Takami Tohyama[4], and Peter Prelovšek[3] — [1]MPIPKS, Dresden, Germany — [2]University of Ljubljana, Faculty of civic and geotedic engineering, Ljubljana, Slovenia — [3]Institute "Jožef Stefan", Ljubljana, Slovenia — [4]Science universigy of Tokyo, Tokyo, Japan

Recent experiments on novel materials, best described by easy-axis spin models on a triangular lattice, stimulated renewed theoretical interest in basic properties of anisotropic spin models on frustrated planar lattices. While the thermodynamic properties of the model on the Kagome lattices are consistent with the spin-liquid scenario in the whole range of anisotropies, the case of the triangular lattice is more complex. Several numerical studies indicate that anisotropic systems should follow the supersolid scenario with broken translation symmetry in the ground state, as well as the transverse magnetic order, implying a gapless Goldstone mode. Confirming this scenario at finite magnetic fields, we find numerically that at zero field, the available evidence points instead to a solid with a finite gap.

TT 23.3 Mon 18:00 P1

Observation of spin-glass behavior in Nd — •Lorenz Pech[1], Lukas Bauer[1], Jiří Pospíšil[4], Christoph Franz[1], Leo Maximov[1], Andreas Bauer[1,3], Marc A. Wilde[1,3], and Christian Pfleiderer[1,2,3] — [1]Technical University of Munich (TUM) — [2]MCQST, Munich — [3]TUM Center for Quantum Engineering — [4]Charles University, Prague

Frustration and effective disorder in Nd are expected to produce frozen, disordered spins with slow, history-dependent dynamics [1]. We investigate the low-temperature magnetic and electronic properties of single-crystal neodymium to map its complex phase behavior and search for a spin-glass like state. To identify such phases, we combine temperature and field sweeps with ac magnetization (frequency-resolved), dc magnetization (ZFC/FC), and relaxation measurements. From anomalies in $\chi'(T)$, $\chi''(T)$, $M(H)$, and $\mathrm{d}M/\mathrm{d}H$ along principal crystallographic directions, we construct a T–B phase diagram. Established spin glass freezing criterias are the presence of a ZFC/FC bifurcation, a frequency-dependent shift of the χ' and χ'' peak, and slow non-exponential relaxation [2]. These benchmarks, together with more recent perspectives on complex low-temperature phases in correlated systems, provide the framework for interpreting our Nd data and distinguishing glassy behavior from conventional long-range magnetic order.
[1] Kamber, Umut et al. Science 368, eaay6757 (2020).
[2] K. Binder and A. P. Young, Rev. Mod. Phys. 58, 801 (1986).

TT 23.4 Mon 18:00 P1

Exploring Quantum Phases of Magnetic Skyrmions — •Marc Currle, Sopheak Sorn, and Markus Garst — Karlsruhe Institute of Technology, Karlsruhe, Germany

The topological skyrmion density in the continuum theory of two-dimensional magnets obeys both a dipole conservation law and the Girvin-MacDonald-Platzman algebra, suggesting a close correspondence with the quantum Hall problem [1]. Motivated by this observation, we explore quantum phases of skyrmions using analogies with integer and fractional quantum Hall states. Employing an effective description in terms of collective coordinates for skyrmions, we demonstrate that quantum states of the skyrmion many-body system can be represented as holomorphic wavefunctions similar to the states within the lowest Landau level. We highlight the consequences of this correspondence, in particular, the possibility of systematically applying methods from quantum Hall physics to identify skyrmion liquid states.
[1] S. Sorn, J. Schmalian, M. Garst, Phys. Rev. X 15, 041037 (2025)

TT 23.5 Mon 18:00 P1

Quantum Phase Transitions of Kitaev's Toric Code on a Honeycomb lattice — •Viktor Kott, Matthias Mühlhauser, Jan Alexander Koziol, and Kai Phillip Schmidt — Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)

We investigate the robustness of the topological phase of Kitaev's toric code in a uniform magnetic field on the honeycomb (and triangular) lattice using perturbative linked-cluster expansions (LCEs) based on a hypergraph decomposition, together with quantum Monte Carlo (QMC) simulations. The LCE approach allows us to correctly account for the nontrivial mutual exchange statistics of elementary anyonic excitations. By extracting the ground-state energy and excitation energies of the topological phase, we determine the quantum phase transitions out of the topologically ordered state. In addition, we use QMC to explore the full quantum phase diagram. In contrast to the conventional toric code on the square lattice, the ground-state phase diagram depends on the sign of the magnetic field, which distinguishes between unfrustrated and frustrated parameter regimes. This leads to distinct quantum-critical properties and a richer phase diagram.

TT 23.6 Mon 18:00 P1

The XY Toric Code on the Kagome lattice — •Constanze Kölbl, Maximilian Vieweg, and Kai Phillip Schmidt — Department Physik, Staudtstraße 7, 91058 Erlangen

This theoretical work investigates the XY toric tode on the Kagome lattice, constituting a generalisation of the 2024 introduced XY checkerboard toric code on the square lattice [1]. Main objectives are deriving ground state and low-excitation properties and further extracting the parameter-dependent quantum phase diagram of the model. Besides a four-spin z-flavour star operator, two kinds of plaquette operators are introduced, including both Pauli x and y interactions and realising a bipartition. Due to the geometry of the lattice, the plaquette operators connect three and six spins each. Star operators still act as symmetries of the Hamiltonian, whereas different plaquette operator types generally do not commute. The behaviour in the limit of isolated plaquettes is examined analytically using first-order perturbation theory, checking for topological order. Further intuition is gained from exact diagonalisation of the full Hamiltonian for a system comprising 24 spins. A duality mapping is performed, giving rise to a self-dual

model built from four- and six-spin Ising interactions. Symmetries of the dual model are investigated, and high-order perturbation theory is performed. The general goal is to understand the influence of geometry on the physical properties of topological codes.
[1] M. Vieweg, K.P. Schmidt, Phys. Rev. Res., 7 (2025)

TT 23.7 Mon 18:00 P1

Stochastic series expansion quantum Monte Carlo for quantum lattice models beyond spin 1/2 — •Melanie A. R. Wolf, Anja Langheld, Calvin Krämer, Jan Alexander Koziol, and Kai Phillip Schmidt — Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtdtr. 7, 91058 Erlangen, Germany
Stochastic series expansion quantum Monte Carlo is a well established method for the quantitative investigation of quantum spin models with spin 1/2. Especially, the sampling of quantum Ising models with arbitrary interactions [1] without a sign problem, constitutes an important milestone in the development of the method. Therefore, it follows naturally to ask how to transfer this efficient sampling scheme to quantum systems with a larger local Hilbert space like spin-one or quantum Potts models. In our work we implement the stochastic series expansion quantum Monte Carlo scheme [2] and explore the quantum and thermal properties of quantum Potts models.
[1] A. Sandvik, Phys. Rev. E 68, 056701
[2] C. Ding et al., arXiv:1702.02675

TT 23.8 Mon 18:00 P1

Convergence behavior of non-perturbative linked-cluster expansions at criticality — •Harald Leiser, Max Hörmann, and Kai Phillip Schmidt — Chair for Theoretical Physics V, FAU Erlangen-Nürnberg, Germany
Non-perturbative linked-cluster expansions (NLCE) provide a systematic framework for computing properties of quantum lattice models directly in the thermodynamic limit. For applying it to excited states, we use a transformation T that block-diagonalizes cluster Hamiltonians, like the Schrieffer-Wolff transformation, while satisfying cluster-additivity. In perturbative linked-cluster expansions up to order N, certain classes of transformations all yield identical and exact results at order N. However, in non-perturbative LCE this equivalence breaks down entirely, as the hierarchical structure of contributions is absent. As a result, the non-perturbative effects introduced by different transformations can produce different convergence behavior, also depending on the observable under study. Our goal is to understand how different choices of T influence the convergence behavior and what these differences reveal about the transformations themselves. Furthermore, we aim to understand the role of the transformation T in extracting quantum-critical behavior from NLCEs. For that, we analyze the energy gap of the transverse-field Ising chain at its quantum critical point, since its exact solution reduces the computational complexity to polynomial, enabling comparison up to large system sizes.

TT 23.9 Mon 18:00 P1

Optimized Crystal Synthesis and Anistropic Magnetism of the 2D Layered Magnets $M\mathbf{PSe_3}$ (M = Fe, Ni, Mn) — •Masoumeh Rahimkhani[1], Saicharan Aswartham[2], Martin Kostka[1], Ashwini Balodhi[1], Andreas Kreyssig[1], and Anna E. Böhmer[1] — [1]Experimental Physics IV, Ruhr-University Bochum, Bochum, Germany — [2]International Centre for Interfacing Magnetism and Superconductivity with Topological Matter, Institute of Physics, Polish Academy of Sciences, Warszawa, Poland
Transition-metal phosphochalcogenides $M\mathrm{PSe_3}$ (M = Fe, Ni, Mn) are important layered van der Waals materials with rich magnetic and electronic behavior. Among them, $\mathrm{FePSe_3}$ is a much investigated layered antiferromagnet with strong potential for applications in two-dimensional spintronics and quantum devices.

Here, we use an additive-free chemical vapor transport technique for growth of single crystals of $\mathrm{FePSe_3}$. Single crystals reach up to 3 mm in length and show nearly ideal atomic ratio composition in energy-dispersive x-ray spectroscopy. Magnetic measurements reveal an antiferromagnetic transition around 120 K. We studied the effect of substitution at the Fe site on the anistropic magnetism. We will discuss how substituted $\mathrm{Fe_{1-x}}M_x\mathrm{PSe_3}$ single crystals can be prepared and how substitution at the Fe site affects the anisotropic magnetism.

TT 23.10 Mon 18:00 P1

Electronic and Magnetic Properties of $\mathbf{CaMn_2P_2}$ and $\mathbf{SrMn_2P_2}$ Single Crystals — •Jule Kirschke, Joscha Grunwald, T. R. Thomas, N. S. Sangeetha, Ashiwini Balodhi, Andreas Kreyssig, and Anna E. Böhmer — Experimental Physics IV, Ruhr-University Bochum, Bochum, Germany
$\mathrm{CaMn_2P_2}$ and $\mathrm{SrMn_2P_2}$ are insulators that adopt the trigonal $\mathrm{CaAl_2Si_2}$-type structure containing corrugated Mn honeycomb layers. Here, we report a systematic study of single crystals grown from Sn flux, including attempts to synthesize $\mathrm{Sr_{1-x}K_xMn_2P_2}$, which revealed that K does not substitute in the $\mathrm{SrMn_2P_2}$ structure. In contrast, $\mathrm{CaMn_2P_2}$ exhibits an unexpected sensitivity to the Ca content used during growth. While powder x-ray diffraction confirms identical crystal structures for all batches, their transport properties differ drastically. Samples prepared with high Ca content during the growth anomalously show almost metallic temperature dependence of the resistivity, whereas others show the insulating behavior commonly reported in the literature. The electronic and magnetic properties of different samples were studied by heat capacity and magnetization measurements.
We acknowledge support by the Deutsche Forschungsgemeinschaft (DFG) under CRC/TRR 288.

TT 23.11 Mon 18:00 P1

Quantum effects in the magnon spectrum of 2D altermagnets on a square lattice and anisotropic honeycomb lattice via continuous similarity transformations. — •Dag-Björn Hering[1], Vanessa Sulaiman[1], Raymond Wiedmann[3], Matthias R. Walther[2], Götz S. Uhrig[1], and Kai P. Schmidt[2] — [1]Condensed Matter Theory, Technische Universität Dortmund, Otto-Hahn-Straße 4, 44221 Dortmund, Germany — [2]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany — [3]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569, Stuttgart, Germany
We investigate quantum effects on magnon excitations in a minimal spin-1/2 Heisenberg model for 2D altermagnets on the square lattice and for an anisotropic honeycomb lattice. For both, a continuous similarity transformation is applied in momentum space to derive an effective Hamiltonian that conserves the number of magnon excitations. This allows us to quantitatively calculate the one-magnon dispersion, the effects of magnon-magnon interactions, and the dynamic structure factor in a certain range of parameters. For the altermagnet, we focus on the altermagnetic spin splitting of the magnon bands and the size of the roton minimum. For the honeycomb, we additionally analyze the ground state energy and the staggered magnetization. We further analyze the stability of the assumed long-range order and the magnons by different generators.

TT 23.12 Mon 18:00 P1

Spectral densities for inelastic scattering in anisotropic Heisenberg models on mono- and bilayer square lattices and the honeycomb lattice via continuous similarity transformations — •Vanessa Sulaiman[1], Dag-Björn Hering[1], Matthias R. Walther[2], Kai P. Schmidt[2], and Götz S. Uhrig[1] — [1]Condensed Matter Theory, Technische Universität Dortmund, Otto-Hahn-Straße 4, 44221 Dortmund, Germany — [2]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany
We apply a continuous similarity transformation (CST) [1] with a magnon-conserving generator to the antiferromagnetic anisotropic XXZ model. For the square lattice, the resulting effective Hamiltonian has already been analyzed [2]. We extend the approach by applying the CST to observables as well. Using the continuous fraction representation, we calculate spectral densities for these observables on the square and honeycomb lattice, as well as the bilayer square lattice. These are compared to experimental data from RIXS measurements [3], for example with single-layered $\mathrm{Ca_2CuO_2Cl_2}$ and bilayer $\mathrm{Sr_3Ir_2O_7}$.
[1] M. Powalski et al., Phys. Rev. Lett. **115**, 207202 (2015) and SciPost Phys. **4**, 001 (2018)
[2] M. R. Walther et al., Phys. Rev. Research **5**, 013132 (2023)
[3] K.-J. Zhou et al., J. Synchrotron Rad. **29**, 563 (2022)

TT 23.13 Mon 18:00 P1

Hall Response, Angular Magnetoresistance, and Field-Induced Metamagnetism in $\mathbf{Sr_4Ru_3O_{10}}$ — •Ilke Masa[1], Simone Seipel[1], Lara Pätzold[1], Zahra Ghazinezhad[1], Agustinus Agung Nugroho[2], Markus Braden[1], and Thomas Lorenz[1] — [1]Institute of Physics II; University of Cologne, Germany — [2]Bandung Institute of Technology, Indonesia
$\mathrm{Sr_4Ru_3O_{10}}$ is a ferromagnetic metal with $T_C \approx 105$ K and exhibits an additional metamagnetic transition below 50 K, whose microscopic origin remains unclear. We investigate single crystals to characterize the anisotropy of magnetization and electrical transport. For in-plane currents, we measure both the normal and anomalous Hall effects, finding a non-monotonic temperature dependence and a low-temperature sign reversal of the anomalous Hall signal, similar to behavior known from $\mathrm{SrRuO_3}$ and associated with Weyl points in its band structure. Due to the layered crystal structure, the out-of-plane resistivity is highly anisotropic ($\rho_c \gg \rho_{ab}$) and shows pronounced changes across the metamagnetic transition. From magnetoresistance data, we extract the field-induced metamagnetic transition at low temperatures and analyse the angular dependence of both the transition fields and the in-plane magnetoresistance. We also identify a clear angular magnetoresistance response in $\mathrm{Sr_4Ru_3O_{10}}$. Possible low-temperature phases remain subjects of ongoing research.
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TT 23.14 Mon 18:00 P1

Heat Transport and Thermodynamic Properties of the Quasi-Two-Dimensional Quantum Magnet $Cu_2(OH)_3Br$ — •Nainish Tickoo[1], Rohit Sharma[1], Lucas Berger[1], Zhiying Zhao[2], Zhe Wang[3], and Thomas Lorenz[1] — [1]Institute of Physics II, University of Cologne, D-50937 Cologne, Germany — [2]State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, China — [3]Department of Physics, TU Dortmund University, D-44227 Dortmund, Germany

$Cu_2(OH)_3Br$ is a quasi-two-dimensional quantum magnet that can be seen as a system of coupled antiferromagnetic spin-1/2 chains. Specific heat, magnetisation and magnetostriction measurements have shown pronounced anomalies at T_N = 9.3 K. These measurements, along with Monte Carlo simulations, have shown that below the T_N, the system undergoes a field-induced transition from a 3D ordered state to a partially decoupled state when a magnetic field (B_c = 16.3 T) is applied transverse to the ordered spins. This transition is interpreted as a dimensional reduction arising from the distinct responses of the AFM chains to an external magnetic field [1]. This study examines the thermal conductivity κ (T, B) of $Cu_2(OH)_3Br$ single crystals under magnetic fields applied along the crystallographic b axis. Strong anomalies in κ near T_N reveal a significant interplay between phonons and magnetic excitations in low-temperature heat transport

Funded by the DFG via CRC 1238 Projects A01, B01 and B04.

[1] A. Reinoldet al., Phys. Rev. B 111, L100405 (2025)

TT 23.15 Mon 18:00 P1

Magnetic and Electronic Transport Behavior in Cr-Based Quantum Materials — •Shitao Qu, Ran Tao, Mengmeng Long, Mads Fonager Hansen, and F. Malte Grosche — Cavendish Laboratory, University of Cambridge, Cambridge, United Kingdom

Unconventional superconductivity among transition metal compounds is seen in Cu-, Fe- and most recently Ni-based materials. What about other transition metal systems? There are a surprising number of **chromium**-based superconductors, often in conjunction with applied pressure: CrAs, $A_2Cr_3As_3$ (with A an alkaline metal), ACr_3As_3, and $CsCr_3Sb_5$. Moreover, CrSb is one of the best-studied metallic altermagnets. These findings motivate a wider study of Cr-based correlated electron materials.

We initially investigate (i) CrP – an isostructural and isoelectronic relative to CrAs, (ii) CrSe – an altermagnet candidate, and (iii) the Kagome lattice systems $CsCr_3Sb_5$ and $CsCr_6Sb_6$.

Single crystals are prepared via flux and vapour-transport techniques and characterised in standard X-ray, magnetometry and transport measurements. They enable studies of the electronic structure and magnetic/superconducting phase diagram, forming a promising basis for exploring correlated-electron behavior in Cr-based quantum systems more widely.

TT 23.16 Mon 18:00 P1

Correlated Electronic Structure of Layered Cathode Material LiMnO2 — •Owen Colire, Francesco Cassol, and Silke Biermann — Centre de Physique Théorique (CPHT), Ecole Polytechnique, Institut Polytechnique de Paris, CNRS, Palaiseau, France

Electronic Coulomb correlations are ubiquitous in transition metal compounds. Our work focuses on layered LiMnO2, a cathode material used in Li-ion batteries, which crystallizes in a monoclinic structure with alternating Lithium and MnO6 layers. The compound is a Mott insulator with a high-spin d4 configuration undergoing a transition to an antiferromagnetically ordered state below the Néel temperature of 250 K. We investigate the electronic structure using Density Functional Theory calculations and combined Density Functional - Dynamical Mean Field Theory, with an emphasis on the interplay of the intra-atomic Hund's exchange coupling and crystal field splittings.

TT 23.17 Mon 18:00 P1

Non-equilibrium Charge Dynamics at the metal-insulator transition in κ-$(BETS)_2Mn[N(CN)_2]_3$ — •Sangeeta Panwar[1], Tim Thyzel[1], Jens Müller[1], Mark Kartsovnik[2], and Natalia Kushch[3] — [1]Institute of Physics, Goethe-Universität Frankfurt, Frankfurt (Main), Germany — [2]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften,Garching, Germany — [3]private

Low-dimensional molecular conductors have been shown to host electronic ferroelectricity, where electronic degrees of freedom cause polar order, allowing for fast switching and phase control [1]. Using fluctuation spectroscopy, we recently investigated the nature of electronic ferroelectricity in the organic conductor κ-$(BETS)_2Mn[N(CN)_2]_3$ [2], representative of a broader class of quasi two-dimensional correlated electron systems. Here, we explore how these phenomena evolve when tuning the bandwidth by applying hydrostatic pressure. We will investigate the slow dynamics of polar nanoregions (PNR) and the evolution of drastic changes in the dynamics as the system is tuned from the insulating to the superconducting phase. By employing fluctuation spectroscopy under pressure, we aim to study how superconductivity emerges from the ferroelectric/multiferroic insulating state and to examine how PNR formation and glassy dipolar freezing evolve [3].

[1] Lang et al., J. Electronic Materials 54, 5087 (2025)
[2] Thomas et al., npj Spintronics 2, 24 (2024)
[3] Zverev et al. PRB 82, 155123 (2010)

TT 23.18 Mon 18:00 P1

Ru L-edge RIXS on the dimer compound $Ba_3CeRu_2O_9$: a cluster Mott insulator? — •Lara Pätzold[1], Frederik Paech[1], Enrico Bergamasco[1], Henrik Schilling[2], Anna Sandberg[3], Hlynur Gretarsson[4], Petra Becker-Bohatý[2], Maria Hermanns[3], and Markus Grüninger[1] — [1]II. Physikalisches Institut, University of Cologne, Germany — [2]Kristallographie, University of Cologne, Germany — [3]KOMKO, University of Stockholm, Sweden — [4]DESY, Hamburg, Germany

Cluster Mott insulators host charge carriers in quasi-molecular orbitals on, e.g., dimers or tetramers [1-2]. With strong spin-orbit coupling, this may yield unconventional quasi-molecular magnetic moments tunable via, e.g., intracluster hopping. Cluster Mott insulators emerge in 5d transition-metal compounds due to large hopping, whereas in 3d materials one expects conventional Mott behavior with carriers localized on individual sites. To clarify whether cluster Mott insulators are realized in 4d compounds, we address the electronic structure of $Ba_3CeRu_2O_9$ that hosts Ru_2O_9 dimers with 4 t_{2g} holes. Ru L-edge RIXS and exact diagonalization reveal a rich excitation spectrum on top of an intricate nonmagnetic ground state in the intermediate regime. Compared to 5d cluster Mott insulators, $Ba_3CeRu_2O_9$ shows reduced intracluster hopping, smaller spin-orbit coupling, and larger electronic correlations, realizing an intriguing part of phase space.

[1] Revelli *et al.*, Sci. Adv. **5**, eaav4020 (2019).
[2] Magnaterra *et al.*, PRL **133**, 046501 (2024).

TT 23.19 Mon 18:00 P1

Sample-Based Quantum Diagonalization of Similarity-Transformed Hamiltonians for Strongly Correlated Systems — •Emanuele Ricci[1,2] and Werner Dobrautz[1,2,3,4] — [1]Technical University Dresden, 01069 Dresden, Germany — [2]Center for Scalable Data Analytics and Artificial Intelligence Dresden/Leipzig, 01069 Dresden, Germany — [3]Center for Advanced Systems Understanding, 02826 Görlitz, Germany — [4]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

One of the central challenges in electronic structure theory is the accurate description of strongly correlated systems. We address this using a hybrid quantum-classical scheme, sample-based quantum diagonalization, in which a quantum computer acts as a dedicated sampler to identify a compact, problem-adapted subspace of important Slater determinants. The corresponding reduced Hamiltonian is then diagonalized classically to obtain the ground state. To mitigate quantum errors, we apply a classical post-processing step that projects samples onto the correct particle-number sector.

Before sampling, we perform a similarity transformation of the Hamiltonian that concentrates the ground-state weight into a smaller set of determinants, reducing the relevant subspace and improving accuracy at the cost of a non-Hermitian effective Hamiltonian. While non-Hermiticity would ordinarily hinder quantum algorithms, we demonstrate that it can still be exploited within a sampling-based framework using the UCJ (unitary cluster Jastrow) ansatz initialized with single and double amplitudes from the transformed Hamiltonian.

TT 23.20 Mon 18:00 P1

A Local-Wave Basis for the Hubbard Model — •Leon Wastl[1,2] and Werner Dobrautz[1,2,3,4] — [1]Center for Advanced Systems Understanding, 02826 Görlitz, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [3]Center for Scalable Data Analytics and Artificial Intelligence Dresden/Leipzig, 01069 Dresden, Germany — [4]Technical University Dresden, 01069 Dresden, Germany

The Fermi-Hubbard model is the prototypical model for interacting electrons and can be employed to describe a wide variety of physical phenomena. Its 2D version is believed to contain the fundamental physics describing low-temperature superconductivity. We present a new basis for the two-dimensional Hubbard model which we call the local-wave basis as it is a hybrid between real space and momentum space. We numerically study the advantages of our newly found transformation using the density matrix renormalization group (DMRG). Since DMRG in its more recent form is a method that is inherently one-dimensional as it is built on top of the matrix product state (MPS) formalism, we combine our local-wave basis with a new way of ordering the sites in the MPS based on a modified version of simulated annealing (SA) using the two-site mutual information as its objective function. Combined with this approach to find the optimal ordering, we show that our method yields lower energies for the same maximal bond dimension than both the pure momentum space and the real space formulation in the low to intermediate U/t regime.

TT 23.21 Mon 18:00 P1

Calculating Moments for Many-Electrons Systems — •Elaheh Adibi and Erik Koch — Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany

We describe an approach for computing the M^{th} moment of an N-electron system, defined as $\langle E^M \rangle = \mathrm{Tr}\, H^M$. Since the Hamiltonian H consists of pairs of creation-annihilation operators and the calculation is performed in the basis of Slater determinants $\{|\mathrm{I}\rangle\}$, the matrix element $\langle \mathrm{I}|H^M|\mathrm{I}\rangle$ contributes to the moment only when the orbital indices of the creation operators form a permutation of those of the annihilation operators. Writing the permutations in cycle notation, the simplest contributions arise from permutations creating a single cycle in which all orbitals are different. These permutations are classified by their number of descents. Permutations with the same number of descents contribute equally to $\sum_{\mathrm{I}} \langle \mathrm{I}|H^M|\mathrm{I}\rangle$. Since the number of permutations with the same number of descents is given by the Eulerian numbers, it suffices to compute the trace for one permutation and multiply the result by this number. In this way the trace can be evaluated combinatorially, without explicitly constructing the many-body Hilbert space. We are able to calculate the all other permutations with respect to these permutations. Finally, we present a recursive formula for the moment that is computationally efficient.

TT 23.22 Mon 18:00 P1

Polynomial Neural Networks in Quantum Many-Body Physics — •Ashish Yashwanth Kangen[1,2] and Werner Dobrautz[1,2,3,4] — [1]Technical University Dresden, 01069 Dresden, Germany — [2]Center for Scalable Data Analytics and Artificial Intelligence Dresden/Leipzig, 01069 Dresden, Germany — [3]Center for Advanced Systems Understanding, 02826 Görlitz, Germany — [4]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Polynomial neural networks were originally derived by applying tensor decompositions to high-order weight tensors. This derivation yields a model architecture that is inherently non-linear through Hadamard products, effectively eliminating the need for standard, tensor-unfriendly activation functions like ReLU.

In this work, we investigate the utility of this architecture within the context of quantum many-body physics and chemistry. We demonstrate that the algebraic properties of these polynomial expansions allow them to serve as robust, activation-free representations of complex quantum correlations. We explore two specific applications: (1) as a standalone wave function ansatz, which can be optimised via both deterministic Density Matrix Renormalization Group sweeps and Variational Monte Carlo, and (2) as a Jastrow correlation factor within the Transcorrelated approach for Quantum Chemistry, trainable via standard gradient-based machine learning optimisation. This framework suggests that the tensor structure underlying polynomial networks offers a flexible and numerically stable bridge between classical deep learning and quantum simulation.

TT 23.23 Mon 18:00 P1

Quantics tensor trains: Quantifying entanglement across length scales — Stefan Rohshap[1], Jheng-Wei Roshap[2], •Alena Lorenz[3], Serap Hasil[1], Karsten Held[1], Anna Kauch[1], and Markus Wallerberger[1] — [1]TU Wien — [2]Univ. Grenoble Alpes — [3]JMU Würzburg

Understanding entanglement remains one of the most intriguing problems in physics. In contrast to particle and site entanglement, length or energy scale entanglement, quantifying the information exchange between different length scales, has received far less attention. Here, we identify the quantics tensor train (QTT) technique, a matrix product state-inspired approach for overcoming computational bottlenecks in resource-intensive numerical calculations, as a renormalization group method by analytically expressing an exact cyclic reduction-based real-space renormalization scheme in QTT language. We precisely match the QTT bond dimension, a measure of length scale entanglement, to the number of rescaled couplings generated in each coarse-graining renormalization step and present our results for the one-dimensional tight-binding model with n-th-nearest-neighbor hopping. Furthermore, though analytically unfeasible, we numerically generate the bond-dimension of the two- and three-dimensional case of the interacting and non-interacting Green's function in momentum space and find, that for the interacting as well as for the one-dimensional non-interacting Green's function, the bond dimension saturates when lowering the temperature.

TT 23.24 Mon 18:00 P1

DMFT-Lanczos study of Alkali-Doped Fullerides: Superconductivity across the (U,J) plane — •Lara Bremer, Lorenzo Crippa, Igor Krivenko, and Tim O. Wehling — I. Institute of Theoretical Physics, University of Hamburg, Notkestraße 9-11, 22607 Hamburg

Alkali-doped fullerides (A_3C_{60}) provide a versatile platform for studying unconventional s-wave superconductivity in a strongly correlated setting, where superconducting phases emerge in close proximity to Mott insulating states. These molecular superconductors exhibit critical temperatures up to about 40 K. Theoretical descriptions of alkali-doped fullerides commonly employ a three-orbital Hubbard-Kanamori model whose defining feature is an effective negative Hund's coupling arising from the coupling of the electronic states to intramolecular Jahn-Teller phonon modes, thereby reversing the usual Hund's rules.

In this contribution we present calculations performed with the multi-orbital Lanczos impurity solver of the EDIpack library within a dynamical mean-field theory framework. We explore the (U, J) interaction space, focusing on the evolution from the regime of weak negative Hund's coupling to regimes with strongly negative Hund's coupling. We analyze how the interplay between the Mott insulating phase present for large Hubbard interaction U and the charge-disproportionated insulating phase present for large negative values of J influences the character of the superconducting states and ehances critical temperatures.

TT 23.25 Mon 18:00 P1

Investigating Non-Hermitian Dynamics in Neural Quantum States — •Mohammed Boky[1,2] and Werner Dobrautz[1,2,3,4] — [1]Center for Scalable Data Analytics and Artificial Intelligence Dresden/Leipzig, 01069 Dresden, Germany — [2]Technical University Dresden, 01069 Dresden, Germany — [3]Center for Advanced Systems Understanding, 02826 Görlitz, Germany — [4]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Both the Neural Quantum States (NQS) and the Transcorrelated (TC) method have proven to be impactful approaches in Ab Initio quantum chemistry and quantum many-body settings. The potential of combining these methods remains largely unexplored. In this work, the application and impact of the combination of these methods are explored with a focus on the computational cost.

The application of the similarity transform in the TC method yields non-Hermitian Hamiltonians. The optimization and impact of this non-Hermiticity on NQS dynamics pose both a great challenge and a source of unexplored possibilities to navigate physics with correlations that differ in magnitude.

In order to investigate both the impact and challenges of these methods, a study is done on a variety of different systems. These systems range from Ab Initio quantum chemistry problems such as hydrogen chains, to lattice models such as the non-Hermitian Transverse Field Ising and the Hubbard model.

TT 23.26 Mon 18:00 P1

Non-equilibrium DMFT solved with the help of Tensor Cross Interpolation — •Bastian Schindler[1], Eva Paprotzki[1,2], and Martin Eckstein[1,2] — [1]I. Institute for Theoretical Physics, University of Hamburg, Notkestraße 9-11, 22607 Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany

The non-perturbative solution of the quantum impurity problem provides the biggest computational challenge when DMFT is applied in non-equilibrium. Most applications of non-equilibrium DMFT are based on simplified perturbative solutions [1]. In diagrammatic approaches to the impurity model, the numerical integration of high-dimensional expressions poses the main computational bottleneck, limiting feasible expansion orders and the number of accessible time steps. Tensor Cross Interpolation (TCI) has recently emerged as a powerful technique to mitigate the exponential scaling of computational cost with dimensionality [2]. In this work, we apply TCI to diagrammatic expressions obtained from a pseudo-particle expansion of the hybridization around the atomic limit in the non-equilibrium steady state. We demonstrate that, with an appropriate parametrization and an FFT-based integration scheme [3], TCI yields a significant speed-up for higher-order contributions. Moreover, we employ TCI to efficiently evaluate the multidimensional integrals required for higher-order spectroscopy, in particular time-resolved resonant inelastic x-ray scattering.

[1] Murakami et al., Rev. Mod. Phys. 97.3 (2025)
[2] Núñez Fernández, et al., SciPost Physics 18.3 (2025)
[3] Eckstein, arXiv:2410.19707 (2024)

TT 23.27 Mon 18:00 P1

Stochastic semiclassical electron-lattice dynamics with DMFT — •Tom Kahana, Francesco Valiera, and Martin Eckstein — I. Institute of Theoretical Physics, University of Hamburg, Hamburg, Germany

The interplay between lattice motion and strongly correlated electronic phases poses a major challenge in nonequilibrium condensed-matter systems, especially near phase transitions where ionic distortions strongly affect the electronic state. We address this problem by solving the coupled electron-lattice dynamics using a quasi-equilibrium (adiabatic) Dynamical Mean-Field Theory on an inhomogeneous lattice defined by the instantaneous phonon configuration. Conservative forces, friction, and stochastic contributions to the lattice dynamics are obtained from the electronic correlation functions. Because each lattice site must be treated as an impurity embedded in a self-consistent bath, this approach is computationally demanding. To make it feasible, we replace the DMFT impurity solver with a trained neural-network emulator that reproduces high-order impurity solutions. This NN-accelerated DMFT loop enables computationally efficient simulations of the coupled electron-lattice dynamics on inhomogeneous lattices. We present benchmarks for the Hubbard-Holstein model. The method provides a path toward simulations of photo-induced transitions in correlated materials, such as Mott and charge-ordered states.

TT 23.28 Mon 18:00 P1

Superradiance in Higher-Order Correlated Collective Emission — •Daniil Platonov[1,2], Xin H. H. Zhang[1,2,3], and Peter Rabl[1,2,3] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany

We investigate supercorrelated decay of an initially inverted ensemble of two-level emitters, where cooperative emission is governed by higher powers of the collective decay operator beyond conventional Dicke superradiance. We develop a qualitative theoretical framework that captures the essential mechanism of generalized supercorrelated decay and predicts the corresponding scaling laws. This framework clarifies the physical distinctions between conventional superradiance and higher-order supercorrelated emission. We further analyze the phenomenon in a waveguide quantum electrodynamics setting, where guided modes mediate strong collective interactions. By deriving an effective semiclassical theory, we obtain a computationally efficient description that enables large-scale simulations of the dynamics.

TT 23.29 Mon 18:00 P1

Hierarchy of timescales in a disordered spin-1/2 XX ladder — •Kadir Çeven, Lukas Peinemann, and Fabian Heidrich-Meisner — Institut für Theoretische Physik, Georg-August-Universität Göttingen, Göttingen, Germany

Understanding the timescales associated with relaxation to equilibrium in closed quantum many-body systems is one of the central focuses in the study of their non-equilibrium dynamics. At late times, these relaxation processes exhibit universal behavior, emerging from the inherent randomness of chaotic Hamiltonians. In our work [1], we investigate a disordered spin-1/2 XX ladder – an experimentally realizable model known for its diffusive dynamics – to explore the connection between transport properties and spectral measures derived solely from the system's energy levels via these relaxation timescales. We begin by analyzing the spectral form factor, which yields the time when the system begins to follow the random matrix theory (RMT) statistics, known as the RMT time. We then determine the Thouless times – the average times for a local excitation to diffuse across the entire finite system – through the linear-response theory for both spin and energy transport. Our numerical results confirm that the RMT time scales quadratically with system size and upper bounds the Thouless times. Interestingly, we also find that, unlike other non-integrable models, spin diffusion proceeds faster than energy diffusion.

Supported by the DFG via FOR 5522.

[1] K.Çeven,L.Peinemann,F.Heidrich-Meisner,arXiv:2509.20078(2025).

TT 23.30 Mon 18:00 P1

Charge carrier relaxation dynamics in the one-dimensional Kondo lattice model — •Arturo Perez Romero, Mica Schwarm, and Fabian Heidrich-Meisner — Institut for Theoretical Physics, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany

A generic question in the field of ultrafast dynamics is concerned with the relaxation dynamics and the subsequent thermalization of optically excited charge carriers. Among several possible relaxation channels available in a solid-state system, we focus on the coupling to magnetic excitations. In this paper, we study the real-time dynamics of a paradigmatic model, the Kondo lattice model in one dimension. We conduct a comprehensive study of the relaxation processes by evaluating the spin polarization of the conduction electron, the local spin-spin correlation between localized and conduction electrons, and the electronic momentum distribution. While in the well-studied cases of one or two charge carriers in a ferromagnetic background, no thermalization occurs, we demonstrate that the stationary state is compatible with thermalization if either the electronic filling is finite or the magnetic background is in the singlet sector. Our real-time simulations using the time-dependent Lanczos method are corroborated by a direct comparison with finite-temperature expectation values and an analysis of the spectrum in terms of the gap ratio.

This work was funded by the Deutsche Forschungsgemeinschaft (DPG, German Research Foundation) via CRC 1073.

TT 23.31 Mon 18:00 P1

Collective dynamics in $SmNiC_2$ probed by time resolved spectroscopy — •Priyanka Yogi[1], Chandra V Kotyada[1], Bhageerath Swaraj[1], Amon. P Lanz[1], Amir.A Haghighirad[2], Sofia. M Souliou[2], Matthieu Le Tacon[2], and Jure Demsar[1] — [1]JGU Mainz — [2]KIT

Rare-earth transition-metal carbides $RNiC_2$ are a unique class of intermetallic compounds that crystallize in a non-centrosymmetric orthorhombic $CeNiC_2$-type structure. Except for $LaNiC_2$ and $CeNiC_2$, where exotic superconductivity has been reported, most members of this family exhibit quasi-1D charge-density-wave (CDW) order and competing magnetic order at low temperature. $SmNiC_2$ is unique, where an incommensurate CDW order appearing below $T_{CDW} \approx 148$ K gets fully suppressed below a first-order transition into a ferromagnetic (FM) phase at $T_M \approx 18$ K.

Here, we employ optical pump-probe spectroscopy to investigate the interplay between the FM and CDW phases by probing single-particle and collective dynamics as a function of temperature. The FM phase is characterized by rather slow (10 ps) demagnetization dynamics, while in the CDW phase, we observe characteristic CDW collective modes. The dominant amplitude mode is found at 1.45 THz, showing pronounced softening towards T_{CDW}. Excitation density-dependent studies provide additional information on the strength of the two phases.

TT 23.32 Mon 18:00 P1

High precision physics in Anderson impurity models, from neutrino mass to axion production in the sun. — •Vera Butz and Maurits W Haverkort — Universität Heidelberg, Institut für theoretische Physik, Philosophenweg 19, 69120 Heidelberg

High-precision comparisons between experimental measurements and numerical simulations not only test the accuracy of computational methods but also offer deeper insights into fundamental physics. In this work, we investigate how charged ions with multiple electrons interact with continuum states, such as photons, free electrons, or as-yet-unobserved particles. This is achieved by using a generalized Anderson impurity model, in which the interactions can be described via the self-energy or hybridization function. The real part of the self-energy induces energy shifts in atomic multiplets, such as the Lamb shift, while the imaginary part results in finite lifetimes for excited states, leading to phenomena like fluorescence or Auger-Meitner decay. Using this method of high-precision calculations of decay rates, on highly charged heavy ions in laboratory or astrophysical settings, allows us to probe the Standard Model. Be that by measuring unknowns, like the neutrino mass [1] or discovering new potential particles like dark matter candidates [2].

[1] Nat. Phys. 20, 921 (2024)
[2] JCAP 09 (2021) 006

TT 23.33 Mon 18:00 P1

Critical dynamics at isostructural instabilities — •Nick Sander — Karlsruhe Institute of Technology

At an elastic structural instability at least one of the elastic moduli vanishes. An acoustic phonon only softens at such an instability if it is accompanied with a change of crystal symmetry. At isostructural transitions with vanishing bulk modulus, however, no softening occurs and all microscopic phonon modes remain non-critical [1]. Nevertheless, we demonstrate that there exist four macroscopic critical elastic modes that will determine the critical dynamics at such an instability. These modes represent conformal symmetry transformations and the displacement vector satisfy a corresponding Killing equation, whose exact form depends on the crystal symmetry. We discuss implications for instabilities in correlated materials like the Mott metal-insulator transition, and realizations with mechanical metamaterials.

[1] R. A. Cowley, Phys. Rev. B 13, 4877 (1976)

TT 23.34 Mon 18:00 P1

Quantum geometry in the context of many-body perturbation theory — •Mario Geoffroy and Corentin Morice — Laboratoire de Physique des Solides, Université Paris-Saclay, CNRS, Orsay, France

Quantum geometry gives rise to some of the most topical physical phenomena in the past decades, but our current understanding of it remains based on single-particle topological band theory, and fails in the presence of electronic correlations [1]. This is particularly problematic given the overwhelming usage of density functional theory for the diagnosis of topological states in materials [2]. Many-body generalizations of the Chern number and other invariants have been put forward, but many-body quantum geometry remains elusive. We study the influence of electronic interactions on the Berry curvature in tractable systems, in view of developing formalisms adapted to accurate predictions in real materials.

[1] J. Vidal et al., PRB 84, 041109(R) (2011)
[2] B. Bradlyn et al., Nature 547, 298 (2017)

TT 23.35 Mon 18:00 P1

Higher-harmonic generation in the driven Mott-Hubbard model — •Abdelrahman Azab, Friedemann Queisser, and Ralf Scheutzhold — Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany

Motivated by recent experiments, we study the generation of higher harmonics in the Mott insulator state of the Fermi-Hubbard model under the influence of an oscillating external electromagnetic field, see also [1]. We find a strong dependence of the higher-harmonic intensity on the spin order (e.g., antiferromagnetic versus paramagnetic phase).

Funding by the DFG through the SFB 1242 is gratefully acknowledged.

[1] F. Queisser and R. Schützhold, Phys. Rev. B 109, 205110 (2024).

TT 24: Focus Session: Quantum Sensing with Solid State Spin defects I (joint session TT/MA)

The electron spins of defects in solid state materials show remarkable quantum coherence, making them excellent sensors. Recent advances in material engineering and measurement techniques lead to continuous improvements in the sensitivity and resolution of established single spin sensors such as the Nitrogen-Vacancy center in diamond, and the development of new defect sensors in materials such as Silicon Carbide and hexagonal Boron Nitride. In condensed matter physics, such sensors are often being used for exploring the structure of magnets, superconductors, topological phases, etc. This focus session will highlight most of the recent experimental and theoretical advances, current challenges, and emerging directions, focusing both on the improvements of the defects themselves, and their use for exploring novel phenomena in condensed matter physics.

Coordinators: Aparajita Singha (TU Dresden), Uri Vool (Max Planck Institute for Chemical Physics of Solids)

Time: Tuesday 9:30–12:45 Location: HSZ/0003

Topical Talk TT 24.1 Tue 9:30 HSZ/0003

Exploring nanoscale van der Waals magnetism using single spin microscopy — •Patrick Maletinsky — Basel University, Departement of Physics, Klingelbergstrasse 82, 4056 Basel

Atomically thin van der Waals (vdW) magnets provide a unique platform to explore magnetism in the ultimate two-dimensional limit [1]. Their weak interlayer coupling, tunable anisotropy, and gate sensitivity enable engineering of magnetic order and spin textures at the atomic scale. However, their small magnetic moments, nanoscale domains, and complex coupling make them difficult to probe experimentally [2].

I will present recent progress in understanding vdW magnetism using single-spin magnetometry based on nitrogen-vacancy centers in diamond. This quantum-sensing technique enables nanoscale imaging of magnetic order, phase transitions in few-layer systems under ambient and cryogenic conditions. I will show how this approach reveals microscopic mechanisms of magnetism in layered materials and uncovers phenomena such as "lateral exchange bias" and spin-reorientation transitions in ultrathin magnets [3,4].

I will conclude with an outlook on how quantum sensors can advance the study of correlated and topological magnetism in vdW materials [5], and how combining them with strain, gating, or optical control may enable designer spintronic and magnonic systems.

[1] Science 363, 706; Nat. Nanotechnol. 14, 408 [2] Science 364, 973 [3] Nat. Commun. 15, 6005 [4] Nat. Commun. 16, 9725 [5] Nat. Rev. Phys. 6, 753

Topical Talk TT 24.2 Tue 10:00 HSZ/0003

Optically addressable spin defects in two-dimensional materials — •Vladimir Dyakonov — Julius-Maximilians-Universität Würzburg, 97074 Würzburg, Germany

Two-dimensional (2D) materials have emerged as the new playground for quantum photonics devices. Among them, hexagonal boron nitride (hBN) is an interesting candidate, mainly because of its crystallographic compatibility with different 2D materials, but also because of its ability to harbour optically active defects generating single photons. The negatively charged boron vacancy was the first intrinsic, optically addressable spin defect in hBN that allows coherent control at room temperature, as reported in 2020. [1] Although other types of spin centers have been found in this material since then, this spin-1 color center remains the only one with a clearly elucidated structure. Practical applications of hBN spin centres as intrinsic magnetic field, temperature, etc. sensors in van der Waals heterostructures are hence envisioned. To further boost the quantum sensing applications of this spin defect in hBN, we investigated the dynamics of the intermediate state, because it is likely to trap electrons for a certain time, which affects the subsequent sensing protocol when the pulsed magnetic resonance experiment is designed.[2] Finally, we found that spin defects exhibit a direct correlation between Raman features and PL intensity, which allowed us to develop an all-optical method for determining the absolute spin defect density in flakes. [3]

[1] A. Gottscholl et al., Nat. Mater. 19, 540 (2020)
[2] P. Konrad et al., arXiv:2503.22815 [quant-ph] (2025)
[3] A. Patra et al., Adv. Funct. Mater. e17851 (2025).

Topical Talk TT 24.3 Tue 10:30 HSZ/0003

Nitrogen vacancy centers in diamond as novel sensing and imaging tool for magnetic nanostructures, in life science and chemistry — Sebastian Westrich[1], Nikhita Khera[1], Emma Resmann[1], Ephraim Spindler[1], Kristin Kühl[1], Alena Erlenbach[1], Mathias Weiler[1], Georg von Freymann[1], Artur Widera[1], Maria Wächtler[2], Stefanie Müller-Schüssele[3], and •Elke Neu-Ruffing[1] — [1]Department of Physics and Research Center Optimas, RPTU Kaiserslautern Landau, Erwin-Schrödinger-Straße 56 67663 Kaiserslautern — [2]Institut für Physikalische Chemie, Christian-Albrechts-Universität zu Kiel — [3]Department of Biology, RPTU Kaiserslautern Landau

Nitrogen vacancy centers (NV centers) locally probe magnetic fields, electric fields and temperature. Advantages of NV sensors include their sensitivity for fluctuating magnetic fields, which can be harnessed e.g. to detect free radicals. Additionally, near field based energy transfer serves as sensing resource to detect optically-active dipoles in close proximity. The talk will summarize our work on using scanning NV-based magnetometry to characterize magnetic nanostructures, including calibrating the scanning NV's position with respect to the sample. We highlight work on imaging frustrated magnetic systems (spin ice) as well as magnetic structures obtained via Direct Laser Writing. As another route towards broadening the field of applicability, we demonstrate for the first time near field energy transfer between NV centers and a naturally occuring fluorophore, namely chlorophyll. We furthermore explore routes to employ NV centers as sensor in photocatalysis.

15 min. break

Topical Talk TT 24.4 Tue 11:15 HSZ/0003

Electron spin, nuclear spin, and optical properties of transition-metal defects in silicon carbide with perspectives for quantum technologies — •Guido Burkard — Department of Physics and IQST, University of Konstanz, 78457 Konstanz, Germany

Transition-metal (TM) defects in silicon carbide (SiC) have emerged as a promising solid-state platform for quantum technologies, particularly because certain species, such as vanadium, provide optical emission in the telecom band and thus enable efficient spin-photon interfaces and quantum memories. In parallel, high-spin nuclei in solids are attracting growing interest for quantum information processing due to their long coherence times and intrinsically large Hilbert spaces, which support advanced protocols in quantum communication, measurement-based quantum computing, and quantum sensing, as well as explorations of fundamental quantum phenomena. A scalable route toward quantum networking relies on modular devices that combine an optically addressable electronic spin with one or more nuclear-spin qudits. We present a theoretical framework for TM defects in SiC. We model the spin and optical structure of a single active 3d electron, revealing how crystal fields and spin-orbit coupling modify selection rules, the g-tensor, and Rabi dynamics. We derive the effective hyperfine interaction within the spin-orbit-induced Kramers doublets and analyze nuclear-electron state transfer. Building on these insights, we propose a driven, dissipative protocol for robust nuclear-spin polarization and investigate how strain engineering can tailor electronic levels, optical Λ systems, and spin initialization pathways.

Topical Talk TT 24.5 Tue 11:45 HSZ/0003

Statics and dynamics of complex magnetic states in microstructures — •Aurore Finco — Laboratoire Charles Coulomb, CNRS and University of Montpellier, Montpellier, France

Scanning NV center microscopy is a versatile technique allowing both the mapping of static magnetic textures [1] and of microwave fields, which can be generated for example by spin waves. Here I will focus on the investigation of microstructures.

I will first show how we can use magnetoelectric coupling in the antiferromagnetic multiferroic bismuth ferrite to pattern a thin film using electric field and create whirling textures of both electric polarization and magnetization [2].

In a second part, I will discuss ferromagnetic microstructures, in the room-temperature van der Waals magnet Fe_5GeTe_2, demonstrating the stabilization of vortices [3], and in permalloy, which hosts either a S state or a vortex. In this material and when choosing the appropriate dimensions for the microstructures, spin wave modes with frequencies in the vicinity of 2.87 GHz are present and can therefore be probed and imaged. Through the handedness of the stray field that these spin wave mode produce, we can even discriminate between several modes with similar frequencies.

[1] Finco and Jacques, APL Materials 11, 100901 (2023)
[2] Chaudron et al, Nature Materials 23, 905 (2024)
[3] Sfeir et al, Physical Review Materials 9, 114003 (2025)

TT 24.6 Tue 12:15 HSZ/0003

Probing Vortex Dynamics in 2D Superconductors with Scanning Quantum Microscope — •Malik Lenger[1], Sreehari Jayaram[1], Lucas Pupim[2], Ruoming Peng[1], Mathias Scheurer[2], Jurgen Smet[3], and Jörg Wrachtrup[1,3] — [1]3rd Institute of Physics, University Stuttgart, Stuttgart, Germany — [2]Institute for Theoretical Physics III, University Stuttgart, Stuttgart, Germany — [3]Max Planck Institute for Solid State Research, Stuttgart, Germany

Magnetic dynamics at the nanoscale provide crucial insight into the behavior of superconductors. Using single-spin scanning quantum microscopy, we probe vortex dynamics in the two-dimensional superconductor NbSe2. Our measurements reveal a disordered vortex glass phase that melts near the critical temperature and displays cooling-rate-dependent configurations. Surprisingly, magnetic noise persists well below Tc, with a strength that increases at lower temperatures - contrary to expectations. This behavior, detected via spin decoherence, points to an intrinsic origin driven by competition between supercurrent density and thermal fluctuations. Our results establish single-spin microscopy as a powerful platform for investigating fluctuations in 2D superconductors.

TT 24.7 Tue 12:30 HSZ/0003

Quantum sensing of a synthetic 3D spin texture — •R. J. Peña Román[1,2,3], S. Maity[1,2], F. Samad[4,5], S. Josephy[6], A. Morales[6], S. Chattopadhyay[1,3], A. Kákay[4], K. Kern[2,7], O. Hellwig[4,5], and A. Singha[1,2,3] — [1]IFMP, Dresden University of Technology — [2]Max Planck Institute for Solid State Research — [3]Wurzburg-Dresden Cluster of Excellence (ct.qmat) — [4]Institute of Ion Beam Physics and Material Research, Helmholtz-Zentrum Dresden-Rossendorf — [5]Insititute of Physics, Chemnitz University of Technology — [6]QZabre AG, Zurich — [7]Institute de Physique, École Polytechnique Fédérale de Lausanne

Multilayered synthetic antiferromagnets (SAFs) are artificial three-dimensional (3D) architectures engineered to create novel, complex, and stable spin textures. Magnetic imaging of the spin texture is a crucial step for achieving tailored material performance and new functionalities. However, the deterministic detection of the magnetic textures and their quantitative characterization at the nanoscale remains challenging. Here, we use nitrogen-vacancy scanning probe microscopy under ambient conditions to perform quantitative vector-field magnetometry in a multilayered SAF. We demonstrate distinct fingerprints emerging from spin noise and constant stray fields, providing insights into the structure of domains and domain walls, as well as into magnetic noise associated with thermal spin waves. Combined with modern machine learning approaches, this work opens up new possibilities for quantitative magnetometry in materials with tailored and complex 3D spin textures.

TT 25: f-Electron Systems

Time: Tuesday 9:30–12:30 Location: HSZ/0101

TT 25.1 Tue 9:30 HSZ/0101

Strong correlations in rare earth intermetallic compounds — •Payel Shee[1], Chia Jung Yang[2], Tanaya Halder[1], Nainish Tickoo[1], Shishir Kumar Pandey[3], Ashis Kumar Nandy[1], Ruta Kulkarni[4], Arumugam Thamizhavel[4], Manfred Fiebig[2], Anamitra Mukherjee[1], and Shovon Pal[1] — [1]National Institute of Science Education and Research, Bhubaneswar, India — [2]ETH Zurich, Zurich, Switzerland — [3]Artificial Intelligence for Science Institute, Beijing, China — [4]Tata Institute of Fundamental Research, Mumbai, India

In rare-earth intermetallic compounds, the strong correlations between magnetic ordering and the crystal electric field (CEF) are essential to understand their many-body ground states. The CEF excitations at a low energy scale becomes crucial to study as it leaves its fingerprints on the exotic magnetic behaviour in rare-earth intermetallics. Using THz time-domain spectroscopy, we have directly probed the underlying CEF states in two distinct material system: a prototype Kondo lattice system ($CeAg_2Ge_2$) and a metallic ferromagnet (PrSi). In $CeAg_2Ge_2$, we elucidate the low lying CEF state to strongly couple with the Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction, evidenced by a distinct blueshift in the transition frequency [1]. However, in PrSi, we identify a prominent increase in the population of the higher CEF state at the curie temperature, showcasing an intricate interplay between CEF and magnetic ordering in these strongly correlated systems[2].

[1] P. Shee et al., Phys. Rev. B 109, 075133 (2024)
[2] P. Shee et al. manuscript submitted to Advanced Science.

TT 25.2 Tue 9:45 HSZ/0101

Rare-earth nitrides: nitrogen stoichiometry, 4*f* valence, and the role of the rare-earth 5*d* states in SmN — Anna Meléndez-Sans[1], Vanda M. Pereira[1], Chun-Fu Chang[1], Chang-Yang Kuo[1,2,3], Chien-Te Chen[2], Liu Hao Tjeng[1], and •Simone G. Altendorf[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [3]Department of Electrophysics, National Yang Ming Chiao Tung University, Hsinchu, Taiwan

We report on the influence of nitrogen stoichiometry on the electronic structure of epitaxial rare-earth nitride (REN) thin films grown by molecular beam epitaxy under ultra-high vacuum base conditions using moderate growth conditions, i.e., slow deposition rates, and moderate temperatures and pressures. The systematic variation of the growth parameters enables precise control of the nitrogen content and the preparation of near-stoichiometric, well-ordered REN thin films [1,2]. Using samarium nitride as a critical model system, we present a combined x-ray photoelectron spectroscopy and x-ray absorption spectroscopy study that reveals the dependence of the rare-earth valence and electronic structure on the nitrogen content. Our findings suggest that the RE 5*d* states may play a crucial role in the nitrogen-deficient samples, as the empty states can stabilize the RE 4*f* valence by hosting the extra electrons.

[1] V. M. Pereira *et al.*, Phys. Rev. Mater. 7, 124405 (2023)
[2] A. Meléndez-Sans *et al.*, Phys. Rev. B 110, 045120 (2024)

TT 25.3 Tue 10:00 HSZ/0101

Terahertz Signatures of Coupled Topological and Heavy-Fermion States in SmB_6 — •Zekai Chen, Debankit Priyadarshi, Erik W. de Vos, and Manfred Fiebig — Department of Materials, ETH Zurich, Zurich, Switzerland.

We present a THz time-domain spectroscopy study that resonantly probes the conducting surface state of the topological Kondo insulator samarium hexaboride (SmB_6). Previous work on Kondo insulators has shown that the Kondo quasiparticles disintegrate near a quantum critical point (QCP) following THz radiation, leading to a delayed echo-pulse-like signal in the time domain [1]. In contrast to these materials, SmB_6 exhibits an additional in-gap state that is hypothesized to be related to its topological surface conductivity. In the presented experiment, this in-gap state is resonantly probed with THz radiation. Our results show the aforementioned echo-like signal at 3 ps, which matches the theoretical surface Kondo temperature [2]. The link between the topological surface state and the Kondo effect is corroborated by the observation of a transition towards negative optical conductivity of the instantaneous THz reflection, which emerges on the same temperature scale as the echo-response. Our results provide insight into the emergence of a coupling between the in-gap surface state and the underlying correlated Kondo physics in SmB_6.

[1] Nature Physics 14, 1103 (2018)
[2] Physical Review Letters, 114, 177202 (2015)

TT 25.4 Tue 10:15 HSZ/0101

Observation of 5f valence fluctuations in UPd_2Cd_{20} by high-resolution XAS — •Jindřich Kolorenč — Institute of Physics (FZU), Czech Academy of Sciences, Prague, Czech Republic

The regime of valence fluctuations, known from anomalous rare-earth systems, has not yet been identified by microscopic techniques in any uranium compound. It was only suggested in a few of them on the basis of thermodynamic measurements (such as the magnetic susceptibility) and their similarity to the behavior of rare-earth valence fluctuators. Such arguments, however, are hardly unequivocal. We present uranium L_3 and M_4 x-ray absorption spectra taken on UPd_2Cd_{20}, which is a heavy-fermion *antiferromagnet*. Although it has only one type of uranium site in its primitive cell, the spectra obtained in the high-energy-resolution fluorescence-detection mode display two edges, each associated with a different valence state, $5f^2$ and $5f^3$. Moreover, the shape of the M_4 spectrum is well approximated by a combination of UCl_3 ($5f^3$) and UCl_4 ($5f^2$) spectra. This suggests $5f^2 \leftrightarrow 5f^3$ fluctuations on a timescale longer than the characteristic time of the spectroscopy technique. Unlike 4f systems, in which such fluctuations typically lead to a *destruction of magnetism* due to one of the involved $4f^n$ configurations being non-magnetic, the $5f^2$ and $5f^3$ states are both magnetic, allowing for a magnetic ordering in the fluctuating state.

This contribution is a result of a collaboration between Niigata University, Japan Atomic Energy Agency, Kyushu University, Japan Synchrotron Radiation Research Institute, Helmholtz-Zentrum Dresden-Rossendorf, ESRF in Grenoble, and Charles University in Prague.

TT 25.5 Tue 10:30 HSZ/0101

Stoichiometry control of the magnetic structure and crystalline electric field effects in the Kondo lattice CeAlGe — •Soohyeon Shin and Yixi Su — Juelich Center for Neutron Sciense at MLZ, Lichtenbergstrasse 1, Garching 85748, Germany

CeAlGe crystallizes in the LaAlSi-type tetragonal structure, where spatial inversion symmetry is broken. This system is expected to host Weyl fermions near a Fermi surface that becomes more stable when time-reversal symmetry is broken. The magnetic ground state and associated topological properties of CeAlGe are known to depend sensitively on chemical stoichiometry. For instance, crystals grown by the flux method typically contain 5-15% excess Al on the Ge site and exhibit commensurate antiferromagnetic order below T=5.1 K. In contrast, crystals prepared by the floating-zone method under 30 bar of Ar gas yield stoichiometric compositions and display incommensurate order below T=4.4 K, where topological Hall effects are induced by external magnetic fields.

In this presentation, we report recent neutron-scattering experiments. Small-angle scattering reveals the emergence of additional incommensurate magnetic ordering associated with Al substitution. Furthermore, time-of-flight measurements suggest the presence of a magnetoelastic bound state between the first excited crystal-field level and an optical phonon mode near 17 meV. We will discuss the implications of this magnetoelastic bound state for the magnetic structures in CeAlGe.

TT 25.6 Tue 10:45 HSZ/0101

Acoustic signatures of field-induced electronic topological transitions in $YbNi_4P_2$ — •Jérémy Sourd[1], E.O. Eljaouhari[2], B.V. Schwarze[1], K. Kliemt[3], C. Krellner[3], F. Husstedt[1,4], J. Wosnitza[1,4], S. Zherlitsyn[1], and G. Zwicknagl[2,5] — [1]Dresden High Magnetic Field Laboratory (HLDEMFL), HZDR, Germany — [2]Institut für Mathematische Physik, TU Braunschweig — [3]Physikalisches Institut, Johann Wolfgang Goethe-Universität, Frankfurt am Main — [4]Institut für Festkörper- und Materialphysik, TU Dresden — [5]Max Planck Institute for Chemical Physics of Solids, Dresden

The Fermi surface is a central concept to elaborate the physical properties of correlated electron systems. While resulting from the precise chemistry of a given material through its crystal and electronic structures, the Fermi-surface shape and topology can evolve drastically upon varying a control parameter leading to an electronic-topological transition (ETT). In heavy-fermion systems the strong electronic correlations generate renormalized flat bands close to the Fermi level, leading to effective Fermi energies of the order of 10 T. Thus, in these systems the Zeeman energy from moderate magnetic field is enough to induce an ETT, as observed for example in $YbNi_4P_2$. We used acoustic waves in order to probe the sequence of ETT in $YbNi_4P_2$, by performing ultrasound experiments at low temperature. By comparing the observed anomalies of the sound velocity for different acoustic modes, we show how ultrasound permits to better explore the reciprocal space structure of the ETTs in $YbNi_4P_2$.

15 min. break

TT 25.7 Tue 11:15 HSZ/0101

Tuning quadrupolar order in $YbRu_2Ge_2$ using uniaxial stress — •Arindam Ghara[1], Caitlin I. O'Neil[1], Elena Gati[1,2], You-Sheng Li[3], Nubia Caroca-Canales[1], Christoph Geibel[1], Hilary Noad[1], and Michael Nicklas[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Goethe University Frankfurt, Germany — [3]National Taiwan University, Taiwan

Multipolar order has gained renewed attention due to its close connection with nematicity, altermagnetism, and quantum criticality. $YbRu_2Ge_2$ exhibits a ferroquadrupolar transition at $T_Q = 10.2$ K accompanied by a tetragonal-to-orthorhombic structural distortion [1,2]. Experimental studies [2] have proposed a B_{1g} order parameter for the ferroquadrupolar ground state. According to theoretical work [3], a transverse field, such as a magnetic field along the c axis or a B_{2g} stress, can drive $YbRu_2Ge_2$ towards a quantum critical point. This makes $YbRu_2Ge_2$ a model system for studying quadrupolar fluctuations under symmetry-resolved tuning parameters.

We used these tuning parameters to map the phase diagram of $YbRu_2Ge_2$ via resistance and Young's modulus measurements. While the data under c-axis magnetic field behave as expected for a transverse field, the response to B_{2g} stress is unexpected: the resistivity anomaly broadens, whereas the Young's modulus anomaly stays sharp. This behaviour challenges the assumption that B_{2g} stress acts purely as a transverse field.

[1] Jeevan *et al.*, *Phys. Rev. B* **73**, 020407 (2006)
[2] Rosenberg *et al.*, *PNAS* **116**, 7232 (2019)
[3] Maharaj *et al.*, *PNAS* **114**, 13430 (2017)

TT 25.8 Tue 11:30 HSZ/0101

$Yb_5Rh_6Sn_{18}$: a valence fluctuating system with ultra-low thermal conductivity — •Oleksandr Bolielyi[1], Volodymyr Levytskyi[1], Kristina O. Kvashnina[2], Andreas Leithe-Jasper[3], and Roman Gumeniuk[1] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg, 09596 Freiberg, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), 01314 Dresden, Germany — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany

$Yb_5Rh_6Sn_{18}$ obtained by high-frequency melting of elemental metals crystallizes with an unique structural configuration closely related to the $Yb_3Rh_4Sn_{13}$ Remeika prototype. An important feature of this structure is that the small Sn1-atoms reside within enlarged Frank-Kasper polyhedra thus, possessing potential for a "rattling" motion. X-ray absorption spectra of $Yb_5Rh_6Sn_{18}$ indicate Yb-ions to be in the intermediate valence state (IVS), i.e. switching between the $4f^{13}$ (Yb^{3+}) and $4f^{14}$ (Yb^{2+}) configurations. In agreement with this finding temperature dependence of magnetic susceptibility reveals a well pronounced maximum. Both Hall and Seebeck coefficients indicate the change of charge carrier type from electrons to holes between 120 and 220 K. Together with electrical resistivity and theoretical DFT calculations these effects confirm $Yb_5Rh_6Sn_{18}$ to be a metal, which disobeys the free electron gas theory. The ultra-low thermal conductivity is attributed to the appearance of phonon resonance as well as to the "rattling" motion of Sn1 atoms in the studied structure.

TT 25.9 Tue 11:45 HSZ/0101

Antiferromagnetic order and spin excitations in $HoInCu_4$ — •O. Stockert[1], X. Boraley[2], J. Lass[2], R. Sibille[2], Ø. S. Fjellvåg[2,3], S. Moody[2], A. M. Läuchli[2,4], V. Fritsch[5], and D. G. Mazzone[2] — [1]Max-Planck-Institut CPfS, Dresden — [2]Paul-Scherrer-Institut, Villigen, Switzerland — [3]Institute for Energy Technology, Kjeller, Norway — [4]École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland — [5]Universität Augsburg, Augsburg

Magnetic frustration quite often leads to novel quantum phases in condensed matter physics. Here, we focus on the intermetallic compound $HoInCu_4$ with a face-centered cubic structure being prone to frustration.

We performed extensive elastic and inelastic neutron scattering on $HoInCu_4$ to unravel the magnetic structure and to study the underlying exchange interactions [1,2]. Below 0.76 K $HoInCu_4$ orders in a type-III AF structure with a reduced ordered moment and partially disordered Ho spins. Enhanced spin fluctuations due to frustration are detected as a diffuse signal, even well inside the ordered state. In the magnetic field polarized state the spin excitations and the magnetic diffuse scattering can be well modeled using linear spin-wave theory yielding a consistent set of nearest and next-nearest neighbor interactions. In contrast, in zero magnetic field spin-wave theory fully fails to describe the overdamped spin excitations in the AF ordered state. All these findings emphasize the importance of frustration in $HoInCu_4$.

[1] O. Stockert et al., Phys. Rev. Res. 2, 013183 (2020).
[2] X. Boraley et al., Phys. Rev. Lett. 135, 046702 (2025).

TT 25.10 Tue 12:00 HSZ/0101

Single crystal growth and characterization of $EuMn_2Si_2$ and $EuMn_2Ge_2$ — •Janina Strahl[1], Tom Gerntke[1,2], Kristin Kliemt[1], Kurt Kummer[2], and Cornelius Krellner[1] — [1]Institute of Physics, Goethe-University, Frankfurt (Main), Germany — [2]European Synchrotron Radiation Facility (ESRF), F-38043 Grenoble Cedex, France

$EuMn_2Si_2$ exhibits a thermally driven valence transition of the europium ions from Eu^{3+} at low temperatures to $Eu^{2.5+}$ at high temperatures [1]. The isoelectronic and isostructural substitution of silicon with germanium leads to a stabilization of the divalent state of Eu in $EuMn_2Ge_2$ with reported ferromagnetic Eu ordering below 13 K [2]. Both rare earth intermetallic 122 compounds crystallize in the tetragonal $ThCr_2Si_2$ structure type and show antiferromagnetic ordering of the manganese sublattices above room temperature. In literature [1,2], additional Mn spin-reorientation transitions in polycrystalline $EuMn_2Si_2$ samples at low temperatures were observed. In this contribution, we present the single crystal growth and physical properties of both compounds. We found antiferromagnetic ordering of the Eu ions in single crystalline $EuMn_2Ge_2$ below 10.4 K. Furthermore, there is evidence that previously reported Mn reorientation transitions are absent in pure $EuMn_2Si_2$ single crystals, and a valence crossover occurs between 350-530 K.

[1] M. Hofmann et al., Phys. Rev. B 69, 174432 (2004)
[2] I. Nowik et al., Phys. Rev. B 55, 3033 (1997)

TT 25.11 Tue 12:15 HSZ/0101

Polaronic quasiparticles in the valence-transition compound $TmSe_{1-x}Te_x$ — •Chul-Hee Min[1,2], Simon Müller[3], Lenart Dudy[4], Michael Heber[5], Woo-Jae Choi[6], Jonathan Denligner[7], Chang Jong Kang[8], Matthias Kalläne[2], Nils Wind[5], Markus Scholz[5], Christoph Schlueter[5], Andrei Gloskovskii[5], Emile Rienks[8], Vladimir Hinkov[3], Hendrik Bentmann[1], Yong Seung Kwon[6], Friedrich Reinert[3], Hyeong Do Kim[9], and Kai Rossnagel[2,5] — [1]FYI, NTNU, Norway — [2]IEAP, CAU Kiel, Germany — [3]Uni. Würzburg, Germany — [4]SOLEIL, France — [5]DESY, Germany — [6]DGIST, South Korea — [7]ALS, USA — [8]BESSY II, Germany — [9]PAL, South Korea

Exotic quasiparticle states have been proposed in mixed-valent compounds exhibiting valence transitions. However, clear spectroscopic evidence identifying these states has remained elusive. Using synchrotron-based photoemission spectroscopy, we have probed the Tm $3d$ and $4f$ emissions in $TmSe_{1-x}Te_x$, where a semimetal–insulator transition occurs. Our photoemission results reveal a novel

quasiparticle excitation in the semimetallic phase: a Holstein polaron. This local lattice distortion, induced by $4f$ photohole, is surprising in a metallic system where efficient screening is expected. We interpret this observation as evidence that, in heavy fermion systems, the conduction electrons' screening response is slower than the characteristic atomic distortion. Our finding underscores the critical role of electron-phonon coupling, which necessitates an extension of the standard Periodic Anderson Model.

[1] Phys. Rev. Lett. 135, 186501 (2025)

TT 26: Correlated Magnetism – Frustrated Systems

Time: Tuesday 9:30–12:15 Location: HSZ/0103

TT 26.1 Tue 9:30 HSZ/0103

Finite-temperature Lanczos approach to frustrated quantum spin systems — •Andreas Honecker[1], Malo Rouxel[1], and Katarína Karľová[2] — [1]Laboratoire de Physique Théorique et Modélisation, CNRS, CY Cergy Paris Université, France — [2]Department of Theoretical Physics and Astrophysics, P.J. Šafárik University, Košice, Slovakia

The finite-temperature Lanczos method or its quantum typicality variants are a method of choice for computing thermodynamic properties of frustrated quantum spin systems, in particular in two dimensions. Here we show that quasi-exact results can be obtained with moderate numerical effort for systems with $N \leq 40$ spins 1/2, even if the method involves Monte Carlo sampling. We illustrate the approach on the diamond-decorated square and honeycomb lattices. These models not only distinguish themselves by the presence of local conservation laws, but also offer a rich phase diagram, including phases with macroscopic ground-state degeneracy. We comment in particular on the resulting enhanced magnetocaloric effect [1].

[1] K. Karľová, A. Honecker, N. Çaçi, S. Wessel, J. Strečka, T. Verkholyak, Phys. Rev. B **110**, 214429 (2024).

TT 26.2 Tue 9:45 HSZ/0103

Quantum annealing for lattice models with long-range interactions — •Jan Alexander Koziol and Kai Phillip Schmidt — Department of Physics, Staudtstraße 7, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), D-91058 Erlangen, Germany

We use superconducting qubit quantum annealing devices to determine the ground state in the thermodynamic limit of Ising models with algebraically decaying long-range interactions. This is enabled by a unit-cell-based optimization scheme, in which the finite optimizations on each unit cell are performed using commercial quantum annealing hardware. To demonstrate the capabilities of the approach, we choose three exemplary problems relevant for other quantum simulation platforms and material science: (i) the calculation of devil's staircases of magnetization plateaux of the long-range Ising model in a longitudinal field on the triangular lattice, motivated by atomic and molecular quantum simulators; (ii) the evaluation of the ground state of the same model on the Kagomé lattice in the absence of a field, motivated by artificial spin ice; (iii) the study of models with modified few-nearest-neighbor interactions relevant for Ising compounds with potential long-range interactions. The approach discussed in this work provides a useful and realistic application of existing quantum annealing technology, applicable across many research areas in which lattice problems with resummable long-range interactions are relevant.

TT 26.3 Tue 10:00 HSZ/0103

Nature of intersite exchange interactions in Ce triangular-lattice delafossites — •Leonid Pourovskii — CPHT, CNRS, Ecole polytechnique, IP Paris, 91120 Palaiseau, France — Collège de France, Université PSL, 75005 Paris, France

Anisotropic intersite exchange interactions (IEI) in frustrated rare-earth magnets are difficult to assess both theoretically and experimentally. We propose an ab initio force-theorem framework combining the quasi-atomic Hubbard-I approach to $4f$ correlations with a static mean-field treatment of the on-site inter-shell Coulomb interaction between rare-earth $4f$ and $5d$ states to simultaneously capture both $4f$ superexchange and $5d$-mediated indirect exchange. Applying it to a set of Ce delafossites – the selenide $CsCeSe_2$, sulfide $KCeS_2$, and oxide $RbCeO_2$ – we find a remarkable qualitative evolution of IEI. While the superexchange is found to dominate over the indirect exchange in the oxide, the situation is reversed in the selenide. Both coupling mechanisms are found to contribute comparably in the sulfide. The calculated IEI place $CsCeSe_2$ and $KCeS_2$ in the yz-stripe region of the published spin-1/2 triangular-lattice model phase diagram, in agreement with experiment, while those for $RbCeO_2$ correspond to the 120° antiferromagnetic order. The magnetic excitation spectra of $CsCeSe_2$ and $KCeS_2$ evaluated from the calculated spin Hamiltonains are in good qualitative and quantitative agreement with experimental data.

TT 26.4 Tue 10:15 HSZ/0103

Quantum Monte Carlo study of the Su-Schrieffer-Heeger model on a triangular lattice — •Disha Hou[1], Anika Götz[1], Jadson Silva[2], Natanael Costa[2], and Fakher Assaad[1] — [1]Institut für Theoretische Physik und Astrophysik, Universitat Würzburg, Würzburg, Germany — [2]Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil

We study the half-filled bond Su-Schrieffer-Heeger (SSH) model on the triangular lattice using sign-problem-free auxiliary-field quantum Monte Carlo methods. By varying the hopping matrix element, we interpolate between the assisted hopping limit — characterized by an emergent local $\mathbb{Z}_2$ symmetry and phases in which the hopping is weakly modulated by phonons. In addition to a s-wave superconducting state and a staggered valence-bond solid state, we observe an emergent flux phase which, in the absence of fluctuations, would exhibit a Dirac dispersion. We find that this phase is gapped and does not appear to break any ultraviolet symmetries of the model, leading us to tentatively identify it as a gapped Z_2 quantum spin liquid phase.

TT 26.5 Tue 10:30 HSZ/0103

Exact nematic and mixed magnetic phases driven by competing orders on the pyrochlore lattice — •Niccolò Francini, Lukas Schmidt, Lukas Janssen, and Daniel Lozano-Gómez — Institut für Theoretische Physik and Würzburg-Dresden Cluster of Excellence ct.qmat, TU Dresden, 01062 Dresden, Germany

Pyrochlore magnets are a paradigmatic example of three-dimensional frustrated systems and provide an excellent platform for studying a variety of exotic many-body phenomena. In recent years, increasing attention has been devoted to bilinear spin models on this lattice, where multiple magnetic phases can be degenerate in energy, often stabilizing unconventional magnetic states. In this work, we focus on one such model, parametrized by the interaction coupling $J_{z\pm}$, which defines a line in parameter space corresponding to the phase boundary between three distinct magnetic phases. Using a combination of analytical and numerical methods, we show that this model exhibits an order-by-disorder mechanism at low temperatures, giving rise to a *mixed* magnetic phase. This represents the first realization of a $\mathbf{q} = 0$ long-range-ordered phase in a pyrochlore magnet characterized by two distinct order parameters, which we denote as the $A_2 \oplus \psi_2$ phase. Furthermore, at $J_{z\pm} = 1/\sqrt{2}$, the model acquires a subextensive number of discrete symmetries, which preclude the stabilization of conventional long-range order and instead lead to the emergence of a novel nematic phase. We characterize this nematic phase, describe how its ground-state configurations are constructed, and analyze its stability at higher temperatures and under small deviations from $J_{z\pm} = 1/\sqrt{2}$.

TT 26.6 Tue 10:45 HSZ/0103

From Open-Shell Nanographenes to Quantum Spin Chains: Controllable Spins in Carbon Ladders — •Andoni Agirre[1,2], Thomas Frederiksen[1,3], Géza Giedke[1,3], and Tobias Grass[1,3] — [1]Donostia International Physics Center (DIPC), Manuel Lardizabal Pasealekua 4, 20018 Donostia, Basque Country — [2]Department of PMAS: Physics, Chemistry and Technology, University of the Basque Country (UPV/EHU), Manuel Lardizabal Pasealekua 3, 20018 Donostia, Basque Country — [3]IKERBASQUE, Basque Foundation for Science, Euskadi Plaza 5, 48009 Bilbao, Basque Country

The low-energy electronic structure of nanographenes with open-shell configurations can be faithfully represented by effective quantum spin models, providing a promising route toward carbon-based quantum simulators. Here we demonstrate this correspondence for an oligo-indenoindene molecule, composed of alternating pentagon-hexagon rings and theoretically mapped to a frustrated Fermi-Hubbard ladder. We show that a spin-1/2 Heisenberg chain consisting of only one spin per pentagon and featuring nearest- and next-nearest-neighbor couplings, quantitatively reproduces the molecular excitation spectrum and entanglement structure obtained from matrix-product-state calculations. By systematically identifying the effective spins with delocalized fermionic modes across the molecular backbone, we achieve near-quantitative agreement in both static and dynamical magnetic properties. Our results establish them as experimentally realizable platforms for exploring frustrated magnetism and correlated spin dynamics in purely carbon-based materials.

15 min. break

TT 26.7 Tue 11:15 HSZ/0103

Single crystal growth and study of the spin gap system Cu_3WO_6 — •Annarose Jose Palliyan[1,2], Nazmul Islam[2], Cintli Aguilar-Maldonado[2], Ralf Feyerherm[2], Andrey Malyuk[3], Sabine Wurmehl[3], and Bella Lake[2,1] — [1]Technische Universität Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [3]Leibniz Institute for Solid State and Materials Research Dresden, Germany

Frustration in magnetic materials is an important phenomena leading to exotic quantum states due to the presence of the competing interactions in those materials. From this point of view, cuprates are interesting because of the possibility of having multiple correlations and interactions resulting in unusual correlated phases[1]. Copper tungstate, Cu_3WO_6, is one such compound where Cu^{2+} (S=1/2) occupies the triangular bipyramidal sites. This cubic system (Pa-3) hosts a unique magnetic lattice consisting of coupled hexagons and equilateral triangles of Cu^{2+} giving rise to multiple exchange interactions. In order to study the magnetic behavior and solve the magnetic Hamiltonian of this material, we have grown the first single crystals of Cu_3WO_6 by several different growth techniques and the high crystalline quality of these crystals has been confirmed. We have also studied the thermodynamic properties on these crystals down to low temperatures and our results confirm the reported singlet ground state with a spin gap of about 130K which suggests a dominant hexagonal interaction[2].
[1] Y. Fudamoto et al., Phy. Rev B 65, 174428 (2002)
[2] M. Hase et al., Phys. B: Condens. Matter 215, 325 (1995)

TT 26.8 Tue 11:30 HSZ/0103

Magnetic frustration and field-induced transitions in the octahedral lattice iridate Ho_3IrO_6 — •Abanoub Hanna[1], Cintli Aguilar Maldonado[1], Ralf Feyerherm[1], A.T. M. Nazmul Islam[1], and Bella Lake[1,2] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Hahn-Meitner Platz 1, D-14109 Berlin, Germany — [2]Institut für Festkörperphysik, Technische Universität Berlin, Germany

Ho_3IrO_6 is a new octahedral lattice compound in which holmium ions form a distorted network of corner sharing octahedra, providing a clean platform to study frustration in rare earth iridates. X ray and neutron powder diffraction confirm a single phase cubic Ia-3 structure with ordered Ho and Ir sites and no detectable impurities, so the magnetic behaviour can be interpreted without structural complications. Low temperature magnetometry shows a sharp transition near 1 kelvin with strong field dependence, and Curie Weiss analysis indicates antiferromagnetic interactions and a large frustration parameter, pointing to competing exchanges on the octahedral lattice. AC susceptibility, nonlinear magnetization curves and field dependent anomalies reveal a genuine thermodynamic transition and metamagnetic steps, while heat capacity data are consistent with a low lying triplet ground state and an additional Schottky like feature around 5 K.

TT 26.9 Tue 11:45 HSZ/0103

Crystal growth, electronic and magnetic Properties of Mn_3Al_9Si — •Ashiwini Balodhi[1], Min Gyu Kim[2], Andreas Kreyssig[1], and Anna E. Böhmer[1] — [1]Experimental Physics IV, Ruhr-University Bochum, Bochum, Germany — [2]University of Wisconsin-Milwaukee, Milwaukee, USA

The Mn-based intermetallic compound Mn_3Al_9Si crystallizes in a hexagonal structure in which the Mn ions form a well-separated triangular network, giving rise to unusual transport and thermodynamic behavior. We have synthesized high-quality single crystals of Mn_3Al_9Si and performed magnetic, transport and heat-capacity measurements. The magnetic susceptibility exhibits isotropic behavior with no evidence of long-range magnetic ordering down to 1.8 K. Low-temperature resistivity measurements reveal a negative magnetoresistance. We further present the critical scaling behavior in applied magnetic fields, in both magnetization and heat-capacity.

We acknowledge funding from the European Research Council through Project 101040811, Distort-to-Grasp.

TT 26.10 Tue 12:00 HSZ/0103

Synthesis and characterization of $Mn_3Al_2Si_3O_{12}$ single crystal — •Marwa Abouelela[1,2], ATM Nazmul Islam[2], Ralf Feyerherm[2], and Bella Lake[1,2] — [1]Institut für Festkörperphysik, Technische Universität, Berlin, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

Geometric magnetic frustration, typically found in materials with triangular and tetrahedral motifs, has attracted significant interest in recent research [1]. The garnet $Mn_3Al_2Si_3O_{12}$ exhibits geometrical frustration, where magnetic Mn^{2+} ($3d^5$) ions that have spin-5/2 form hyper-Kagome structure which is three-dimensional network of corner-sharing triangles [2]. In this study, we synthesized the first single crystals of $Mn_3Al_2Si_3O_{12}$ grown by the optical floating-zone technique. X-ray and neutron diffraction confirmed the garnet space group $Ia\bar{3}d$. Temperature-dependent magnetic susceptibility measurements reveal antiferromagnetic ordering of the Mn^{2+} ions below T_N = 6.5 K, along with an effective moment of 5.85 μ_β and a Curie–Weiss temperature of T_{CW} = −24.48 K, giving a frustration index of $f = |\theta_{CW}/T_N|$ = 3.8. Investigation of the magnetic structure below T_N and the short-range order above T_N is ongoing.
[1] Islam, Manisha et al., Crystals 13 (2023)397
[2] Lau et al., Phys. Rev. B 80 (2009) 214414

TT 27: Focus Session: Tunable Correlations in van der Waals Quantum Materials II (joint session TT/DS/HL)

Time: Tuesday 9:30–10:45 Location: HSZ/0105

Invited Talk TT 27.1 Tue 9:30 HSZ/0105

Simulating high-temperature superconductivity in a triangular moiré lattice — •Kin Fai Mak — Luruper Chaussee 149 Bldg. 900 (MPSD), 22761 Hamburg, Germany

Moiré materials built on transition metal dichalcogenide semiconductors have emerged as a tunable platform for simulating the Hubbard model on a triangular lattice. A natural question arises: Can the platform be tuned to yield a phase diagram similar to that in high-temperature cuprate superconductors? In this talk, I will discuss the emergence of high-temperature superconductivity near the Mott transition in a triangular moiré lattice with intermediate coupling strength. The emergent doping-temperature phase diagram looks remarkably similar to that in cuprate superconductors. I will also discuss the evolution of the phase diagram by tuning the band structure of the material by gating. The results could provide a new angle for understanding the phenomenon of high-temperature superconductivity in strongly correlated materials.

TT 27.2 Tue 10:00 HSZ/0105

Engineering Hubbard models with gated two-dimensional moiré systems — •Yiqi Yang[1], Yubo Yang[2], Miguel Morales[3], and Shiwei Zhang[3] — [1]Lund University, Lund, Sweden — [2]Hofstra University, New York, USA — [3]Flatiron Institute, New York, USA

Lattice models are powerful tools for studying strongly correlated quantum many-body systems, but their general lack of exact solutions motivates efforts to simulate them in tunable platforms. Recently, a promising new candidate has emerged for such platforms from two-dimensional materials. A subset of moiré systems can be effectively described as a two-dimensional electron gas (2D EG) subject to a moiré potential, with electron-electron interactions screened by nearby metallic gates. In this talk, we present the realization of lattice models in such systems [1]. We show that, by controlling the gate separation, a 2D EG in a square moiré potential can be systematically tuned into a system whose ground state exhibits orders analogous to those of the square lattice Hubbard model, including the stripe phase. Furthermore, we study how variations in gate separation and moiré potential depth affect the ground-state orders. A number of antiferromagnetic phases, as well as a ferromagnetic phase and a paramagnetic phase, are identified.We then apply our quantitative downfolding approach to triangular moiré systems closer to current experimental conditions, compare them with the square lattice parameters studied, and outline routes for experimental realization of the phases.
[1] arXiv:2508.13314

TT 27.3 Tue 10:15 HSZ/0105

Dirac quantum criticality in twisted double bilayer transition metal dichalcogenides — •Jan Biedermann and Lukas Janssen — Institut für Theoretische Physik and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01062 Dresden, Germany

We investigate the phase diagram of twisted double bilayer transition metal dichalcogenides with ABBA stacking as a function of twist angle and pressure. At a filling of 2 holes per moiré unit cell, the noninteracting system hosts a Dirac semimetal with graphene-like low-energy bands. At small twist angles however, interactions dominate the low-temperature physics, stabilizing an antiferromagnetic insulating ground state that is characterized by spin density modulations at the moiré scale. The twist-tuned semimetal-to-antiferromagnet transition is shown to be continuous and belongs to the Gross-Neveu-Heisenberg universality class. We propose that this transition may also be realized by applying uniaxial pressure to a sample, raising the intriguing possibility of experimentally measuring the associated critical exponents for the first time.

TT 27.4 Tue 10:30 HSZ/0105

Chemically Tunable Correlation Strength in Breathing Mode Kagome van der Waals Materials $Nb_3(F,Cl,Br,I)_8$ — •Joost Aretz[1], Sergii Grytsiuk[1], Xiaojing Liu[2], Giovanna Feraco[2], Chrystalla Knekna[2,3], Muhammad Waseem[2], Zhiying Dan[2], Marco Bianchi[4], Philip Hofmann[4], Mazhar Ali[5], Mikhail Katsnelson[1,6], Antonija Grubišić-Čabo[2], Hugo Strand[7], Erik van Loon[8], and Malte Rösner[1,9] — [1]Radboud University, Nijmegen, Netherlands — [2]University of Groningen, Netherlands — [3]University of Amsterdam, Netherlands — [4]Aarhus University, Denmark — [5]Delft University of Tech-

nology, Netherlands — [6]Constructor University, Bremen, Germany — [7]Örebro University, Sweden — [8]Lund University, Sweden — [9]Bielefeld University, Germany

Finding tunable correlated electron systems in nature is highly desirable for studying strongly correlated materials. Our recent work demonstrates that the Nb_3X_8-family offers such a platform for tuning correlation effects in van der Waals systems. By using ab initio downfolding and cluster dynamical mean-field theory we show how correlation effects evolve across the halide series. In these materials an intruiging interplay between in-plane trimerization and out-of-plane dimerization leads to correlated insulating behavior, where the strength of correlations can be tuned by switching the halide or by changing the layer number. The predicted trends are supported by ARPES measurements. The correlated electron physics in this system is robust, tunable and layered, which allows studying the role of correlations in devices such as the $NbSe_2/Nb_3Br_8$ Josephson diode.

TT 28: Superconducting Electronics: SQUIDs and other Josephson Circuits and Components

Time: Tuesday 9:30–12:45 Location: CHE/0089

TT 28.1 Tue 9:30 CHE/0089

Gate-controlled switching in non-centrosymmetric superconducting devices - Large output voltage — •Jennifer Koch[1], Leon Ruf[1], Angelo Di Bernardo[1,2], and Elke Scheer[1] — [1]Universität Konstanz, Konstanz, Germany — [2]Università degli Studi di Salerno, Fisciano (SA), Italy

Gate-controlled supercurrent (GCS) devices have become of great interest as a superconducting equivalent to complementary metal-oxide-semiconductor (CMOS) logic. The underlying concept is based on the observation that supercurrent can be controlled electrically through the application of a gate voltage [1,2].

We investigate GCS devices made of the non-centrosymmetric superconductor $Nb_{0.18}Re_{0.82}$. By combining geometric adjustments with the material's high normal-state resistivity, we achieve a significant increase of the output voltage. The resulting voltage is high enough to drive CMOS transistors, demonstrating the potential of GCS devices to interface directly with conventional semiconductor electronics. This finding represents an important step towards hybrid computing architectures.

[1] De Simoni et al., Nature Nanotech 13, 802 (2018)
[2] Paolucci et al., Nano Letters 18, 4195 (2018)

TT 28.2 Tue 9:45 CHE/0089

Chemical-mechanical polishing process for the fabrication of cross-type Nb/Al-AlO$_x$/Nb Josephson tunnel junctions — •Alexander Stoll, Lukas Münch, Daniel Hengstler, Andreas Reifenberger, Andreas Fleischmann, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, Germany

The core elements at the frontier of superconducting electronic devices, such as qubits or superconducting quantum interference devices (SQUIDs), are the Josephson tunnel junctions (JJs). To enable scaling in production of these devices, good parameter control is required, including a uniform quality and reproducibility. We use a cross-type geometry for our JJs so that our junction area is not limited by alignment inaccuracies and, at the same time, parasitic capacitances and thus parasitic LC resonances can be avoided. A sputtered SiO_2 layer used for the insulation of the structured Nb/Al-AlO$_x$/Nb trilayer including its sidewalls usually requires a time-consuming lift-off and leaves behind undesired wings that can compromise the quality of subsequent layers. To mitigate these challenges, we introduced a chemical-mechanical polishing (CMP) step. We present our optimized fabrication process which achieves a well-embedded, smooth, and uniform post-CMP surface and substantially improves the reliability and yield of our JJs on 3 inch wafer-scale. A variety of tests to characterize the JJs based on their IV-characteristics and their Fraunhofer Patterns as well as the electrical properties of the superconducting Nb are discussed.

TT 28.3 Tue 10:00 CHE/0089

Towards the next generation of dc SQUID sensors — •Mauro Esattore[1], Oliver Kieler[1], Michael Paulsen[2], Rainer Körber[2], Patryk Krzysteczko[2], Mark Bieler[1], and Jörn Beyer[2] — [1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany — [2]Physikalisch-Technische Bundesanstalt, Abbestraße 2-10, 10587 Berlin, Germany

This is an update on our path towards next-generation SQUID devices, featuring "fine-pitch" input coils and window-type Nb/Al-AlOx/Nb Josephson junctions (JJs), both realized with sub-micrometer dimensions. The circuit elements are fabricated using electron beam lithography and are integrated into existing sensor designs which are currently fabricated using UV lithography, which limits the minimal dimensions. For current sensor SQUIDs, it is crucial to maximize the inductive coupling k between the signal input coil and the SQUID loop to minimize the coupled energy sensitivity $\varepsilon_c = \varepsilon/k^2$ - with ε being the intrinsic energy sensitivity. The SQUID energy sensitivity $\varepsilon \approx \sqrt{(C_{JJ})}$ can also be lowered by reducing the JJ capacitance C_{JJ}. Our aim is to achieve high sensor compactness as well as reduced coupling losses, without further modifying the sensors design. To that end, we fabricated fine-pitch coils with lateral width down to 0.3 μm - almost an order of magnitude smaller than coils fabricated with UV lithography - with inductance values ranging from 400 nH to 14 μH, depending on the number of coil windings. Details concerning design aspects of both circuit elements, their fabrication and characterization results are provided.

TT 28.4 Tue 10:15 CHE/0089

Tapping-mode SQUID-on-tip Microscopy with Proximity Josephson Junctions — •Matthijs Rog[1], Tycho J. Blom[1], Daan B. Boltje[1,2], Milan P. Allan[1,2,3], and Kaveh Lahabi[1,2] — [1]Institute of Physics, Leiden University, Leiden, The Netherlands — [2]QuantaMap B.V., Leiden, The Netherlands — [3]Faculty of Physics, Ludwig-Maximilians-University Munich, Munich, Germany

Understanding nanoscale dynamics in strongly correlated systems and quantum materials requires investigating the interplay between dissipation, magnetism and electronic transport. The local mapping of transport properties, such as current flow, and their relation to geometry and magnetism still remains a major challenge. Here, we introduce tapping-mode SQUID-on-tip, which combines atomic force microscopy (AFM) with nanoSQUID sensing. This microscope is able to simultaneously image magnetic flux, electrical currents, local heating and sample topography. Our probes minimize nanoSQUID-sample distance, provide in-plane magnetic sensitivity, and operate even on highly corrugated nanostructures and devices. Our fully electronic readout removes the need for optical elements and external radiation. By using proximity-junction nanoSQUIDs with large voltage output, we resolve nanoscale currents down to 100 nA using a simple four-probe electronic readout. In addition to demonstrating the technique, we will show the first applications to strongly correlated electron systems, where our microscope offers immediate new insights into the underlying physics.

[1] M. Rog et al., arXiv:2508.21575

TT 28.5 Tue 10:30 CHE/0089

Nanoscale SQUID on a wireframe tip cantilever by corner lithography — •Thijs Roskamp[1], Tim Horstink[2], Melissa Goodwin[1], Erwin Berenschot[1], Roeland Huijink[2], Edin Sarajilic[2], Niels Tas[1], and Hans Hilgenkamp[1] — [1]MESA+ Institute, University of Twente, Enschede, The Netherlands — [2]Bruker Nederland B.V., Bruker Corporation, Leiderdorp, The Netherlands

Superconducting quantum interference devices (SQUIDs) are the most sensitive magnetic flux sensors and are used in scanning SQUID microscopy (SSM) to spatially resolve and map magnetism. Conventional SSM probes make use of planar silicon substrates which limit their spatial resolution to several micrometers due to an increased sample-pickup area spacing.

Employing ideas from other scanning probe techniques like atomic force microscopy, moving the SQUID to the apex of tip on a scanning probe can significantly increase the spatial resolution.

We have used the principles of corner lithography and molding in silicon wafers to create freestanding superconducting wireframe tips on cantilevers on the wafer scale. With a focused ion beam we pattern superconducting weak links at the apex of the fabricated wireframe tips to create SQUIDs with sizes from sub-100 nm to several micrometers. By integrating the wireframe probe on a silicon nitride cantilever with pre-defined contact pads, leads, and resistive strain gauges, we create a SQUID on cantilever probe which will enable simultaneous magnetic and topographic imaging.

TT 28.6 Tue 10:45 CHE/0089

Low noise amplification using Nb trilayer Dimer Josephson Junction Array Amplifiers — •Bhoomika R Bhat, Asen L Georgiev, Fabian Kaap, Victor Gaydamachenko, Christoph Kissling, Judith Felgner, Mark Bieler, and Lukas Grünhaupt — Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

Minimizing added noise in amplification is crucial for quantum-based devices requiring microwave readout signals in the femtowatt range. For example, in superconducting qubits, it significantly improves readout fidelity. Extensive efforts over the last decade have been made in the development of parametric amplifiers to address this challenge. We develop a Dimer Josephson Junction Array Amplifier (DJJAA) [1], in which parametric amplification in the degenerate four-wave-mixing regime is facilitated by pairs of resonant modes, referred to as dimers. We design it to feature multiple flux-tunable dimers within the 2 to 8

GHz range, each of which could be utilized for parametric amplification. Our DJJAAs have 900 to 3000 dc-SQUIDs, and we fabricate them using Nb/Al-AlOx/Nb trilayer technology. We present the fabrication flow of our devices and provide an overview of the corresponding experimental results. Our devices show gain on the order of 20 dB with bandwidths in the range of 5 to 10 MHz and the typical input saturation powers are on the order of -110 dBm.
[1] P. Winkel et al., Phys. Rev. Applied 13, 024015 (2020).

15 min. break

TT 28.7 Tue 11:15 CHE/0089

Controlling three- and four-wave mixing processes in JTWPAs — •Daniil Bazulin[1,2], Johannes Schirk[1,2], Niklas Bruckmoser[1,2], Leon Koch[3], Yongjie Yuan[4], Michael Haider[4,5], Stefan Filipp[1,2,6], and Kirill G. Fedorov[1,2,6] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [3]Peak Quantum GmbH, 85748 Garching, Germany — [4]TUM School of Computation Information and Technology, Technical University of Munich, 85748 Garching, Germany — [5]Universität der Bundeswehr München, 85579 Neubiberg, Germany — [6]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany

Josephson travelling-wave parametric amplifiers (JTWPAs) are essential for scalable quantum computing with superconducting circuits. Their typical bandwidths of several gigahertz, in combination with quantum-limited noise performance, enable high-fidelity multiplexed readout of qubits. In JTWPAs, amplification occurs due to the interaction between the pump and signal modes in a nonlinear medium provided by superconducting nonlinear asymmetric inductive elements (SNAILs). Here, we experimentally investigate a robust JTWPA design based on SNAILs that is capable of operating in both three- and four-wave-mixing regimes. Our results show that we can fully suppress the three-wave mixing process while observing over 10 dB gain from the four-wave pumping over the bandwidth of 4 GHz.

TT 28.8 Tue 11:30 CHE/0089

Demonstration of natively phase-matched parametric amplification in a left-handed transmission line — •Christoph Kissling[1], Victor Gaydamachenko[1], Fabian Kaap[1], Melanie Ziegler[2], Hannes Toepfer[2], and Lukas Grünhaupt[1] — [1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig — [2]Technische Universität Ilmenau, Ehrenbergstraße 29, 98693 Ilmenau

Wideband amplification of weak microwave signals is a key ingredient for cutting-edge experiments ranging from quantum information processing to the search for dark matter. A class of devices that achieves this is the traveling-wave parametric amplifier (TWPA). So far, all TWPA implementations are based on right-handed transmission lines, which exhibit a positive refractive index. Recently, an alternative approach has been proposed that utilizes left-handed transmission lines, which have a negative refractive index [1]. This property allows for self-phase-matched parametric amplification in the four-wave-mixing regime, eliminating the need for any engineering of nonlinearity or dispersion for phase matching. Here, we present our implementation of this concept, which employs a left-handed transmission line with nonlinear inductors made from a granular aluminum thin film. First results show a signal power gain exceeding 10 dB, dynamically tunable across multiple GHz. With only one lithography step, and an order-of-magnitude reduction in circuit length, the concept is promising to significantly reduce the complexity of designing and fabricating a TWPA.
[1] C. Kow et al., Phys. Rev. Applied 24, 024026 (2025)

TT 28.9 Tue 11:45 CHE/0089

Towards 1 V Josephson Arbitrary Waveform Synthesizer — •Omar M. Aladdin[1], Oliver Kieler[1], Abdulrahman Widaa[1], Hannes Preissler[1], Erasmus Wolf[2], Marco Schubert[2], Judith Felgner[1], Rolf-Werner Gerdau[1], Johannes Kohlmann[1], and Mark Bieler[1] — [1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany — [2]Supracon AG, An der Lehmgrube 11, 07751 Jena, Germany

The Josephson Arbitrary Waveform Synthesizer (JAWS) provides quantum-accurate AC voltage waveforms with high spectral purity, low noise, and inherent long-term stability. Based on pulse-driven Josephson junction (JJ) arrays, JAWS is established as the primary AC voltage standard. Recent JAWS developments at PTB include increasing the output voltage per chip, targeting 1 V RMS to advance its use in high-accuracy metrological applications [1]. Current efforts focus on enhancing the JAWS fabrication process to enable larger array sizes using 5-stacked JJ arrays. The stacked junction technology is combined with improved on-chip Wilkinson power dividers, allowing the incorporation of more than two JJ arrays on one chip [2]. The power dividers have been successfully demonstrated with 3-stacked JJ arrays achieving 600 mV RMS per JAWS chip with a total of 36,000 junctions. In this contribution, we present the recent results of 5-stacked JJ arrays and Wilkinson power dividers with up to 60,000 JJs per JAWS chip.
[1] DOI: 10.1016/B978-0-323-90800-9.00001-9
[2] DOI: 10.1109/TASC.2021.3055161

TT 28.10 Tue 12:00 CHE/0089

Study on the feedthrough error in quantum-based superconducting RF waveform generators — •Michael Haas, Abdulrahman Widaa, Oliver Kieler, Marco Kraus, Ralf Behr, Johannes Kohlmann, and Mark Bieler — Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

Quantum-based signal generators are of great interest for a variety of applications such as electrical metrology or quantum computing. The Josephson Arbitrary Waveform Synthesizer (JAWS) consisting of an array of Josephson junctions is one of such devices. It allows the generation of arbitrary, low-noise waveforms with high spectral purity by utilizing the Josephson effect. This approach is well established for signal frequencies in the kHz to low MHz range. However, modern applications typically demand increasing signal frequencies, reaching the microwave range. To satisfy the need for higher JAWS output frequencies, modified circuit designs and bias schemes are necessary. This is mainly because of the so-called feedthrough error, which denotes an input signal being fed through to the output. We will present recent developments of GHz-JAWS at PTB, comprising detailed investigations on the feedthrough error and methods for its reduction.

TT 28.11 Tue 12:15 CHE/0089

Nonequilibrium plasmon fluid in a Josephson junction chain — Anton V. Bubis[1], •Lucia Vigliotti[1], Maksym Serbyn[1], and Andrew P. Higginbotham[2] — [1]Institute of Science and Technology Austria, Am Campus 1, Klosterneuburg, 3400, Austria — [2]James Franck Institute and Department of Physics, University of Chicago, 929 E 57th St, Chicago, Illinois 60637, USA

With the recent push towards the development of quantum technologies, multimode quantum systems, such as superconducting resonators, have drawn considerable attention. These systems can be generally described as weakly nonlinear bosonic modes coupled to a thermal bath and subject to coherent driving. As the number of modes grows and extrinsic decoherence is reduced, understanding the mode-to-mode interaction becomes increasingly relevant, especially far from equilibrium. We consider the interacting plasmonic modes emerging in a long chain of Josephson junctions (JJs), probed via multitone microwave spectroscopy. We investigate the nonequilibrium kinetics of the resulting one-dimensional quantum fluid both theoretically and experimentally, focusing on four-wave-mixing processes. Under two coherent drives, we observe cascaded coupling between plasmonic modes, reproduced using input-output theory applied to nonlinear mode multiplets. Under incoherent broadband drive, we explore the kinetics of weakly populated modes and numerically implement a kinetic equation that predicts the non-equilibrium steady state and captures the excess linewidth of non-driven modes. Our work establishes the key role of four-wave-mixing nonlinearities in the non-equilibrium response of JJ chains.

TT 28.12 Tue 12:30 CHE/0089

Superconducting non-volatile memory device based on charge trapping in Al_2O_3. — •Leon Ruf[1], Jennifer Koch[1], Angelo Di Bernardo[1,2], and Elke Scheer[1] — [1]Department of Physics, University of Konstanz, 78464 Konstanz, Germany — [2]Department of Physics, University of Salerno, 84084 Salerno, Italy

Gate-controlled supercurrent (GCS) is a debated research topic. Experiments on three-terminal devices have shown that applying a gate voltage can modulate the supercurrent [1]. The authors interpret their findings as a direct electric-field effect, suggesting potential for CMOS-compatible superconducting transistors.

In contrast, other studies suggest that the observed modulation stems from a small leakage current flowing within the substrate [2,3], which can be as small as a few fA causing nonequilibrium phonons and/or electrons suppressing the supercurrent. A leakage current flowing through the substrate is typically undesirable for applications.

Here, instead, we show that the charge-trapping properties of the Al_2O_3 substrate can be harnessed to realize a non-volatile superconducting memory device based on the GCS effect [4]. We outline the device concept and operating principle and provide an outlook on future avenues for device optimization.
[1] De Simoni et al., Nat. Nanotechnol. 13, 802 (2018).
[2] Ritter et al., Nat. Electron. 5, 71 (2022).
[3] Basset et al., Phys. Rev. Research 3, 043169 (2021).
[4] Ruf et al., arXiv:2503.17241 (2025).

TT 29: Unconventional Superconductors

Time: Tuesday 9:30–12:45 Location: CHE/0091

TT 29.1 Tue 9:30 CHE/0091

Investigation of the field-dependent phase diagram of UTe_2 — •F. Husstedt[1,2], M. Kimata[3], S. Naduvile Thadathil[1,2], M. König[5], G. Lapertot[4], J.-P. Brison[4], G. Knebel[4], J. Wosnitza[1,2], and T. Helm[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL) and Würzburg-Dresden Cluster of Excellence ctd.qmat, HZDR, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Institute for Materials Research, Tohoku University, Japan — [4]Centre CEA de Grenoble, France — [5]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

While the general shape of the UTe_2 superconducting (SC) phase diagram is already known, there are still investigations ongoing regarding the details of the SC states. This includes, for example, the shape and nature of the high-field reentrant SC phase near the crystallographic *b* axis as well as multiple superconducting phases at lower fields. Especially interesting is the case for field applied parallel to the *b* axis. The phase diagram proposed by Rosuel *et al.* [1] contains two second-order phase transition lines meeting, which is thermodynamically forbidden [2]. This problem could be resolved by a fourth line emerging from this point. The first indication of such a line was proposed by Sakai *et al.* [3]. We performed transport studies on a microfabricated sample to get deeper insight in the phase diagram for both the *a* axis and *b* axis as well as the angle-dependent behavior of the emergent phases.

[1] Rosuel *et al.*, PRX **13**, 011022 (2023)
[2] Yip *et al.*, PRB **43**, 2742 (1991)
[3] Sakai *et al.*, PRL **130**, 196002 (2023)

TT 29.2 Tue 9:45 CHE/0091

Determining the superconducting order parameter of UPt_3 using scanning tunneling microscopy — •Rebecca Bisset[1], Luke C. Rhodes[1], Hugo Decitre[1], Matthew Neat[1], Ana Maldonado[1], Andrew Huxley[2], Carolina A. Marques[1], and Peter Wahl[1,3] — [1]SUPA, School of Physics and Astronomy, University of St Andrews, North Haugh, St Andrews, KY16 9SS, United Kingdom — [2]SUPA, School of Physics and Astronomy, University of Edinburgh, Kings Buildings, Edinburgh, EH9 3FD, United Kingdom — [3]Physikalisches Institut, Universität Bonn, Nussallee 12, 53115 Bonn, Germany

The hunt for spin-triplet superconductors has excited researchers for decades, with new candidates regularly being proposed as others are ruled out. This pairing of electrons into a Cooper pair state with total spin of one is allowed theoretically but has yet to be confirmed in a material. A system with these characteristics would have profound fundamental and technological implications. Here, we use ultra-low temperature scanning tunneling microscopy to measure the superconducting gap of UPt_3, which reveals a zero-bias Andreev bound state in the surface perpendicular to the *c*-axis. The superconducting origin of the gap is confirmed via observation of a vortex lattice, as well as by suppression of the gap above the expected critical field and temperature. For triplet pairing, such an Andreev state is fragile against Rashba spin-splitting, whereas for singlet pairing it remains robust, strongly suggesting that UPt_3 is a spin-singlet superconductor.

TT 29.3 Tue 10:00 CHE/0091

Study of tri-layer Bismuth-based Cuprates through ARPES measurement — •Elisa Auffray[1,2], Lenart Dudy[2], and Siham Benhabib[1] — [1]Laboratoire de Physique des Solides, CNRS, Orsay, France — [2]Synchrotron Soleil, CEA, CNRS, St Aubin, France

It is now well established that three-layer cuprates exhibit the highest critical temperature within each family, making them particularly interesting systems for studying superconductivity. Due to the presence of an underdoped inner CuO_2 plane, the magnetic environment is expected to differ from that of two-layer cuprates, a feature that has indeed been demonstrated by nuclear magnetic resonance measurements. This doping imbalance has also been revealed by ARPES measurements on the three-layer compound Bi2223. The bismuth-based three-layer cuprate is one of the most accessible in terms of synthesis and experimental investigation, and together with Hg1223 it belongs to the cuprates with the highest critical temperatures across the entire family. This makes it an excellent candidate for understanding three-layer physics, as highlighted by the number of recent publications devoted to it. Among these ARPES studies, only a few focus on the antinodal region where superconductivity truly emerges, so systematic comparisons between nodal and antinodal behavior are still lacking. In this presentation, we report our ARPES measurements on Bi2223. We present the momentum dependence of the 70 meV kink, which has previously been studied in the nodal region in superconducting state, as well as a comparison between the normal and superconducting phases.

TT 29.4 Tue 10:15 CHE/0091

Boundary critical temperature in unconventional superconductors and effects of impurities — •David Haink[1,2] and Benedikt Fauseweh[1,2] — [1]High-performance Computing, Institute of Software Technology, German Aerospace Center (DLR), 51147 Cologne, Germany — [2]Condensed Matter Theory, TU Dortmund University, Otto-Hahn-Straße 4, 44227 Dortmund, Germany

In BCS theory, s-wave superconductors have a higher critical temperature at their boundaries than in their bulk [PRB 101, 134512 (2020)]. We show that this boundary behavior does not hold for p-wave, but for d-wave superconductors and for coexisting phases. We further investigate the effects of randomly distributed impurities in the chemical potential on the critical temperature of the edge.

TT 29.5 Tue 10:30 CHE/0091

Weak competition between magnetism and superconductivity in the heavy-fermion compound $CeRh_2As_2$ — •Pavlo Khanenko[1,2], Javier F. Landaeta[2], Simon Ruet[2], Thomas Lühmann[2], Konstantin Semeniuk[2,3,6], Max Pelly[4], Andreas W. Rost[4], Grzegorz Chajewski[5], Dariusz Kaczorowski[5], Christoph Geibel[2], Seunghyun Khim[2], Elena Hassinger[3,6], and Manuel Brando[2] — [1]Helmholtz Zentrum Dresden Rossendorf, Germany — [2]MPI CPfS, Germany — [3]TUD, Germany — [4]University of St. Andrews, United Kingdom — [5]Institute of Low Temperature and Structure Research, Poland — [6]KIT Karlsruhe, Germany

The heavy-fermion superconductor $CeRh_2As_2$ shows superconductivity at T_c = 0.35 K, which is preceded by another phase (phase I) at T_0 = 0.54 K. Recent μSR studies detected an internal magnetic field within phase I and suggested its coexistence with superconductivity. When a magnetic field is applied parallel to the *c* axis of its tetragonal unit cell, a second superconducting (SC) phase is observed at $\mu_0 H^* \approx 4$ T. An earlier study has shown that phase I persists up to $\mu_0 H_0 \approx 6$ T, larger than H^*. However, the phase transition disappeared upon entering the SC dome, contradicting thermodynamic considerations. Here, we report magnetic field-dependent ac-susceptibility and magnetostriction measurements on high-quality single crystals. We observed clear evidence of the singularity at H_0 in fields up to 7 T and inside the SC dome. Analysis of the phase boundaries in terms of the Ginzburg-Landau theory of coupled order parameters shows a weak competition between phase I and superconductivity.

TT 29.6 Tue 10:45 CHE/0091

Entropy-rich superconductivity and unconventional vortex dynamics in $CeRh_2As_2$ — •Shuai Zhang, Xinyang Liu, Enke Liu, and Peijie Sun — Institute of Physics and Beijing National Laboratory for Condensed Matter Physics, Chinese Academy of Sciences, Beijing 100190, China

We investigate the multiple superconducting (SC) phases SC1 and SC2 of $CeRh_2As_2$ using high-resolution magnetocaloric-effect (MCE) measurements. Pronounced temperature hysteresis observed during quasiadiabatic field sweeps provides direct thermodynamic evidence that both the SC1-normal (NS) and SC2-NS transitions are first order. In contrast, a continuous yet asymmetric entropy evolution across the SC1-SC2 boundary reveals a change in the superconducting order parameter, consistent with a second-order transition. The observed temperature dips in field-sweep traces identify SC2 as a higher-entropy phase compared with SC1 and NS. Furthermore, the two-step resistive transitions and enhanced ΔT near the SC2-NS boundary highlight the unconventional and current-sensitive nature of SC2. These results establish a comprehensive thermodynamic phase diagram for $CeRh_2As_2$ and demonstrate that MCE is a powerful probe of entropy discontinuities and symmetry reconstruction in locally noncentrosymmetric superconductors.

TT 29.7 Tue 11:00 CHE/0091

Chiral topological superconductivity in hole-doped Sn/Si(111) — •Matthew Bunney[1,2], Lucca Marchetti[1], Domenico Di Sante[3], Carsten Honerkamp[2], and Stephan Rachel[1] — [1]School of Physics, University of Melbourne, Australia — [2]Institute for Theoretical Solid State Physics, RWTH Aachen University, Germany — [3]Department of Physics and Astronomy, University of Bologna, Italy

A third monolayer of tin atoms on the semiconductor substrate Si(111) has been shown to become superconducting upon six to ten percent hole doping. Experiments have reported promising results hinting at a superconducting chiral *d*-wave order parameter. Here we examine Sn/Si(111) by combining most recent ab initio results, quasi-particle interference calculations, state-of-the-art truncated-unity functional renormalization group simulations and Bogoliubov-de Gennes analysis. We show remarkable agreement between experimental and theoretical quasi-particle interference data both in the metallic and superconducting regimes. The interacting phase diagram reveals that the superconductivity is indeed chiral *d*-wave with Chern number $C = 4$. Surprisingly, magnetically ordered phases are absent, instead we find charge density wave order, as observed

in related compounds, as a competing phase. Our results substantiate further that Sn/Si(111) is a promising candidate material for chiral topological superconductivity.

15 min. break

TT 29.8 Tue 11:30 CHE/0091

Point-contact spectroscopy of atomic contacts from the non-centrosymmetric superconductor $Nb_{18}Re_{82}$ — •Tiark Tiwary, Elias Hadzic, Marcel Strohmeier, and Elke Scheer — University of Konstanz, 78457 Konstanz, Germany

Revealing various properties of unconventional superconductivity, the non-centrosymmetric superconductor $Nb_{18}Re_{82}$ (Nb-Re) has become of great interest in the recent years. A key feature is the absence of inversion symmetry which is causing a Rashba-type spin-orbit coupling. Theoretically, this lack of symmetry allows for an admixture of spin-singlet and spin-triplet states. While previous measurements [1] on point contacts with Nb-Re single crystals stated the existance of two distinct BCS-like superconducting energy gaps, measurements on Nb-Re thin films [2] are showing a single s-wave gap. To address these inconsistencies, we utilised the mechanically controlled break junction technique to characterise Nb-Re atomic contacts. We observe the typical features of Andreev refelctions for atomic contacts with high transmission as well as tunneling spectra for contacts with low transmission. As a result the two distinct gaps observed in [1] can be reproduced. While the temperature dependencies of both gaps follow an BCS-like behaviour, the magnetic field dependent measurements shows a non-BCS-like behaviour.

[1] Cirillo et al., Phys. Rev. B, **91**, 134508 (2015)
[2] Cirillo et al., Phys. Rev. B, **94**, 104512 (2016)

TT 29.9 Tue 11:45 CHE/0091

Unconventional superconductivity in monolayer transition metal dichalcogenides — •Subhojit Roy[1], Andreas Kreisel[2], Brian Andersen[3], and Shantanu Mukherjee[4] — [1]University of Regensburg, Regensburg, Germany — [2]Niels Bohr Institute, University of Copenhagen, Denmark — [3]Niels Bohr Institute, University of Copenhagen, Denmark — [4]Indian Institute of Technology Madras, Chennai, India

The observation of a Leggett mode, nodal superconducting gaps in STM measurements, unusually large in-plane upper critical fields far exceeding the Pauli limit, and a two-fold gap anisotropy in magnetoresistance experiments all point toward an unconventional pairing mechanism. Ab-initio calculations have further revealed a strongly anisotropic Eliashberg electron-phonon spectral function in monolayer $NbSe_2$, with a significant contribution arising from same-spin K-K′ scattering. In this work [1], we consider the interplay of electron-electron and electron-phonon interactions. Starting from the ab-initio phonon spectrum, we compute the effective phonon-mediated interaction and incorporate it into an RPA-based description of the screened Coulomb interaction. Our framework captures the full lattice structure, the multi-orbital character of the relevant d-band states, and phonon retardation effects within a unified microscopic model. Using this model, we address key magnetic-field-dependent phenomena in Ising superconductors, including the enhanced Pauli limit and the two-fold magnetoresistance anisotropy.

[1] S. Roy et al., arXiv:2509.03907 (2025).

TT 29.10 Tue 12:00 CHE/0091

Effects of YIG exchange field on TMDC superconductor $NbSe_2$ — •Alfredo Spuri[1], Marcin Faitsch[1], Christian Wiedemann[1], Wolfgang Belzig[1], Elke Scheer[1], and Angelo Di Bernardo[1,2] — [1]Universität Konstanz, Konstanz, Germany — [2]Università degli studi di Salerno, Fisciano, Italy

Yttrium iron garnet (YIG) [1] is a heavily investigated material for application in spintronic devices as a ferromagnet with high critical temperature (T_C ~ 560 °C), insulating properties due to a large bandgap of ~ 2.85 eV, and a strong local in-plane exchange field (H_{ex} ~ 10^2 T). Coupling YIG with a natural 2D Ising superconductor like $NbSe_2$, with a very high in-plane critical field (H_C ~ 40 T in the monolayer limit) [2], offers the possibility of novel unconventional superconducting states.

We have assembled YIG/$NbSe_2$ heterostructures and investigated their superconducting properties. $NbSe_2$ with a YIG flake on top reveals features in the T_C(B) curve that are not found on bare $NbSe_2$, We tentatively attribute the features in the heterostructures to scattering between two different energy bands in $NbSe_2$, enhanced by the strong exchange field of the YIG.

[1] R. Hartmann et al., APL Mater. 12, 031121 (2024).
[2] X. Xi et al., Nature Phys. 12, 139 (2016).

TT 29.11 Tue 12:15 CHE/0091

Effects of disorder on the superconducting properties of YFe_2Ge_2 — •Mads Hansen[1], Han Zong[1], Jiasheng Chen[1], Romian Grasset[2], Siham Benhabib[3], and Malte Grosche[1] — [1]University of Cambridge, Cambridge, United Kingdom — [2]Laboratoire des Solides Irradies, École Polytechnique, CNRS, Institut Polytechnique de Paris, Palaiseau, France — [3]Laboratoire de Physique des Solides, Orsay, France

YFe_2Ge_2 has been reported as an unconventional superconductor [1-3]. The non-Fermi liquid behavior observed in the normal state, as well as enhanced magnetic fluctuations [4,5] evidence the strongly correlated nature of the electron system. The pairing mechanism remains unknown, however, theoretical proposals hypothesize two different scenarios: an $s^{+/-}$ [6] or a triplet pairing wavefunction [7]. We have grown high quality crystals and induced point-like defects at various concentrations, using the electron irradiation facility SIRIUS. Here, we present a study on the effect of disorder on the Sommerfeld coefficient and the transport properties of YFe_2Ge_2 to address the outstanding question of the pairing mechanism.

[1] Y. Zou et al., Phys. Status Solidi RRL 8, 928 (2014)
[2] J. Chen et al., Phys. Rev. Lett. 116, 127001 (2016)
[3] J. Chen et al., Phys. Rev. Lett. 125, 237002 (2020)
[4] N. Sirica et al., Phys. Rev. B 91, 121102 (2015)
[5] H. Wo et al., Phys. Rev. Lett. 122, 217003 (2019)
[6] A. Subedi, Phys. Rev. 89, 024504 (2014)
[7] D. J. Singh, Phys. Rev. B 89, 024505 (2014)

TT 29.12 Tue 12:30 CHE/0091

Inverse proximity effect and unconventional superconductivity in the Pb/CrTe hybrid thin films — •Lichen Ji[1,2], Wei Chen[2], Xinyu Zhou[2], Xusheng Wang[2], Yi Hu[2], Xiaopeng Hu[2], Qinghua Zhang[3], Ding Zhang[2], Qi-kun Xue[2], and Shuai-Hua Ji[2] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden 01187, Germany — [2]State Key Laboratory of Low-Dimensional Quantum Physics, Department of Physics, Tsinghua University, Beijing 100084, China — [3]Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

Two-dimensional (2D) heterostructures provide an important platform for exploring unconventional quantum states. Here, we investigate molecular-beam-epitaxial 2D vertical superconductor (S)/ferromagnet (F) hybrids composed of superconducting Pb and ferromagnetic CrTe using in situ scanning tunneling microscopy and ex situ transport measurements. We observe an unconventional superconducting gap structure accompanied by a pronounced inverse proximity effect. Transport data further show strong suppression of both the critical temperature and upper critical field. Importantly, the critical temperature exhibits an oscillatory dependence on the CrTe thickness, and re-entrant superconductivity emerges within a finite magnetic-field window. These results offer new insights into the unconventional superconducting properties of Pb/CrTe hybrids, underscoring the crucial role of interfacial effect and inverse proximity effect.

TT 30: Caloric Effects in Ferromagnetic Materials (joint session MA/TT)

Time: Tuesday 9:30–11:30 Location: POT/0151

Invited Talk TT 30.1 Tue 9:30 POT/0151

Magnetic Cooling: From applications at room temperature to hydrogen liquefaction — •T. Gottschall[1], E. Bykov[1], M. Strassheim[1], T. Platte[2], C. Fujta[2], D. Benke[2], M. Fries[2], W. Liu[3], A. Döring[3], K. Skokov[3], O. Gutfleisch[3], and J. Wosnitza[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]MAGNOTHERM Solutions GmbH, Darmstadt, Germany — [3]Technical University of Darmstadt, Darmstadt, Germany

Magnetic cooling can be utilized to construct environmentally friendly cooling devices, air conditioners, and heat pumps. Recently, low temperatures became the focus of attention as an area of application for magnetocaloric cooling, namely for hydrogen liquefaction. The conventional liquefaction process uses up to 40 % of the lower heating value of the gas we are compressing, just to liquefy it! Magnetocaloric materials enable an alternative and more efficient approach. A large number of compounds are already known that show magnetocaloric effects in the desired temperature range and new candidates are constantly being added. In this work, we would like to discuss our current progress for the creation of a materials library for cryogenic applications. The basis for this is our characterization infrastructure for materials research at TU Darmstadt and the Dresden High Magnetic Field Laboratory in static and pulsed magnetic fields. Furthermore, we also provide an overview of the recent results in the demonstrator development of a magnetic hydrogen liquefier within the framework of the European project HyLICAL.

TT 30.2 Tue 10:00 POT/0151

Hydrogen tunned transition temperature of GdFeSi for magnetocaloric hydrogen liquefaction application — •Allan Döring[1], Wei Liu[1], Marc Strassheim[2], Tino Gottschall[2], Konstantin Skokov[1], and Oliver Gutfleisch[1] — [1]Institute of Materials Science, Functional Materials, Technical University of Darmstadt, Darmstadt, Germany — [2]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany

Hydrogen can play an important role in the future carbon-neutral society. Among several alternatives to store this energy carrier, the liquid H2 (LH2) stands out for its higher volume-to-energy ratio. However, the actual method of H2 liquefaction sums up to 34% of the costs of LH2. The magnetocaloric cooling could be one alternative to improve the efficiency of the process. Thus, it is essential to conduct research on materials exhibiting a strong magnetocaloric effect (MCE) within the temperature range of 20 K to 77 K. The peak of the MCE is at transition temperatures, such as the Curie temperature (TC). The magnetocaloric effect peak of GdFeSi is at 125 K. In this study, the TC of GdFeSi was shifted to lower temperatures by hydrogenation process, achieving a shift of over 90 K. By the anisotropic crystal expansion, GdFeSiH exhibited and higher magnetocaloric effect than the pristine alloy, not only by the isothermal entropy change, but also directly measured adiabatic temperature change. We acknowledge the HyLICAL project for the funding of this research through grant 101101461, and Deutsche Forschungsgemeinschaft (DFG) within the CRC/TRR 270 (Project-ID 405553726).

TT 30.3 Tue 10:15 POT/0151

First-principles investigation of chemical substitution and interstitial doping in La(Fe,Si)$_{13}$ — •Anita Yadav and Markus E. Gruner — University of Duisburg-Essen, 47057 Duisburg, Germany

La(Fe$_x$Si$_{1-x}$)$_{13}$ is a prominent magnetocaloric material, characterized by a sharp first-order phase transition and a large associated entropy change. Its behavior arises from an intricate coupling among the magnetic, electronic, and lattice degrees of freedom, which makes the material highly responsive to external factors and enables targeted tuning of its magnetocaloric response [1,2]. The operating range can be modified through substitution and interstitial loading, which can alter the local atomic environment and reshape the coupling between structural and magnetic subsystems. In this work, we employ first-principles calculations in the framework of density functional theory (DFT) to systematically screen the impact of chemical substitution and loading of light elements on interstitial sites with respect to structural stability, lattice expansion, magnetic interactions, and thermodynamic behavior. Furthermore, we explore the benefits of machine-learning force-fields based on our DFT results for an efficient modeling of the thermodynamic properties of La(Fe$_x$Si$_{1-x}$)$_{13}$-based compounds. Funding by the DFG via TRR270 (B06) is gratefully acknowledged.

[1] M. E. Gruner *et al.*, Phys. Rev. Lett. **114**, 057202 (2015)
[2] K. P. Skokov *et al.*, Appl. Phys. Rev. **10**, 031408 (2023)

TT 30.4 Tue 10:30 POT/0151

Magnetocaloric Laves phases based on light rare earths: Addressing Criticality — •M. Strassheim[1,2], L. Beyer[3,4], J. Wosnitza[1,2], and T. Gottschall[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Leibniz Institute for Solid State and Materials Research Dresden, Germany — [4]TU Bergakademie Freiberg, Germany

Laves-phase intermetallic compounds based on heavy rare-earth elements have long been recognized for their excellent magnetocaloric performance at low temperatures, making them promising candidates for cryogenic cooling applications. However, the reliance on heavy rare earths poses challenges in terms of cost, availability, and sustainability. In this work, we explore the magnetocaloric properties of the light rare-earth-based Laves phase $CeFe_2$. By the substitution of Al, its unstable ferromagnetism can be disturbed enough to establish an antiferromagnetic phase below 80 K. Using a combination of structural, magnetic, and direct adiabatic temperature change measurements at the Dresden High Field Laboratory, we investigate the potential of this antiferromagnetic state for its potential in magnetocaloric hydrogen liquefaction.

TT 30.5 Tue 10:45 POT/0151

Pressure effect on the magnetocaloric response of RCo$_2$ Laves Phases — •Catalina Salazar-Mejia[1], E. Bykov[1], W. Liu[2], K. Skokov[2], O. Gutfleisch[2], J. Wosnitza[1,3], and T. Gottschall[1] — [1]High Magnetic Field Laboratory (HLD-EMFL), Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]Institut für Materialwissenschaft, TU Darmstadt, Germany — [3]Institut für Festkörper- und Materialphysik, TU Dresden, Germany

Rare-earth Laves phases are potential candidates for magnetic refrigeration at cryogenic temperatures. They exhibit large magnetocaloric effects and their transition temperatures can be tuned through elemental substitutions. In this work, we investigate the effect of hydrostatic pressure on the magnetism and magnetocaloric effect of RCo$_2$ Laves phases with rare-earth elements R = Tb, Dy, Ho, and Er. In general, we observe that the Curie temperature, T_C, decreases with applied pressure in all alloys. T_C is most sensitive to pressure in TbCo$_2$, with $dT_C/dp \approx -22$ K/GPa, and this value decreases systematically along the series, reaching $dT_C/dp \approx -7.7$ K/GPa in ErCo$_2$. More interestingly, hydrostatic pressure has an almost negligible effect on the magnetocaloric response - specifically on the isothermal entropy change, ΔS_T, with the exception of HoCo$_2$, where ΔS_T increases by about 26% under an applied pressure of approximately 1 GPa and for a magnetic field change of 5 T.

TT 30.6 Tue 11:00 POT/0151

Manipulating Magnetocaloric Properties Through Magnetic Exchange at Mn$_{3-x}$GaC/Fe Interfaces — •Ivan Tarasov and Ulf Wiedwald — Faculty of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany

Magnetocaloric materials enable solid-state cooling by exploiting temperature changes under magnetic-field variation. Manganese-based antiperovskites (APVs, Mn_3AX) are promising materials due to their sharp, tunable first-order magnetostructural transition (FOMST). A key challenge is to control the working temperature window and enhance the magnetocaloric response within a given material system. Tailoring magnetic exchange interactions offers a new strategy.

Here, we investigate APV/Fe bilayers, focusing on interface-driven exchange effects. Uncoupled $Mn_2GaC_{1.1}$ films show a sharp FOMST at 189 K with a strong $\partial M/\partial T$ peak. A 5 nm Fe cap lowers the transition to 175 K, broadens hysteresis, and suppresses the $\partial M/\partial T$ peak above 1 T. The bare APV exhibits $\Delta S_m \approx 10$ J kg^{-1} K^{-1} at $B = 6$ T, whereas coupling reduces this to ~ 1 J kg^{-1} K^{-1} at $B = 5$ T. In multi-domain bilayers, $\partial M/\partial T$ increases by 15% (AFM–FM) and 46% (FM–PM) for a Fe film thickness of $t = 2.6$ nm, but disappears for $t = 21$ nm, accompanied by an anomaly near 50 K linked to interfacial AFM ordering.

Funding by the Deutsche Forschungsgemeinschaft (DFG) within CRC/TRR 270, project B02 (Project-ID 405553726) is gratefully acknowledged.

TT 30.7 Tue 11:15 POT/0151

Frustration and Antiferromagnetic Ordering in Low-Temperature Materials for Adiabatic Demagnetization — •Anton Jesche, Tim Treu, Marvin Klinger, Jorginho Villar Guerrero, and Philipp Gegenwart — EP VI, Institute of Physics, University of Augsburg, Germany

The development of improved materials for adiabatic demagnetization refrigeration (ADR) has been driven increasingly by research on magnetically frustrated systems, where competing interactions can suppress magnetic ordering to very low temperatures [1]. Such behavior is particularly attractive for low-temperature cooling and has led to several promising rare-earth-based compounds. Notable examples include $KBaYb(BO_3)_2$, which reaches temperatures near 20 mK [2], and $NaGdP_2O_7$, which demonstrates extended hold times below 2 K in standard cryogenic environments [3].

This contribution will highlight selected Yb- and Gd-based materials and discuss the influence of frustration and antiferromagnetic (AFM) ordering on their cooling performance. Using $NaGdP_2O_7$ as a representative case, we examine how magnetic entropy near AFM transitions affects ADR behavior under varying magnetic fields and temperatures. We further show that high-resolution thermodynamic information, such as heat capacity, can be extracted directly from ADR curves.

[1] M. E. Zhitomirsky, Phys. Rev. B, 2003, 67, 104421, [2] Y. Tokiwa, Commun. Mater. 2021, 2, 42, [3] P. Telang, Phys. Rev. B, 2025, 111, 064434

TT 31: Frustrated Magnets I (joint session MA/TT)

Time: Tuesday 9:30–12:30 Location: POT/0361

TT 31.1 Tue 9:30 POT/0361

Spontaneous symmetry breaking in the Heisenberg antiferromagnet on a triangular lattice — •Bastian Pradenas[1,2], Grigor Adamyan[1,3], and Oleg Tchernyshyov[1] — [1]William H. Miller III Department of Physics and Astronomy, Johns Hopkins University, Baltimore, USA — [2]Leibniz Institute for Solid State and Materials Research, IFW, Dresden, Germany — [3]Department of Physics, Massachusetts Institute of Technology, Cambridge, USA

We present a detailed investigation of an overlooked symmetry structure in non-collinear antiferromagnets that gives rise to an emergent quantum number for magnons. Focusing on the triangular-lattice Heisenberg antiferromagnet, we show that its spin order parameter transforms under an enlarged symmetry group, $SO(3)_L \times SO(2)_R$, rather than the conventional spin-rotation group SO(3). Although this larger symmetry is spontaneously broken by the ground state, a residual subgroup survives, leading to conserved Noether charges that,

upon quantization, endow magnons with an additional quantum number—*isospin*—beyond their energy and momentum. Our results provide a comprehensive framework for understanding symmetry, degeneracy, and quantum numbers in non-collinear magnetic systems, and bridge an unexpected connection between the paradigms of symmetry breaking in non-collinear antiferromagnets and chiral symmetry breaking in particle physics.

TT 31.2 Tue 9:45 POT/0361

Antiferro octupolar order in the $5d^1$ double perovskite Sr_2MgReO_6 and its spectroscopic signatures — •Dario Fiore Mosca[1] and Leonid Pourovskii[2,3] — [1]University of Vienna, Faculty of Physics and Center for Computational Materials Science, Vienna, Austria — [2]CPHT, CNRS, Ecole polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France — [3]College de France, Université PSL, 11 place Marcelin Berthelot, 75005 Paris, France

Hidden-order phases governed by high-rank multipolar order parameters have recently been identified in several cubic 5d double perovskites. Because experimental probes often couple weakly to high-rank moments, multipolar orders can remain elusive or be misinterpreted as lower-rank phases. A notable example is the $5d^1$ double perovskite Sr_2MgReO_6, originally proposed as a spin glass and later reclassified as a conventional dipolar antiferromagnet.

In this work, we show instead that Sr_2MgReO_6 hosts a hidden antiferroic order of magnetic octupoles. The dominant tetragonal crystal field isolates a doublet carrying octupolar degrees of freedom, while weak dipolar moments arise only through admixture of the excited j = 1/2 spin-orbit multiplet. This octupolar order produces characteristic quasigapless magnetic excitations and superstructural neutron-diffraction intensities that peak at large scattering momenta.

This results highlights the tunability of multipolar interactions in spin-orbit entangled materials and places Sr_2MgReO_6 with unconventional octupolar phases.

TT 31.3 Tue 10:00 POT/0361

Field-dependent CEF excitations in Ce_2Bi — •Nikolai Pavlovskii[1], Alexander Sukhanov[2], Anton Kulbakov[1], Michael Smidman[3], Federico Mazza[4], Darren Peets[1], Kaushick Parui[1], Ross Stewart[5], Ross Piltz[6], and Dmytro Inosov[1] — [1]TU Dresden, Germany — [2]University of Augsburg, Germany — [3]Zhejiang University, China — [4]TU Vienna, Austria — [5]ISIS, UK — [6]ANSTO, Australia

Ce_2Bi is a cerium-based intermetallic compound where crystal-field (CEF) splitting and anisotropic magnetic interactions occur on comparable energy scales. To identify the relevant low-energy degrees of freedom, we investigate the field dependence of CEF-related excitations in single-crystalline Ce_2Bi using neutron-scattering techniques. Single-crystal diffraction establishes the crystallographic symmetry at the Ce site, providing the structural framework required for interpreting the magnetic excitations. The excitation spectrum shows a clear magnetic mode within the $J = 5/2$ manifold whose energy and intensity vary strongly with applied field. Crucially, the mode displays clear dispersion, demonstrating the presence of exchange interactions; as a result, what was previously interpreted as a localized CEF level is revealed to be a dispersive magnetic exciton. The field-induced evolution of this exciton constrains the mixing within the CEF manifold and the anisotropy of the ground-state Kramers doublet.

TT 31.4 Tue 10:15 POT/0361

High-field magnetic excitations in a kagome antiferromagnet — •Yoshihiko Ihara[1], Dmytro Inosov[2], Darren Peets[2], Moyu Kato[1], and Hiroyuki Yoshida[1] — [1]Hokkaido University, Sapporo, Japan — [2]TU Dresden, Dresden, Germany

Magnetic ground states in kagome antiferromagnets have been intensively studied to reveal the quantum mechanically disordered magnetic states. By applying high magnetic fields, further intriguing phenomena have been introduced such as the plateau in magnetization curve at the 1/9 of the full saturation value in $YCu_3(OH)_{6.5}Br_{2.5}$. [S. Jeon et al., Nat. Phys. **20**, 435 (2024), S. Suetsugu et al., PRL **132**, 226701 (2024), G. Zheng et al., PNAS **122**, e2421390112 (2025)]. Although higher magnetic fields induce another magnetization plateau at the 1/3 of the full saturation, the field strength required to access the 1/3 plateau is more than 50 T and is too large to perform most of the microscopic experiments. Thus, we focus on another Cu-based mineral $InCu_3(OH)_6Cl_3$, which shows the 1/3 plateau around 10 T due to smaller energy scale of exchange interactions [M. Kato et al., Commun. Phys. **7**, 424 (2024)]. This allows us to perform NMR experiments in the entire field range reaching the full saturation. The measured nuclear spin-lattice relaxation rate demonstrates that the magnetic excitations are gapped in the 1/3 plateau state and the gap size increases with fields [M. Kato et al., JPSJ **94**, 083704 (2025)]. We will also discuss the magnetic excitations above the 1/3 plateau based on the results obtained in the high-field magnet in Tohoku Univ.

TT 31.5 Tue 10:30 POT/0361

Evidence for a Near-Ideal Jeff = 1/2 Ground State in Triangular-Lattice Na2BaCo(PO4)2 — •Miguel M. F. Carvalho[1,2], Sheng H. Chen[1], Yu C. Ku[3,4], Anagha Jose[5], Ryan Morrow[5], Chang Y. Kuo[3,4], Chun F. Chang[1], Zhiwei Hu[1], Maurits W. Haverkort[6], and Liu H. Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids,Dresden — [2]Institute of Physics II, University of Cologne — [3]Department of Electrophysics, National Yang Ming Chiao Tung University, Hsinchu, Taiwan — [4]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [5]Institut fuer Festkoerperphysik, Leibniz IFW, Dresden — [6]Institute for theoretical physics, Heidelberg University

We investigated the local Co 3d electronic structure of Na2BaCo(PO4)2 using polarization-dependent X-ray absorption spectroscopy (XAS) together with full multiplet cluster calculations. To obtain reliable spectra from this strongly insulating material, we employed the line-fitting inverse partial fluorescence yield (IPFY) method. Our combined experimental and theoretical analysis shows that the CoO6 octahedra exhibit only a very small effective trigonal distortion of about 11 meV, placing the system close to the ideal conditions for a Jeff = 1/2 ground state. Using our cluster model, we are also able to simulate the magnetic susceptibility along different crystallographic directions, . Overall, these results establish Na2BaCo(PO4)2 as a promising platform for investigating exotic magnetic behavior linked to Jeff = 1/2 states on triangular lattices.

TT 31.6 Tue 10:45 POT/0361

Dimensional reduction and fractionalized magnetization plateaus in the scalene-distorted triangular-lattice magnet kobyashevite — •Kaushick Parui[1], Anton Kulbakov[1], Roman Gumeniuk[2], Maria Teresa Fernandez-Diaz[3], Sergey Granovsky[1], Sergei Zvyagin[4], Dmytro Inosov[1], and Darren Peets[1,5] — [1]TU Dresden, Germany — [2]TU Bergakademie Freiberg, Germany — [3]ILL, France — [4]HZDR, Germany — [5]ct.qmat, TU Dresden, Germany

Quantum magnetism intertwined with lattice distortion can give rise to exotic ground states, yet studies on scalene-distorted triangular-lattice antiferromagnets remain scarce. Here, we report the crystal and magnetic structures, as well as magnetic and thermodynamic properties, of kobyashevite, $Cu_5(SO_4)_2(OH)_6{\cdot}4H_2O$. This compound hosts a scalene-distorted triangular lattice and exhibits antiferromagnetic order at 4 K, with a possible second transition at 0.64 K. High-field magnetization and specific-heat measurements reveal a cascade of field-induced states, manifested as magnetization plateaus, suggestive of a rich magnetic phase diagram. Neutron diffraction uncovers a dimensionally-reduced commensurate magnetic structure with propagation vector $\mathbf{k} = (0\,0\,\frac{1}{2})$, consisting of coupled alternating ferromagnetic and antiferromagnetic spin chains, while the Cu4 spins remain idle at 1.5 K. Collectively, these results establish kobyashevite as a promising platform for exploring the interplay of frustration, distortion, and dimensional reduction in quantum magnets.

15 min break

TT 31.7 Tue 11:15 POT/0361

Atomically sharp magnetic solitons for racetrack memory at the spatial limit — K Allen[1], K Du[2], J Bouaziz[3], S Mishra[1], G Bihlmayer[3], Y Zhang[1], Y Hao[4], V Ukleev[5], C Luo[5], F Radu[5], Y Gao[1], Ch Lane[6], J-X Zhu[6], M Yi[1], H Cao[4], S-W Cheong[2], •Stefan Blügel[3], and Emilia Morosan[1] — [1]Dept. of Physics and Astronomy & Rice Center for Quantum Materials, Rice University, Houston, 77005, TX, USA — [2]Dept. of Physics and Astronomy, Rutgers University, Piscataway, 08854, NJ, USA — [3]Peter-Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany — [4]Neutron Scattering Division, Oak Ridge Natl Lab, Oak Ridge, 37831, TN, USA — [5]Helmholtz-Zentrum Berlin, 14109 Berlin, Germany — [6]Theoretical Division, Los Alamos Nat. Lab., Los Alamos, 87545, NM, USA

We discuss the physics of a metallic square-net lattice rare-earth compound that exhibits RKKY interactions leading to magnetic frustration whose effective exchange interactions competes with the uniaxial anisotropy resulting in a rare ferrimagnetic up-up-down phase. Applying magnetic fields, atomically sharp solitons can be precipitated that have all the foundational credentials for a racetrack memory at the spatial limit. We present DFT calculations relating the RKKY interaction and the magnetic anisotropy to the electronic structure. We performed atomistic spin-dynamics calculations relating the interaction parameters to the soliton formation. A combination of experiments will be presented that provide evidence of the 1D magnetic solitons.

TT 31.8 Tue 11:30 POT/0361

Guest*Controlled Quantum Magnetism in a Flexible Metal-Organic Framework — •Fang Liu[1], Armin Schulz[2], Axel Lubk[4], Alexej Pashkin[3], Sergej Granovski[1], Shuhan Wang[1], Weinel Kristina[4], Herzog Max[4], and Stefan Kaiser[1] — [1]Institute of Solid State and Materials Physic, Dresden University of Technology — [2]Max Planck Institute for Solid State Research, Stuttgart — [3]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [4]Leibniz Institute for Solid State and Materials Research, Dresden

Metal-organic frameworks provide an unusual setting where magnetic frustration and structural flexibility coexist. In our system, two distinct states emerge: a guest-stabilized regime with signatures of a potential quantum spin liquid, and a guest-free state exhibiting weak magnetic ordering. Raman and infrared spectroscopy reveal pronounced differences in lattice modes between these phases. Complementary Raman and THz measurements further uncover contrasting magnetic backgrounds. These findings establish a guest-controlled route to tuning magnetic quantum states in MOFs.

TT 31.9 Tue 11:45 POT/0361

Investigation of spin-correlated phases in quasi two-dimensional layered honeycomb oxide — •Aprajita Joshi[1], Anjali Kumari[2,3], Shalini Badola[1], Anup Kumar Bera[2,3], and Surajit Saha[1] — [1]Indian Institute of Science Education and Research Bhopal, 462066, India — [2]Bhabha Atomic Research Centre, Mumbai 400085, India — [3]Homi Bhabha National Institute, Mumbai 400094, India

Honeycomb oxides are an intriguing class of materials characterised by low dimensionality and strong magnetic frustration, which leads to exotic quantum spin correlations. Here, we investigated a quasi-two-dimensional magnetic oxide Na2Co2TeO6, which exhibits several intriguing magnetic phases, including the zigzag antiferromagnetic interaction and Kitaev paramagnetic spin interactions. We explored the intricate relationship between these phases and phonons using temperature-dependent Raman measurements. Our findings reveal the signature of magnetoelastic coupling across the long-range and short-range magnetic ordering temperatures. Furthermore, Na2Co2TeO6, which has a noncentrosymmetric crystal structure, showcases ferroelectric order below 80 K. The evolution of Raman spectra reveals the presence of a ferroelectric order coupled phonon mode in Na2Co2TeO6 below this temperature.

TT 31.10 Tue 12:00 POT/0361

Characterizing entanglement at finite temperature: how does a paramagnet become a quantum spin liquid? — Snigdh Sabharwal[1,2], •Matthias Gohlke[1], Paul Skrzypczyk[2], and Nic Shannon[1] — [1]Okinawa Institute of Science and Technology, Onna, Japan — [2]H. H. Wills Physics Lab., University of Bristol, Bristol, UK

Quantum spin liquids (QSL) are generically many body entangled states of matter that form when quantum fluctuations meet the extensive ground state degeneracy of a classical spin liquid. Entanglement properties have enabled to characterise gapped QSL at zero temperature, however, much less is known about how quantum many body entanglement evolves at finite temperature.

Here, we use entanglement depth and genuine multipartite entanglement (GME) to study how entanglement and its local structure emerge when cooling a frustrated magnet from the high-temperature paramagnet down to the low-temperature QSL state. Within a case study on the Kitaev Honeycomb model, we obtain two characteristic bounds: (1) a lower bound on the upper temperature below which separability breaks and quantum entanglement must be present, while (2) a lower temperature scale is obtained when GME on plaquettes becomes finite signifying the coherent, structured entanglement that is characteristic for QSL ground states [1], i.e. the flux free state of the Kitaev spin liquid. We provide a framework to discuss the relevant temperature scales for QSL in frustrated magnets [2].

[1] L. Lyu, D. Chandorkar, et al., arXiv:2505.18124
[2] S. Sabharwal, M. Gohlke, et al., arXiv:2511.15144

TT 31.11 Tue 12:15 POT/0361

Fate of the Triangular Dirac spin liquid under an external magnetic field — •Sasank Budaraju[1,2], Josef Willsher[3], Federico Becca[4], Johannes Knolle[1,2], and Frank Pollmann[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany — [3]Max-Planck-Institut fur Physik komplexer Systeme, 01187 Dresden, Germany — [4]Dipartimento di Fisica, Universita di Trieste, Strada Costiera 11, I-34151 Trieste, Italy

We investigate the J1-J2 Heisenberg model under an external Zeeman field using the Variational Monte Carlo approach. Simple variational ansatzes are proposed for several candidate ordered states, and their energetics are compared on large clusters to obtain the phase diagram for small/moderate fields. For small J2, we capture a continuous transition from the Y to the "Up-Up-Down" (UUD) states as predicted by spin-wave theory. Additionally, around the highly frustrated region, we demonstrate that the ground state in the presence of a small field is a condensate of monopoles, which are gapless gauge excitations of the U (1) spin liquid. The monopole condensate is shown to be the ground state for a significant region of phase diagram, which we estimate using finite size numerics. Our results imply that the Dirac spin liquid is unstable to a condensation of monopoles in the presence of external fields.

TT 32: Nanomechanical systems (joint session HL/TT)

Time: Tuesday 10:00–12:45 Location: POT/0051

TT 32.1 Tue 10:00 POT/0051

Mechanical characterization of freely-suspended crystalline YIG nanodevices — •Jonny Qiu[1,2], Matthias Grammer[4,5], Sebastian Sailler[6], Sebastian T. B. Goennenwein[6], Michaela Lammel[6], Hans Huebl[3,4,5], and Eva Weig[1,2,3] — [1]TUM School of Computation, Information and Technology, Garching, Germany — [2]Zentrum für Quantum Engineering, Garching, Germany — [3]Munich Center for Quantum Science and Technology, Munich, Germany — [4]TUM School of Natural Sciences, Garching, Germany — [5]Walther-Meißner-Institut, BAdW, Garching, Germany — [6]University of Konstanz, Department of Physics, Konstanz, Germany

Efficient quantum transduction, the reciprocal conversion of quantum signals from one energy level to another, is an ongoing challenge in quantum network applications. Engelhardt et al. [1] proposed a microwave to optical converter (MWOC) that co-localizes microwave, magnetic and elastic excitations within a suspended optomechanical crystal (OMC) made of crystalline yttrium iron garnet (YIG).

In this talk, we report our progress towards realizing the MWOC and present freely-suspended YIG nanodevices. We fabricated YIG cantilevers and beams using an electron beam lithography process and a subsequent crystallization by annealing approach. Piezo-driven interferometric spectroscopy reveals the mechanical response modes of these devices, from which we extract Young's modulus and internal stress to design the OMC as a MWOC. We visualize and thus confirm the corresponding mode shapes via laser doppler vibrometry.

[1] F. Engelhardt, et al., Phys. Rev. Appl. 18, 044059 (2022).

TT 32.2 Tue 10:15 POT/0051

Sensing local temperature changes of a silicon nitride nanomembrane under large-amplitude vibration — •Valentin Barth, Mengqi Fu, and Elke Scheer — University of Konstanz, Konstanz, Germany

In MEMS and NEMS, changes in environmental conditions (e.g., a global change in temperature [1]) can alter the motion properties of silicon nitride (SiN) membranes. Vibrational motion may cause the membrane to experience local heating effects.

SiN square membranes (side length: 450 μm, thickness: 500 nm) are used and driven with a piezoelectric actuator. The motion is monitored using digital holographic microscopy. The measurements are carried out with a strong drive, resulting in vibration amplitudes on the order of hundreds of nanometers. Local temperatures are measured via the Seebeck effect using permalloy ($Ni_{81}Fe_{19}$) and gold as thermocouple, which provides a sensitivity of 20 μV/K and is suitable for micrometer-scale measurements [2]. To improve the signal-to-noise ratio and suppress unwanted contributions, the measurement is performed with a lock-in amplifier, where the temperature signal is demodulated at twice the drive frequency. The measured temperature depends on both the position of the thermometer and the vibration amplitude, with values reaching up to 0.5 mK. Besides the temperature signal of the membrane, signals caused by vibrations from neighboring membranes (distanced 1.5 mm) are also detected.

[1] F. Yang et al., Sens. Actuators A Phys. 354, 114307 (2023).
[2] F. L. Bakker et al., J. Appl. Phys. 111, 084509, (2012)

TT 32.3 Tue 10:30 POT/0051

FEBID and FIBID nanowire field emitters integrated with microcantilevers - fabrication and characterization — •Ewelina Gacka[1,2], Gregor Hlawacek[1], Krzysztof Kwoka[2], Tomasz Piasecki[2], Bartosz Pruchnik[2], René Hübner[1], and Teodor Gotszalk[2] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328, Dresden, Germany — [2]Department of Nanometrology, Wroclaw University of Science and Technology, 50-370, Wroclaw, Poland

Because micro- and nanomechanical systems are continuously evolving, there is a need to leverage various fabrication technologies. A scanning electron microscope with a gallium focused ion beam, as well as a helium ion microscope, were used to integrate platinum-carbon (Pt-C) and tungsten-carbon (W-C) nanowire field emitters with microcantilevers, serving as deflection sensors. Pt-C and W-C nanocomponents were fabricated using an additive, direct-writing method - focused-electron-/ion-beam-induced deposition (FEBID/FIBID)[1,2]. After growth calibration, the field emission behavior was studied in situ inside a vacuum chamber. The deposited Pt-C and W-C materials were characterized using Kelvin probe force microscopy and transmission electron microscopy. [1] T. Piasecki et al., Nanotechnology 35 (2024), doi: 10.1088/1361-6528/ad13c0. [2] E. Gacka et al., Measurement 234 (2024), doi: 10.1016/j.measurement.2024.114815.

TT 32.4 Tue 10:45 POT/0051

Optimization of Faraday Cage Angled Etching and Its Application Prospects in Silicon Carbide — •Wuzheng Ge[1,2], Ciaran Fowley[1], Jens Zscharschuch[1], Claudia Neisser[1], Artur Erbe[1,2], Philipp Bredol[3], Felix David[3], and Eva Weig[3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany — [2]Dresden University of Technology, Faculty of Electrical and Computer Engineering, 01069 Dresden, Germany — [3]Technical University of Munich, Chair of Nano and Quantum Sensors, 85748 Munich, Germany

This work presents the optimization of a Faraday Cage Angled Etching (FCAE) approach for ICP-RIE. By reshaping the plasma potential through the cage's mesh geometry, FCAE steers ions along the cage-wall normal, enabling controllable ion incidence angles. Reproducible 3D triangular cross-section structures were demonstrated on silicon, confirming the effectiveness of ion-direction tuning. The results were also applied to silicon carbide nanomechanical resonators. The enhanced directional ion flux enables direct fabrication of free-standing, stress-free structures in bulk, undoped SiC. This capability offers new pathways for advanced SiC-based MEMS.

15 min. break

TT 32.5 Tue 11:15 POT/0051

Probing Mechanical Nonlinearities with Quantum Dots — •Noah Spitzner, Jona Richter, Emeline Denise Sophie Nysten, Matthias Weiss, and Hubert Krenner — Universität Münster, Münster, Germany

The coupling of quantum dots to mechanical resonances is a well-established approach to investigate the behaviour of mechanical resonators and crystals. Within that approach, the quantum dots (QDs) act as point-like sensors sensitive to dynamical changes to their lattice constant. Vibrations in the host structure modulate the emission energy of the quantum dot, enabling readout of mechanical modes via ultrafast optical detectors. In our hybrid structures, mechanical excitation is achieved by integrating the QD-membrane onto a lithium niobate substrate equipped with finger-like electrodes called interdigitated transducers (IDTs). Applying a radio-frequency (RF) signal to the IDTs generates surface acoustic waves, which propagate on the surface of the substrate, coupling to quantum dots in their path.

This hybrid platform was taken a step further by structuring the QD-membrane into rings hosting mechanical resonances. Frequency sweeps of the RF signal applied to the IDT revealed sharp resonances in the emission-energy modulation exclusively for the quantum dots located within the rings. Interestingly, the resonances appear over a large region of SAW frequencies from 200 MHz to 900 MHz. Moreover, we detect clear signatures of a nonlinear mechanical response e.g. asymmetric lineshapes in the time-modulated optical signal of the QD when the external drive by the IDT is increased.

TT 32.6 Tue 11:30 POT/0051

Dry processing of 3C-silicon carbide nanostring resonators — •Felix David[1,2,3], Yannick Klass[1], Philipp Bredol[1,2,3], and Eva Weig[1,2,3] — [1]Technische Universität München, School of Computation, Information and Technology, Garching, Germany — [2]Technische Universität München, Zentrum für QuantumEngineering (ZQE), Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), München, Germany

We fabricate string resonators from strongly stressed 3C-silicon carbide (SiC) grown on a silicon substrate. In conventional fabrication processes, electron-beam lithography with PMMA is employed to define a metallic hard mask for the subsequent dry etching step via a liftoff process. This requires some wet-chemical process steps, such as HF etching and metal removal, which can destroy samples. Here, we describe an alternative process that avoids all wet-chemical process steps, enabling superior quality. It involves the use of a negative electron-beam resist as an etch mask, as well as the completely reactive-ion etching-based release of the nanostrings. The dry-processed nanostrings can be fabricated with a high yield and exhibit high mechanical quality factors at room temperature. Due to its high reliability, combined with high process speed, it also allows for quick adaptation to new projects, such as multilayer and hybrid mechanical systems.

TT 32.7 Tue 11:45 POT/0051

The best of two worlds: hexagonal boron nitride exfoliated on stressed silicon carbide string resonators — •Philipp Bredol[1], Felix David[1], Junhui Wu[2], Andrey N. Anisimov[2], Takashi Taniguchi[3], Kenji Watanabe[3], Georgy V. Astakhov[2], Artur Erbe[2], and Eva M. Weig[1] — [1]TU Munich, Chair of Nano and Quantum Sensors, 85748 Munich, Germany — [2]HZDR, Institute of Ion Beam Physics and Materials Research, 01328 Dresden, Germany — [3]National Institute for Materials Science, 1-1 Namiki, Tsukuba 305-0044, Japan

The boron vacancy (VB) of hexagonal boron nitride (h-BN) is a promising single photon emitter for applications in quantum technologies. Nanomechanical control of the VB would greatly enhance its versatility in such applications, therefore nanomechanical h-BN resonators are of great interest. Here we demonstrate that h-BN can be exfoliated on a chip with a pre-stressed silicon carbide thin-film and subsequently patterned into nanomechanical string resonators with high tensile stress. The resulting h-BN covered string resonators have high mechanical quality factors due to dissipation dilution and show the optically detected magnetic resonance signature of the VB of h-BN. Our fabrication approach allows to decouple the choice of the defect hosting 2D-material from the engineering of the mechanical mode and paves the way to nanomechanical control of single photon emitters in h-BN and other 2D materials.

TT 32.8 Tue 12:00 POT/0051

Cavity optomechanics with van der Waals materials — •Aloysius Farrel[1,3], Lukas Schleicher[1,3], Irene Sánchez Arribas[1,3], Leonard Geilen[2,3], Alexander Musta[2,3], Alexander Holleitner[2,3], and Eva Weig[1,3] — [1]Chair of Nano and Quantum Sensors, TU Munich, Germany — [2]Walter Schottky Institute, TU Munich, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Munich, Germany

Freely suspended two-dimensional materials are promising platforms for hybrid quantum systems that combine mechanical, optical, and electronic properties. Coupling the optical and mechanical modes of the resonators would be the first step towards such hybrid quantum system.

Here, we present studies of the mechanical resonators with van der Waals materials, such as hBN, on a SiN membrane. We map the spatial mechanical modes of the freestanding and supported 2D materials. Furthermore, we observe an optical nonlinearity in our high-finesse fiber optic cavity setup, which could couple to the mechanical modes. This result helps us understand the optomechanical coupling of the system and leads the way for a hybrid quantum device by incorporating quantum emitters in the system.

TT 32.9 Tue 12:15 POT/0051

Imaging GHz surface acoustic waves in epitaxial graphene cavities — •Mingyun Yuan[1], Alberto Hernández-Mínguez[1], Yi-Ting Liou[2], Jens Herfort[1], Joao M. J. Lopes[1], and Paulo V. Santos[1] — [1]Paul-Drude-Institut, Leibniz Institut im Forschungsverbund e.V., Berlin, Germany — [2]Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany

The imaging of sound has fascinated scientists and the public alike, dating back to Chladni's demonstrations in the 19th century. Nowadays, it is possible to image mechanical vibrations at the nanoscale, enabling direct probing of propagation, scattering and diffraction for high-frequency acoustic waves with short wavelengths. Here, we present the imaging of GHz surface acoustic waves (SAWs) in an epitaxial monolayer graphene nanostructure, based on thermal decomposition of SiC, using atomic-force microscopy (AFM). We observe a near-perfect strain transfer that gives rise to rich acoustic patterns in the phononic cavity formed by the graphene nanostructure. Furthermore, the enhanced acoustic intensity in the graphene region indicates a waveguiding effect, with graphene serving as an atomically thin, embedded shorting layer. Within the cavity, signatures of quantum chaos are observed. The high spatial resolution of AFM enables the investigation of SAW strain transferred onto 2D materials with high precision. The results also demonstrate an epitaxial nanophononic platform for both functional acoustic devices and fundamental studies of quantum phenomena.

TT 32.10 Tue 12:30 POT/0051

Nonlinear vibrational dynamics locally probed by time-resolved electron diffraction — •Kai Nettersheim[1], Alexander Schröder[1], and Sascha Schäfer[1,2] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Regensburg Center for Ultrafast Nanoscopy (RUN), Regensburg, Germany

Nonlinear dynamics of micro- and nanoscale electro-mechanical systems can be observed using electrical or optical methods. However, these approaches are often limited in their spatial resolution, which leaves the underlying mechanics only partially accessible. Recent advances in ultrafast electron microscopy (UTEM) enable the highly localized probing of nanoscale oscillators, allowing to retrieve detailed information about their atomic structure and material defects.

Utilizing stroboscopic UTEM imaging techniques, we present the characterization of nonlinear mode dynamics in free-standing silicon membranes employing an event-based electron detector with nanosecond temporal resolution [1]. The high-Q resonator is excited using an optical pulse train driving the sample into the nonlinear regime. Due to the use of event-based converged electron beam diffraction (CBED), phase-accurate measurements of the nanoscale structural motion are provided. Whereas at weak driving, the oscillator displays a simple Duffing-type bistability, higher harmonic overtones as well as period doubling dynamics emerge at higher driving amplitudes.

[1] A. Schröder et al., Ultramicroscopy 256, 113881 (2024)

TT 33: Correlated Magnetism – Dynamics and Spectroscopy

Time: Tuesday 11:00–12:30 Location: HSZ/0105

TT 33.1 Tue 11:00 HSZ/0105

Nonlinear spectroscopy of spiral magnets — •Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, D-38106 Braunschweig, Germany

Spin systems with noncollinear long range order (NCLRO) allow for light-matter coupling via effective dipole moments which stem from the inverse Dzyaloshinskii-Moriya interaction. This permits to explore spin excitations of quantum magnets using time-dependent electric fields, which is of particular interest in the nonlinear regime, where second harmonic generation and two-dimensional spectroscopy may provide insight into the dynamics beyond linear probes. Here, we present results for such nonlinear response functions, using spin-wave theory and considering quasi two-dimensional magnets with NCLRO arising from frustration.

TT 33.2 Tue 11:15 HSZ/0105

Third-Order Nonlinear Response in Frustrated Magnets: Efficient Calculation in the Frequency Domain — •Marius Möller, Roser Valentí, and David A.S. Kaib — Institut für Theoretische Physik, Goethe-Universität Frankfurt, Max-von-Laue-Strasse 1, 60438 Frankfurt am Main, Germany

Techniques measuring higher-order response functions, such as two-dimensional coherent spectroscopy (2DCS) were proposed as powerful tools to provide deeper insights into the excitations of a system. However, calculating nonlinear response functions can be computationally intensive. Recently, we proposed an efficient Lanczos-based approach to calculate the second order susceptibility $\chi^2(\omega_t, \omega_\tau)$ [1]. Here, we present different approaches and approximations to compute the more commonly probed third-order susceptibilities $\chi^3(\omega_t, \omega_\tau)$ directly in the frequency domain. We compare them in terms of convergence, numerical stability and computational cost. Finally, we apply these techniques to frustrated magnets.

M.M., D.K. and R.V. gratefully acknowledge funding by the DFG (German Research Foundation): TRR 288-422213477.

[1] D.A.S. Kaib, M. Möller, R. Valentí, arXiv:2502.01746 (2025.

TT 33.3 Tue 11:30 HSZ/0105

Terahertz Time-Domain Spectroscopy of Coupled Spin and Low-Energy Excitations in $CeCoGe_3$ — •Debankit Priyadarshi[1], Zekai Chen[1], Erik W. de Vos[1], Geetha Balakrishnan[2], and Manfred Fiebig[1] — [1]ETH Zurich, Switzerland — [2]University of Warwick, United Kingdom

We present a direct observation of the interaction between a low-frequency excitation and a spin-wave resonance [1] in the intermetallic heavy-fermion compound $CeCoGe_3$ using terahertz time-domain spectroscopy. $CeCoGe_3$ exhibits three low-temperature magnetic transitions at 21 K, 12 K and 8 K [2]. In addition to the observation of a magnon mode below the Nèel temperature at 1.04 THz, we find a temperature-independent low-frequency excitation at 0.4 THz. The absorption intensities of the low-frequency mode and the magnon mode suggest an inverse coupling effect which becomes strongest below the second magnetic transition at 12 K. This hints at strong magnon-phonon coupling emerging at low-temperatures. These results can therefore shed light on how lattice vibrations influence heavy-fermion magnetism. Additionally, optical-pump THz-probe measurements are performed to investigate the role of electronic excitations in order to understand the cross-talk between these three different fundamental degrees of freedom in inter-metallic systems.

[1] M. Smidman et al., *PRB* 88, 134416 (2013).
[2] A. Thamizhavel et al., *J. Phys. Soc. Jpn.* 74, 1858 (2005).

TT 33.4 Tue 11:45 HSZ/0105

Exploring the Nonlinear Magnetic Response of FeI_2 via Two-Dimensional Coherent Spectroscopy — •Sagar Ramchandani[1], Yoshito Watanabe[1], Simon Trebst[1], and Ciarán Hickey[2] — [1]Institute for Theoretical Physics, University of Cologne, Cologne, Germany — [2]School of Physics, University College Dublin, Belfield, Dublin 4, Ireland

Nonlinear THz spectroscopy has emerged as a powerful method to extract new information beyond conventional linear response. In this work, we employ a semi-classical approach to 2-dimensional coherent spectroscopy (2DCS), implemented in the context of the Sunny Julia package for modelling atomic-scale magnetism. We apply this framework to explore the nonlinear response of FeI_2, a 2D spin-1 antiferromagnet with hybridized dipolar-quadrupolar fluctuations, to reveal its rich nonlinear dynamics.

TT 33.5 Tue 12:00 HSZ/0105

Measuring Anyonic Exchange Phases Using Two-Dimensional Coherent Spectroscopy — •Nico Kirchner[1], Wonjune Choi[2], and Frank Pollmann[1] — [1]Technical University of Munich, TUM School of Natural Sciences — [2]Theoretical Division, T-4 and Center for Nonlinear Studies, Los Alamos National Laboratory

Identifying experimental signatures of anyons, which exhibit fractional exchange statistics, remains a central challenge in the study of two-dimensional topologically ordered systems. Previous theoretical work has shown that the threshold behavior in linear response spectroscopy can reveal the fractional exchange statistics between an anyon and its antiparticle. In this work, we extend this framework to nonlinear, two-dimensional coherent spectroscopy. We demonstrate by analyzing time-ordered four-point correlation functions that the threshold behavior of nonlinear response functions encodes the fractional statistics between general pairs of anyons that can combine to any composite topological charge. This feature in particular provides a powerful probe for unambiguously distinguishing non-Abelian anyons, which can form multiple composite charges with distinct nontrivial braid statistics. Our approach is validated using numerical simulations that are consistent with the correct fractional exchange statistics for both the Abelian anyons in the toric code and non-Abelian Ising anyons.

TT 33.6 Tue 12:15 HSZ/0105

Control of chiral topological phases: Dynamics of a chiral spin liquid — •Ruben Burkard and Urban Friedrich Peter Seifert — Institut für Theoretische Physik, Universität Köln, Zülpicher Straße 77a, 50937 Köln, Germany

As recent advances in experiment make it increasingly feasible to realize and control unconventional quantum many-body states, we investigate the out-of-equilibrium dynamics of a chiral spin liquid, with the aim of drawing lessons for the control of topologically ordered phases. In particular, we consider the Hubbard model on the triangular lattice near the Mott transition, which can be described by an effective spin model with higher-order interaction terms and is believed to host a CSL phase. In order to drive the system out of equilibrium, we apply ultrafast optical pulses, which couple to the spins in the system via magnetoelectric couplings and induce nonthermal, reversible modifications to the system's effective spin Hamiltonian. These can be derived from an appropriate Hubbard model in a Floquet approach. We then formulate a time-dependent parton mean-field theory to study the light-induced dynamics of the magnetic degrees of freedom. From this study, one might also infer lessons for other systems with chiral topological order, such as fractional quantum anomalous Hall (FQAH) states recently observed (and optically controlled) in twisted $MoTe_2$, or chiral pseudospin liquids in Moiré heterostructures.

TT 34: Members' Assembly

All members of the Low Temperature (TT) Division are invited to join!

Topics:

- Report
- Outlook 2026
- Election Deputy Spokesperson
- Miscellaneous

Time: Tuesday 14:00–15:30 Location: HSZ/0101

TT 35: Cooperative Phenomena: Spin Structures and Magnetic Phase Transitions (joint session MA/TT)

Time: Tuesday 14:00–15:30 Location: POT/0151

TT 35.1 Tue 14:00 POT/0151

Stochastic Simulation of Phase Transitions in the Dissipative 2D XYZ-Model — •Franz Pöschl[1,2,3], Przemyslaw Zielinski[1,2,3], Xin Zhang[1,2,3], and Peter Rabl[1,2,3] — [1]Technical University of Munich, TUM School of Nat- ural Sciences, Physics Department, 85748 Garching, Germany — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany

The simulation of large, open quantum spin systems is a hard problem and for most cases it is not possible to get exact solutions. Therefore, we use methods in the class of the Truncated Wigner Approximations to tackle this problem. In our work we investigated the hybrid discrete-continuous truncated Wigner approximation and used it to determine the phase diagram of the dissipative 2D XYZ-model. We were able to simulate systems with several thousands of spins due to the linear scaling of the method and numerical optimization of our code. Hence we were able to simulate the phase transitions of the model and also characterize the different phases in the open quantum system.

TT 35.2 Tue 14:15 POT/0151

Large magnetoreflectance and optical anisotropy due to 4f flat bands in the frustrated kagome magnet HoAgGe — •Felix Schilberth[1,2], Luke DeFreitas[3], Khan Zhao[4,5], Florian Le Mardelé[6], Ivan Mohelsky[6], Milan Orlita[6], Philipp Gegenwart[5], Hua Chen[3], István Kézsmárki[1], and Sándor Bordács[2] — [1]Experimentalphysik V, Unversity of Augsburg — [2]Department of Physics, BME Budapest — [3]Department of Physics, Colorado State University — [4]School of Physics, Beihang University — [5]Experimentalphysik VI, Unversity of Augsburg — [6]LNCMI, Université Grenoble Alpes

We report peculiar optical properties of the frustrated itinerant magnet HoAgGe, which exhibits multiple magnetically ordered states obeying the kagome spin-ice rule. The optical conductivity is higher for light polarization perpendicular to the kagome plane both for the free carrier response and the interband transitions. The latter have strong contributions from Ho 4f flat bands located near the Fermi level, as revealed by our *ab initio* calculations, explaining the unusual anisotropy of the optical properties and the pronounced temperature dependence of the interband transitions for out-of-plane light polarization. The key role of Ho 4f states is further supported by the large variation of the magneto-reflectivity, following the field dependence of the magnetization in contrast to that of the magnetotransport data. Such heavy-electron bands near the Fermi level offer an efficient way to control transport and optical properties and we show that their ultrafast magneto-optical response is susceptible to the magnetic order.

TT 35.3 Tue 14:30 POT/0151

Transition between critical antiferromagnetic phases in the J1-J2 spin chain — Adam McRoberts[1], •Chris Hooley[2], and Andrew Green[3] — [1]International Centre for Theoretical Physics, Trieste, Italy — [2]Coventry University, Coventry, United Kingdom — [3]University College London, London, United Kingdom

The J1-J2 spin chain is one of the canonical models of quantum magnetism, and has long been known to host a critical antiferromagnetic phase with power-law decay of spin correlations. We show that there are, in fact, two distinct critical antiferromagnetic phases, where the roles of the local dimer field and its dual field are interchanged: the 'Affleck-Haldane' phase near the Heisenberg point J2 = 0, where the dimer field that parametrises local singlet order is gapless and part of a joint O(4) Neel-singlet order parameter; and the 'Zirnbauer' phase which appears at sufficiently large ferromagnetic J2, where the dimer field is gapped out and its dual field - the instanton density of the O(3) Neel field - is critical instead. The phases are so-named because each realises one of the competing pictures for how the O(3) non-linear sigma model with a topological theta term renormalises to the su(2) level 1 Wess-Zumino-Witten model. We support these predictions with density matrix renormalisation group calculations.

TT 35.4 Tue 14:45 POT/0151

Field-induced transitions in the charge-ordered Kagome metal FeGe — •Lilian Prodan[1], Jeremy Sourd[2], Pavlo Khanenko[2], Yurii Skourski[2], Sergei Zherlitsyn[2], and István Kézsmárki[1] — [1]EPV, Institute of Physics, University of Augsburg - Augsburg, Germany — [2]HLD-EMFL, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Kagome metals with strong electronic correlations have recently attracted significant interest as fertile platforms for emergent phenomena such as unconventional magnetism, topological transport, and symmetry-breaking instabilities. Among them, FeGe stands out due to its intriguing combination of noncollinear magnetism and charge ordering, making it a prime candidate for studying the coupling between spin, charge, and lattice degrees of freedom [1]. This compound orders antiferromagnetically below $\sim$ 410 K, develops a charge-density-wave state near $\sim$ 110 K, and forms a noncollinear spin structure below $\sim$ 60 K. To explore how these orders interact, we performed magnetization, sound-velocity, and magnetostriction measurements in static and pulsed magnetic fields up to 60 T. Our results reveal previously unreported transitions at high magnetic fields and allow us to construct an extended H-T phase diagram for FeGe. [1] X. Teng, et al., Nature **609**, 490-495 (2022).

TT 35.5 Tue 15:00 POT/0151

Successive field-induced phase transitions in the kagome magnet $ErMn_6Sn_6$ — •A. Kurtanidze[1,2], Sh. Yamamoto[1], K. Uhlirova[3], Y. Skourski[1], S. Zherlitsyn[1], J. Sourd[1], T. Herrmannsdörfer[1], E. Weschke[4], O. Prokhnenko[4], H. Nojiri[5], B. Eggert[6], A. Aubert[7], K. Kummer[8], K. Skokov[7], H. Wende[6], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Materials Growth and Measurement Laboratory (MGML), Charles University, Prague, Czech Republic — [4]Helmholtz-Zentrum Berlin für Materialien und Energie, BESSY II, Berlin, Germany — [5]Institute for Materials Research, Tohoku University, Sendai, Japan — [6]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Germany — [7]Functional Materials, Material Science, TU Darmstadt, Germany — [8]ESRF, The European Synchrotron, Grenoble, France

The ternary stannides RMn_6Sn_6 (R = Sc, Y, Gd-Lu) with hexagonal $HfFe_6Ge_6$-type structure ($P6/mmm$) are a key platform for exploring coupled topological electronic and magnetic properties. We focused on single crystals of $ErMn_6Sn_6$ and observed successive field-induced phase transitions. Using element-specific x-ray magnetic circular and linear dichroism (XMCD/XMLD) measurements in pulsed magnetic fields up to 30 T, we revealed the microscopic nature of these transitions, supported by thermodynamic data. We discuss Er and Mn moment reorientations and their link to macroscopic results.

TT 35.6 Tue 15:15 POT/0151

Depinning by shaking of skyrmions by oscillating magnetic fields — •Rajendra Loke[1], Alla Bezvershenko[2], Petra Becker Bohaty[3], Achim Rosch[2], and Joachim Hemberger[1] — [1]II. Physikalisches Institut, University of Cologne, Zülpicher Str. 77, 50937 Cologne, Germany — [2]Institut for Theoretical Physics, University of Cologne , Zülpicher Str. 77, 50937 Cologne, Germany — [3]Institut for Geology und Mineralogy, University of Cologne , Zülpicher St. 49b, 50674 Cologne, Germanyy

Here we present our recent result on shaking the skyrmion lattice by oscillating transvers magnetic field. When a transvers field is applied in addition to the longitudinal external field, skyrmion strings try to align themselves parallel to the effective field. To do so, the tips of the skyrmion strings have to move large distances and thus have to overcome pinning forces before being able to follow the field lines. We employ linear and non-linear AC susceptometry as experimental probe. The signature of this pinning-depinning transition is observable as contribution to the magnetic susceptibility, to the magnetic loss, and as well in the higher harmonic susceptibility. According to theoretical predictions, due to the chiral nature of the material the depinning is connected to translational motion of the skyrmions.

[1] Jan Müller et al. PhysRevLett.119.137201 (2017) [2] Felix Rucker et al. arXiv: 2504.01133v1 [3] Nina del Ser et al. SciPost Phys. 15, 065 (2023).

TT 36: Weyl Semimetals (joint session MA/TT)

Time: Tuesday 14:00–15:30 Location: POT/0361

TT 36.1 Tue 14:00 POT/0361

Ferrimagnetism and the causes of discontinuous magnetic behavior in Kagome Weyl-semimetal Co3Sn2S2 — •Abdul-Vakhab Tcakaev[1], Benjamin Katter[1], Stefan Enzner[2], Eugen Weschke[3], Sebastian Wintz[3], Gohil S. Thakur[4], Michael Ruck[4], Giorgio Sangiovanni[2], and Vladimir Hinkov[1] — [1]Experimentelle Physik IV, Fakultät für Physik und Astronomie, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Computational Quantum Materials, Fakultät für Physik und Astronomie, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [3]Helmholtz-Zentrum Berlin for Materials and Energy, Albert-Einstein-Straße 15, 12489 Berlin, Germany — [4]Technical University of Dresden, Helmholtzstr. 10 01069 Dresden

The Kagome Weyl semimetal Co3Sn2S2 shows puzzling magnetic anomalies that have been interpreted as hidden phase transitions. Combining element-specific XMCD, SQUID magnetometry, STXM, DFT, and inelastic neutron scattering, we establish a ferrimagnetic ground state in which Co moments are partially compensated by antiparallel Sn moments and stabilized by strong uniaxial magnetocrystalline anisotropy. Temperature-dependent XMCD and STXM show that the discontinuous drop of remanent magnetization on zero-field warming arises from abrupt domain nucleation controlled by demagnetization effects, rather than from an intrinsic change of the spin structure. This yields a consistent microscopic picture of the magnetism in Co3Sn2S2 relevant for its Weyl and anomalous Hall properties.

TT 36.2 Tue 14:15 POT/0361

High-field THz Probing of the Crossover between Weyl and Weyl-Kondo Physics in $Mn_{3+x}Sn_{1-x}$ — •Erik W. de Vos[1], Zekai Chen[1], Debankit Priyadarshi[1], Anusree V. Puleri[2], Uri Vool[2], Claudia Felser[2], Edouard Lesne[2], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zurich, Zurich, Switzerland — [2]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany

We present temperature-dependent high-field THz spectroscopy measurements on a substitution series of the noncollinear antiferromagnet $Mn_{3+x}Sn_{1-x}$. When the Mn substitution is increased from x=0 to x=0.5, $Mn_{3+x}Sn_{1-x}$ has been found to transition from a pure Weyl semimetal to a Weyl-Kondo insulator. This is accompanied by the emergence of a hybridization gap of 10.2 meV [1]. Our study uses high-field THz radiation to probe and drive the non-linear response of $Mn_{3+x}Sn_{1-x}$ through the onset of Kondo-driven correlations. Via this high-field resonant excitation, we directly probe the dynamic response across the transition from a Weyl semimetal to a Weyl-Kondo insulating state.

[1] Sci. Adv. 6, eabc1977 (2020)

TT 36.3 Tue 14:30 POT/0361

Peierls-induced topological Weyl semimetal in $PtBi_2$ — •Anders C. Mathisen[1], Stefanie S. Brinkman[1], Xin L. Tan[1], Øyvind Finnseth[1], Fabian Göhler[1], Chul-Hee Min[1], Jens Buck[2], Kai Rossnagel[2], Grisha Shipunov[3], Anna Isaeva[3], Jorge I. Facio[4], and Hendrik Bentmann[1] — [1]Center for Quantum Spintronics, Department of Physics, NTNU, Norway — [2]Kiel University & DESY, Germany — [3]Institute of Physics, University of Amsterdam, The Netherlands — [4]Instituto Balseiro, National University of Cuyo, Argentina

$PtBi_2$ is attracting interest because of its exotic electronic properties, including bulk Weyl nodes, Fermi-arc surface states, and unconventional surface superconductivity. The emergence of Weyl nodes in materials is commonly attributed to accidental crossings between non-degenerate valence and conduction bands, while little emphasis has been placed on the physical mechanisms that induce Weyl physics. Recent theory indicates that reduced translational symmetry in the Peierls-distorted crystal structure of $PtBi_2$ constitutes a mechanism for the formation of Weyl nodes [1]. In this talk, we will present an investigation of the bulk electronic structure of $PtBi_2$ using soft X-ray angle-resolved photoelectron spectroscopy. Based on an analysis of the spectral weight across wide regions in momentum space, we show how the Peierls-distortion in $PtBi_2$ promotes the formation of Weyl nodes.

[1] S. Palumbo *et al.*, Interplay between inversion and translation symmetries in trigonal $PtBi_2$. Phys. Rev. B **112**, 205125 (2025)

TT 36.4 Tue 14:45 POT/0361

Phonon-driven axial fields enable terahertz Kerr rotation in WTe2 — •Soma Dutta, Vishal Shokeen, Ruslan Chulkov, David Muradas Belinchón, M. Venkata Kamalakar, Oscar Gränäs, and Hermann Dürr — Department of Physics and Astronomy, Uppsala University, Box 516, 75120 Uppsala, Sweden

Weyl semimetals provide a platform for studying the coupling between lattice dynamics and topological electronic structure through the motion of Weyl nodes and their associated Berry curvature (see Sie et al., Nature 565, 61, 2019). Here we report the observation of terahertz-frequency Kerr rotation in the noncentrosymmetric Weyl semimetal WTe_2, generated in the absence of an external magnetic field. Using ultrafast pump-probe polarimetry, we identify coherent oscillations at 0.24 THz and 2.4 THz that originate from interlayer shear vibrations and optical phonon modes, respectively. The 0.24 THz shear mode exhibits maximum amplitude along the a-axis and is strongly suppressed along b, indicating an odd mirror-symmetry character. By modeling the strain-induced modification of the Weyl-node separation, we show that this shear phonon produces an axial vector potential whose sign depends on the direction of atomic displacement. Spatial gradients of this axial potential generate a pseudo-magnetic field with a sign structure that naturally accounts for the observed phase inversion. Our results provide direct evidence for phonon-driven axial electromagnetic fields in a Weyl semimetal and demonstrate a route for ultrafast control of topological optical responses through coherent lattice motion. *Ab initio* calculations will further clarify the Kerr response mechanism.

TT 36.5 Tue 15:00 POT/0361

Magnetoconductance in Chiral Topological Semimetals — •Ricardo Manuel Sousa Barbosa and Annika Johansson — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle (Saale), Germany

Chiral topological semimetals [1] are a class of quantum materials whose crystal symmetries enforce multifold band crossings with nonzero topological charge, hosting symmetry-protected chiral fermionic quasiparticles, long surface Fermi arcs, and enhanced optical and transport responses. These Weyl semimetals [2] are three-dimensional materials that exhibit multiple Weyl nodes that act as point-like sources and sinks of Berry curvature in momentum space, and provide a condensed-matter realization of the chiral anomaly [3], a field-induced nonconservation of electrons associated with a given Weyl node, which manifests as a positive longitudinal magnetoconductance.

We investigate the magnetotransport properties of compounds in space group 198 [4], which host four- and six-fold degenerate Weyl nodes at the Γ and *R* points, respectively, with Chern numbers up to ±4. Using a semiclassical approach, we compute the resulting magnetoconductance, enabling a detailed analysis of the unconventional electronic responses characteristic of these materials.

[1] N.B.M. Schröter *et al.*, Nature Physics **15**, 759-765 (2019); [2] M. Z. Hasan *et al.*, Annu. Rev. Condens. Matter Phys. **8**, 289-309 (2017); [3] F. Bladuini *et al.*, Nat. Commun. **15**, 6526 (2024) [4] D.A. Pshenay-Severin *et al.*, J. Phys.: Condens. Matter **30**, 135501 (2018)

TT 36.6 Tue 15:15 POT/0361

Giant Anomalous Hall Effect Tuned by Atomic Order in Fe3Pt — •Yibo Wang and Enke Liu — Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

The Berry curvature induced anomalous Hall effect (AHE) has attracted considerable interest in recent years [1,2]. In Fe3Pt, a nodal line situated near the Fermi level generates a pronounced Berry curvature hotspot [3], giving rise to an intrinsic anomalous Hall conductivity (AHC) of 1250 S/cm according to our measurement. Building on this large intrinsic contribution, we sought to enhance the total AHE by deliberately increasing the extrinsic AHC through control of atomic ordering. By annealing Fe3Pt samples at various temperatures and for different durations, we were able to tune the extrinsic AHC continuously from nearly 0 S/cm up to 550 S/cm. The most striking result was obtained for a specimen that was annealed for ten days; at 2 K this sample exhibited a total AHC of 1892 S/cm. This value is a significant value among magnetic topological materials and represents a 50 % increase over the intrinsic contribution alone. These findings confirm the success of the proposed strategy: leveraging a substantial intrinsic Berry curvature AHC and subsequently amplifying the total AHC through extrinsic AHC through mechanisms such as atomic engineering. The approach provides a practical pathway for achieving exceptionally large anomalous Hall responses in magnetic topological systems. [1]Nat. Phys. 14, 1125-1131 (2018). [2] Nat. Phys. 14, 1119-1124 (2018). [3] Adv. Mater. 35, 2301339 (2023).

TT 37: Ultrafast electron dynamics at surface and interfaces – Poster (joint session O/TT)

Time: Tuesday 14:00–16:00 Location: P2

TT 37.1 Tue 14:00 P2

Nonequilibrium phonon dynamics after laser-excitation — Tobias Held, Christopher Seibel, Markus Uehlein, •Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau

Electron-phonon coupling is a fundamental process governing the energy relaxation dynamics of solids excited by ultrafast laser pulses. While this coupling is often described in terms of an effective electron temperature, recent works have highlighted the important roles of both nonequilibrium electronic distributions and detailed phononic properties.

In this study, we investigate how nonequilibrium electron occupations, phonon stiffness, and wavenumber-resolved coupling collectively shape the energy exchange between electrons and the lattice in metals. We find that deviations from thermal electronic distributions can substantially modify the coupling parameter, challenging the conventional assumption that electron temperature alone determines the coupling strength. We further identify a roughly quadratic scaling of the coupling parameter with phonon stiffness, with high-wavenumber phonon modes consistently dominating the interaction. Finally, we demonstrate that this preferential coupling leads to the emergence of hot phonons near the Brillouin-zone boundary, which in turn induces a collapse of the overall energy transfer rate and significantly delays electron-phonon equilibration.

TT 37.2 Tue 14:00 P2

Comparing temperature change during light-matter interaction of thermal and athermal electron systems — •Fabio A. Müller, Tobias Held, Christopher Seibel, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau

When an ultrashort laser pulse irradiates a metal, the electronic system initially absorbs energy and is driven far from equilibrium. This transient nonequilibrium distribution modifies the light-matter interaction, in part through changes in Pauli blocking, while electron-electron scattering concurrently drives the system toward a hot Fermi-Dirac distribution. Consequently, ultrashort laser pulses of the same fluence but different duration lead to different absorption, even in the linear regime.

Here, we investigate how the capability of an electron ensemble to absorb photons depends on its instantaneous energy distribution. Specifically, we compare the absorption arising from nonequilibrium electron distributions with that of Fermi-Dirac distributions carrying the same energy density. Our results show that, for realistic materials, the relative absorption is highly sensitive to the photon energy, a behavior that can be traced back to distinct features in the electronic density of states.

TT 37.3 Tue 14:00 P2

Role of non-thermal electrons on energy dissipation and phase transition in laser excited metals — •Lukas Jonda, Tobias Held, Markus Uehlein, Christopher Seibel, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics andResearch Center OPTIMAS, RPTU Kaiserslautern-Landau

The influence of non-equilibrium electrons on energy dissipation and phase transitions is not well understood. It is known that during femtosecond laser irradiation of a surface, electrons are excited to a state of non-equilibrium in space and energy. These highly excited electrons then transport energy ballistically into the bulk. On a picosecond timescale, electrons transfer energy to the lattice via electron-phonon collisions. If the transferred energy is large enough to reach the melting point, the crystal lattice can undergo a phase transition.

We developed a hybrid model that combines a kinetic Monte Carlo simulation and a two-temperature model. The latter describes diffusive transport as well as electron-phonon equilibration, and the former describes primary electron excitation by the laser pulse, transport of non-equilibrium electrons, and secondary electron generation.

We present results for gold, where the influence of non-equilibrium electrons on energy transport is expected to be significant, due to the long mean free path of its electrons. Finally, we are interested in the influence of non-equilibrium electrons on the melting process.

TT 37.4 Tue 14:00 P2

Capturing thermalization through electron-electron scattering with machine learning — •David L. Kaiser, Tobias Held, Christopher Seibel, Markus Uehlein, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau

Ultrafast excitation of metals by optical laser pulses induces nonequilibrium energy distributions in the electron system. This nonequilibrium gives rise to complex electron-electron scattering processes, which typically restore a Fermi-Dirac distribution on a femtosecond timescale. Accurately modelling the thermalization requires evaluating the full electron-electron collision integral, which is however computationally costly.

In this study, we explore the possibility to use machine learning to emulate the dynamics generated by the full collision integral. Our goal is to significantly accelerate these calculations, enabling efficient simulations of bulk and multilayer systems. This approach opens the door to uncovering new relaxation pathways and predicting the response of complex material systems to ultrafast excitation.

TT 37.5 Tue 14:00 P2

Studies of laser ablation of band-gap materials — •Markus Bonifer[1,2], Sebastian T. Weber[1], Nils Cremer[2,3], Gabriel Schaumann[2,3], and Baerbel Rethfeld[1] — [1]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, Germany — [2]Focused Energy GmbH, Im Tiefen See 45, 64293, Darmstadt, Hessen, Germany — [3]Institute of nuclear physics (IKP), Technische Universität Darmstadt, Darmstadt, Germany

We aim to explore laser ablation as a possible approach for creating clean, well-defined microholes in polymers used for laser fusion targets where symmetry and control of surface roughness are important. Because polymers differ widely in their properties, general insights into laser material interaction are sought through modeling of density-dependent excitation in band-gap materials.

The theoretical models used are based on the density-dependent two-temperature model (nTTM) and extended multiple rate equations (EMRE). These calculations are intended to guide experimental studies carried out in collaboration with Focused Energy to identify suitable processing conditions and improve overall feature quality.

TT 37.6 Tue 14:00 P2

Thermalization of optically excited electrons in metals: electron-electron scattering dynamics — •Stephanie Roden, Christopher Seibel, Tobias Held, Markus Uehlein, Sebastian T. Weber, and Baerbel Rethfeld — Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau

When a metal is irradiated with a short-pulsed optical laser, the electron distribution is disturbed into a state far from equilibrium. On a femtosecond timescale, the non-thermal electrons thermalize by collisions with each other, which drives the electrons towards a hot Fermi distribution.

In this work, we present a derivation of the full electron-electron Boltzmann collision integral within the random-$\boldsymbol{k}$ approximation. Building on this approach, we trace the temporal evolution of the electron energy distribution in metals after ultrafast excitation. Furthermore, we examine to which extent the resulting dynamics can be captured by the numerically simpler relaxation time approach, applying a constant and an energy-dependent relaxation time derived from Fermi-liquid theory.

We find a better agreement with the latter, while specific features caused by the balance of scattering and reoccupation can only be captured with a full collision integral.

TT 37.7 Tue 14:00 P2

Time-resolved PEEM and μARPES using a 100 kHz ToF momentum microscope — •Isabella Alexandra Hofmeister[1,2], Michael Herb[1,2], Maria Federl[1], Franz Seitz[1], and Isabella Gierz[1,2] — [1]University of Regensburg, Regensburg, Germany — [2]Regensburg Center for Ultrafast Nanoscopy - RUN, Regensburg, Germany

Momentum microscopy provides energy-resolved imaging in real and reciprocal space with < 100 meV resolution, combining PEEM ($\Delta x < 40$ nm lateral resolution) and μARPES ($\Delta k < 0.02$ Å^{-1}) capabilities. We implemented an ultrafast setup with a time-of-flight momentum microscope and a 100 kHz laser system delivering 6 eV probe pulses and pump pulses tunable from the mid-infrared to visible range. Procedures for converting time-of-flight to kinetic energy and for establishing spatial and temporal pump-probe overlap are discussed. Proof-of-principle time-resolved PEEM and μARPES experiments on the topological insulator Bi_2Se_3 demonstrate femtosecond-resolved carrier dynamics with high spatial and momentum precision.

TT 37.8 Tue 14:00 P2

First steps with a qPlus-based MIR AFM — •Furkan Özyigit, Lukas Böhm, Leonie Weiss, Jay Weymouth, Rupert Huber, and Franz Giessibl — University of Regensburg, 93053 Regensburg

We report initial progress in an ultrafast non-contact atomic force microscope/scanning tunneling microscope (NC-AFM/STM) platform based on qPlus sensors, integrated with a CEP-stabilized mid-infrared (MIR) pump-probe system and tunable optical parametric amplifier (OPA) for versatile excitation. In first experiments, we successfully induced transient tunneling currents on Cu(111) using MIR pulses, demonstrating precise control of ultrafast electronic

excitation at the atomic scale via laser-coupled tunneling. While the tunneling cur- rent reflects the ultrafast electronic excitation dynamics, the qPlus sensor permits complementary force detection to monitor subsequent structural or electrostatic interaction changes, such as those resulting from induced charge redistribution or lattice relaxation. This enables simultaneous probing of electronic and mechanical dynamics with fem- tosecond time and sub-nanometer spatial resolution. Beyond investi- gations of transient electrostatic forces, this versatile system facilitates a broad class of ultrafast nanoscale experiments, including scattering- type scanning near-field optical microscopy (s-SNOM) for imaging car- rier and phase dynamics, time-resolved tip-enhanced spectroscopy for molecular states, and pump-probe tunneling spectroscopy.

TT 37.9 Tue 14:00 P2

Image potential states of oxide quasicrytals — •Barbara Drobinski[1], Friederike Wührl[1], Richard Kraska[1], Konrad Gillmeister[1], Stefan Förster[1], Cheng-Tien Chiang[2], and Wolf Widdra[1] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany — [2]Institute of Atomic and Molecular Sciences , Academia Sinica, Taipeh, Taiwan

Quasicrystals are aperiodically ordered materials that lack translational symmetry. Their aperiodic potentials give rise to an infinitely dense set of Fourier components, which can induce gaps and mini-gaps in the electronic band structure. Here, we investigate this phenomenon for nearly free-electron-like image-potential surface states, where electrons propagate in front of the surface while experiencing the aperiodic potential. Using momentum-resolved two-photon photoemission, we determine both the electronic dispersion and relaxation dynamics of oxide quasicrystals (OQCs) based on Ba-Ti-O/Pt(111) [1] and Eu-Ti-O/Pt(111). The latter is obtained via Eu decoration of a Ti_2O_3 honeycomb precursor [2]. In both systems, we observe n=1 and n=2 image potential states, located 340 meV (360 meV) and 150 meV (190 meV) below the vacuum level for Ba-Ti-O (Eu-Ti-O), respectively. The states exhibit parabolic dispersions without apparent gap openings. We discuss the momentum-dependent electron lifetimes in the context of possible mini-gaps in the underlying aperiodic potential.

[1] S. Förster *et al.*, Nature **502**, 215 (2013)
[2] M. Haller *et al.*, http://arxiv.org/abs/2510.11426

TT 37.10 Tue 14:00 P2

Ultrafast Electron Diffraction Study of Lattice Dynamics in Elemental Chromium — •Justus Richter[1,2], Victoria Taylor[1], Hyein Jung[1,2], Ralph Ernstofer[1,2], and Yoav William Windsor[1,2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Institut für Physik und Astronomie, Technische Universität Berlin

Femtosecond electron diffraction (FED) allows to quantitively study ultrafast atomic motion. Here we use FED to study photoinduced atomic motion in Cr. We saw that measurements taken above- and below T_N exhibit qualitatively different responses from the lattice, hinting to the effect of the spin-induced periodic lattice distortion within the antiferromagnetic Cr phase, though further investigation is required. A two temperature model (TTM) was used to model the energy flow between the electronic and lattice subsystems by which we extract an estimate for the electron-phonon coupling constant $G_{ep} = (4.8 \pm 0.6) \times 10^{17}$ $Jm^{-3}K^{-1}$, which fits into the wide range of values reported in literature. Finally, we measured Cr side-by-side with Pt and demonstrate qualitative differences in their temporal responses, including a significantly faster thermalization of the Cr lattice and differences in the shape of their temporal response.

TT 37.11 Tue 14:00 P2

Ultrafast electron dynamics in the valence-fluctuating intermetallic $EuIr_2Si_2$ — •Abeer Arora[1], Túlio de Castro[1], Amine Wahada[1], Lawson Lloyd[1], Tommaso Pincelli[2], Kristin Kliemt[3], Cornelius Krellner[3], Denis V. Vyalikh[4,5], Yoav Will Windsor[2], Martin Wolf[1], Ralph Ernstorfer[1,2], and Laurenz Rettig[1] — [1]Fritz Haber Institute of the Max Planck Society, Berlin, Germany — [2]Institut für Physik und Astronomie, TU Berlin, Germany — [3]Physikalisches Institut, Göthe-Universität Frankfurt, Germany — [4]Donostia International Physics Center, San Sebastián, Spain — [5]Ikerbasque, Basque Foundation for Science, Bilbao, Spain

$EuIr_2Si_2$ is a valence-fluctuating intermetallic compound that, despite its non-magnetic bulk, develops 2D ferromagnetic order below 48 K in the topmost Eu layer due to a stable Eu^{2+} configuration. Its heavy Ir ions generate strong Rashba spin-orbit coupling, which interacts with magnetic exchange and influences the surface electronic states. Probing the non-equilibrium dynamics of the 2D electrons in the Si-Ir-Si surface layer offers a direct way to study the coupling of the spin-orbit and surface magnetic interaction. Using femtosecond XUV time- and angle-resolved photoemission spectroscopy, we investigate how the surface states evolve following photoexcitation with a 1.55 eV pulsed laser. Our preliminary results show an ultrafast quenching of the surface-state splitting, which we discuss in terms of demagnetization of the Eu 4f moments and modified spin-orbit coupling.

TT 37.12 Tue 14:00 P2

Ultrafast STEM locked to GHz sample excitation — •Andreas Wendeln[1], Alexander Schröder[1], Sakal Singla[1], and Sascha Schäfer[1,2] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Regensburg Center for Ultrafast Nanoscopy (RUN), Regensburg, Germany

Ultrafast transmission electron microscopy (UTEM) has been an established method for investigating nanoscale dynamics for several years, combining the nanometer spatial resolution of TEM with the femtosecond temporal resolution of a pump-probe approach. In recent years, there have been numerous advances in the development of new femtosecond electron sources, such as laser-driven Schottky [1] or cold-field emitters [2]. A combination of these sources with advanced electron optical elements, such as a probe aberration corrector, is expected to deliver even smaller electron spot sizes and to increase the available pulsed current but was not yet demonstrated. Here, we present a measurement scheme for ultrafast STEM with a focus on magnetic imaging, utilizing an aberration corrector and a laser-driven cold-field emitter. In initial measurements using a continuous photoelectron beam, the measurement method is characterized regarding experimental parameters, such as probe currents, focal spot sizes, and stability. Subsequently, we report the locking of femtosecond electron pulse train at repetition rates between 100 kHz up to 80 MHz to GHz radiofrequency currents which we aim to employ for DPC and ptychography imaging schemes of current-driven magnetic dynamics. [1] Feist et al., Ultramicroscopy, 2017. [2] Schröder et al., Ultramicroscopy, 2025.

TT 37.13 Tue 14:00 P2

Probing Ultrafast Structural Dynamics in Multilayer Graphene Using ULEEM — •Simon Briesenick[1,2,4], Johannes Otto[1,2,4], Leon Brauns[1,2], Philip Schädlich[3], and Claus Ropers[1,2] — [1]Department of Ultrafast Dynamics, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Göttingen, Germany — [3]Institute of Physics, TU Chemnitz, Chemnitz, Germany — [4]authors contributed equally

Multilayers of graphene (MLG) exhibit electronic and structural properties that vary strongly with, e.g., layer number and stacking order, making MLG a suitable model platform for studying ultrafast phenomena in two-dimensional materials [1]. We investigate the behavior of MLG after excitation with ultrashort light pulses using our newly developed ultrafast low-energy electron microscope (ULEEM) [2]. The instrument allows for the investigation of surface structural dynamics with sub-picosecond and nanometer spatial resolution, utilizing low-energy ($\leq$ 100 eV) ultrashort probe electron pulses. We present first data on the light-induced Debye-Waller effect in MLG, demonstrating the potential of ULEEM studies for resolving ultrafast structural behavior in MLG.

[1] K. V. Emtsev, et al. Phys Rev B. 77, 155303 (2008) [2] J. Otto et al. (in preparation)

TT 37.14 Tue 14:00 P2

Hot-electron dynamics in moiré structures studied with resonant scanning tunneling spectroscopy — •Martin Lülff, Marta Przychodnia, Maciej Bazarnik, and Anika Schlenhoff — Institute of Physics, University of Münster, Germany

To study hot-electron dynamics in Gr-metal heterostructures, image-potential states (IPSs) serve as ideal model system. While their energies are known to be highly sensitive to the respective Gr-metal distance variation within the moiré unit cell [1, 2], recent two-photon photoemission experiments suggest moiré-site dependent lifetimes [3].

Here, utilizing the high spatial resolution of resonant scanning tunneling microscopy (STM) and spectroscopy (STS) we study the moiré-site dependent IPSs' lifetimes for highly corrugated Gr/Fe/Ir(111) and Gr/Ir(111), respectively. Comparing these resonant STS data with those recorded on bare Fe/Ir(111) and Ir(111), respectively, enables the influence of the varying Gr-metal distance on the lifetimes to be distinguished from that of the underlying metal substrate. We analyse the IPSs' lifetimes for a Stark shift in their energies by applying various electric field strengths in current-dependent STS series, and discuss the results in terms of their resulting energetic positions with respect to the underlying unoccupied electronic band structure. Our work contributes to an in-depth understanding of electron transfer processes at Gr-metal interfaces.

[1] M. Bazarnik and A. Schlenhoff, ACS Nano **19**, 25812 (2025)
[2] N. Armbrust *et al.*, New J. Phys. **17**, 103043 (2015)
[3] N. Armbrust *et al.*, Phys. Rev. Lett. **108**, 056801 (2012)

TT 37.15 Tue 14:00 P2

Photo-induced electron pressure drives THz phonon in Platinum-Copper superlattice — •Jan-Etienne Pudell[1], Maximilian Mattern[2,3], Marc Herzog[2], Alexander von Reppert[2], Daniel Schick[3], Chandan Singh[4], Peter M. Oppeneer[4], Michel Hehn[5], Ulrike Boesenberg[1], Angel Rodriguez-Fernandez[1], Roman Shayduk[1], Wonhyuk Jo[1], Johannes Möller[1], Jörg Hallmann[1], James Wrigley[1], Matias Bargheer[2,6], and Anders Madsen[1] — [1]European XFEL — [2]University Potsdam — [3]MBI, Berlin — [4]Uppsala University — [5]IJL, Université Lorraine — [6]HZB Berlin

Using ultrafast X-ray diffraction (UXRD) at the MID end-station at the European XFEL, we investigate the ultrafast lattice dynamics of metal-metal superlattice (SL) with few atomic layers of Pt and Cu upon femtosecond photoexcitation. Our results reveal that the absorbed optical energy is rapidly localizes within the Pt layers, driving the excitation of a coherent artificial THz phonon mode defined by the superlattice period. The signal's amplitude and phase modulation of the SL Bragg peaks induced by the lattice excitation i.e. the artificial THz phonon, are predominantly driven by electron pressure within the first picosecond. This response is faster than the Debye-Waller effect, which is limited by the electron-phonon coupling time.

TT 37.16 Tue 14:00 P2

Experimental realization of an interferometric XUV-trARPES experiment with phase-stabilized IR pulses — •Antonius Naujok[1], Gregor Zinke[1,2], Franz Spartz[1], Sebastian Hedwig[1], Tobias Eul[2], Martin Aeschlimann[1], and Benjamin Stadtmüller[2] — [1]Department of Physics and Re search Center OPTIMAS, RPTU University Kaiserslautern- Landau, 67663 Kaiserslautern, Germany — [2]Experimental Physics II, Institute for Physics, University of Augsburg, 86159 Augsburg

Layered 2D van der Waals materials, such as TMDCs, have been extensively studied for their optical properties and coherent responses. However, exploring coherent excitations and dephasing processes in such materials using time-resolved ARPES is challenging because the key points of the materials' band structure cannot be accessed using phase-stabilized pulses in the visible regime, as has been done in most experiments thus far [1]. To overcome this limitation, we introduce a modified version of coherent multidimensional spectroscopy. This new method is based on time-resolved ARPES and utilizes a pair of phase-stabilized femtosecond infrared (fs-IR) pulses in combination with femtosecond XUV pulses for photoionization. We demonstrate the feasibility of our approach by focusing on the A-exciton excitation and the subsequent carrier dynamics in WSe_2. Through temporal Fourier-analysis of the entire ARPES spectrum, we're able to resolve distinct frequency components within characteristic features of the WSe_2 electronic band structure. [1] M. Aeschlimann et al., Phys. Rev. B. 105, 205415 (2022)

TT 37.17 Tue 14:00 P2

Implementation of white light continuum probing for pump-probe spectroscopy — •Joris Wicker, Tim Titze, Maximilian Staabs, Jacob Kutzner, Stefan Mathias, and Daniel Steil — University of Göttingen, 1. Institute of Physics, Göttingen, Germany

We integrated a white-light continuum (WLC) probe together with a prism spectrometer in a conventional two-color femtosecond pump-probe setup. Further, we developed a custom measurement program using Microsoft's .NET Framework and Python, enabling instrument control, automated measurement sequences, and preliminary data analysis. To test the modified setup and software, we investigated the transient evolution of the reflectivity in metallic thin film systems and perovskite oxides using 1030 nm pumping. Spectrally and temporally resolved reflectivity variations were observed, confirming the proper functionality of the system. Furthermore, the stability of the WLC source was characterized. Possible future improvements include integrating a Wollaston prism to enable spectrally and time-resolved magneto-optical Kerr effect (MOKE) measurements.

TT 37.18 Tue 14:00 P2

Investigation of the light-dressed bandstructure of graphene — •Lina Segerer[1], Marco Merboldt[1], Mattis Langendorf[1], Paul Werner[1], Jan Philipp Bange[1], Junde Liu[1], Wiebke Bennecke[1], Marcel Reutzel[2], and Stefan Mathias[1] — [1]Georg-August-Universität Göttingen, I. Physikalisches Institut, Germany — [2]Philipps-Universität Marburg, Germany

Time-periodic driving of solids with strong laser fields enables optical control of material properties. Photon-driven systems not only exhibit replicas of their equilibrium band structure, known as Floquet-Bloch states, but can undergo non-trivial topological phase transitions when excited with circularly polarized light. Recent advances in angle-resolved photoemission spectroscopy (ARPES) have shown that Floquet-Bloch states can be generated in graphene using linear polarized laser pulses [1,2]. However, the oblique incidence angle of the pump pulse so far has limited the realization of a purely circularly polarized light field. In this study, we overcome this challenge by integrating an extra beam path in our ultrafast momentum microscopy (MM) setup enabling backside normal-incidence excitation with linearly and strictly circularly polarized IR pump pulses. We observe light-induced Floquet-Bloch states and investigate the polarization dependence of Floquet-Volkov interference as well as modifications in the light-dressed band structure of epitaxial graphene.

[1] M. Merboldt *et al.*, Nat. Phys. **21**, 1093 (2025).
[2] D. Choi *et al.*, Nat. Phys. **21**, 1100 (2025).

TT 37.19 Tue 14:00 P2

Table-top 3D ultrafast momentum microscopy with a time-preserving EUV-monochromator — •Lennart Weinhagen[1], Wiebke Bennecke[1], Jan Philipp Bange[1], David Schmitt[1], Marco Merboldt[1], Bent van Wingerden[1], Thi Lan Dinh[2], Fabio Frasetto[3], Luca Poletto[3], Marcel Reutzel[1], Daniel Steil[1], D. Russel Luke[2], Stefan Mathias[1], and G.S. Matthijs Jansen[1] — [1]1st Institute of Physics, University of Göttingen, Göttingen, Germany — [2]Institute for Numerical and Applied Mathematics, University of Göttingen, Göttingen, Germany — [3]Institute for Photonics and Nanotechnologies CNR-IFN, Padova, Italy

Photoemission momentum microscopy with tunable probe-photon energy gives unique access to electronic and molecular structures, enabling Fermi-surface imaging, photoemission electron diffraction (PED) and 3D orbital tomography (3D-POT). However, such measurements have largely relied on synchrotron radiation, thus limiting their use in femtosecond-resolved experiments. Here, we present a table-top EUV source with a time-preserving monochromator driven by a 1030 nm femtosecond laser, using an off-plane grating at grazing incidence to reduce spatial chirp. Integrated into our time-resolved momentum microscope [1], it delivers femtosecond, photon-energy-tunable EUV probe pulses. Demonstrated on PTCDA/Ag(110), the setup enabled full 3D reconstruction of the frontier orbitals highlighting the potential of laboratory-scale, energy-selective momentum microscopy [2].

[1] Schmitt *et al.*, Nature 608, 499-503 (2022).
[2] Bennecke *et al.*, arXiv:2502.18269 (2025).

TT 37.20 Tue 14:00 P2

Multimode momentum microscopy of cleaved 1T-TaS_2 crystals — •Bent van Wingerden[1], Olena Tkach[2], Hashima Marukara[1], Jan Philipp Bange[1], Wiebke Bennecke[1], Marcel Reutzel[3], Junde Liu[1], Gerd Schönhense[2], and Stefan Mathias[1] — [1]Georg-August-Universität Göttingen, Germany — [2]Johannes Gutenberg-Universität Mainz, Germany — [3]Philipps-Universität Marburg, Germany

Ultrafast momentum microscopy has evolved as one of the most powerful tools to study non-equilibrium electronic structure dynamics of 2D quantum materials [1]. However, the large electric field strength generated by the immersion lens limits its versatility in terms of sample systems. One critical issue is related to vacuum-cleaved van-der-Waals-crystals that often show microscopic protrusions, which are prone to field-induced electron emission and flashovers, both of which can destroy the sample itself as well as the microscope's electronics. In our work, we test the momentum imaging capabilities of a newly designed multimode momentum microscope [2,3] in combination with an EUV table-top HHG source. Using vacuum-cleaved bulk crystals of *1T*-TaS_2, we show that operating in modes of reduced electric field strength at the sample position suppresses field emission, while still preserving the field-of-view and imaging quality. We carry out detailed comparisons of different operating modes with the new lens system.

[1] Reutzel, Jansen, Mathias, *Adv. in Phys. X* 9, 2378722 (2024).
[2] Tkach & Schönhense, *Ultramicroscopy* 276, 114167 (2025).
[3] Tkach et al., arXiv:2401.10084 (2024).

TT 37.21 Tue 14:00 P2

Towards time-resolved momentum microscopy of plasmon excited quantum materials — •Mattis Langendorf[1], Lina Segerer[1], Paul Werner[1], Marco Merboldt[1], Jonas Pöhls[1], Tobias Meyer[1], Daniel Steil[1], Junde Liu[1], Jan Philipp Bange[1], Wiebke Bennecke[1], G. S. Matthijs Jansen[1], R. Thomas Weitz[1], Marcel Reutzel[2], and Stefan Mathias[1] — [1]Georg-August-Universität Göttingen, Germany — [2]Philipps-Universität Marburg, Germany

For the realization of Floquet*Bloch engineering as well as for the study of formation and propagation of excitons in two-dimensional quantum materials using time- and angle-resolved photoemission spectroscopy (ARPES), a highly localized excitation on a micron scale seems ideal [1]. However, achieving such spatial confinement poses a significant experimental challenge. Surface plasmon polaritons (SPPs) offer a promising solution, as these collective charge-carrier oscillations enable strong electromagnetic field localization and can therefore provide the required tightly focused excitation conditions [2]. In combination with femtosecond momentum microscopy that enables spatiotemporal access to electron and exciton dynamics [3], we investigate the concept of exploiting SPPs as a driving field to excite quantum materials.

[1] Merboldt *et al.*, Nat. Phys. **21**, 1093*1099 (2025).
[2] Dreher *et al.*, Nanophotonics **11**, 3687-3694 (2022).
[3] Reutzel, Jansen, Mathias, Adv. in Phys. X **9**, 2378722 (2024).

TT 38: Topology and symmetry protected materials & Topological insulators – Poster (joint session O/TT)

Time: Tuesday 14:00–16:00 Location: P2

TT 38.1 Tue 14:00 P2

Manipulation of topological surface states by switchable molecules. — Lukas Staiger[1], Jannis Lessmeister[1], •Ralf Hemm[1], Juliusz Wolny[1], Volker Schünemann[1], Martin Aeschlimann[1], and Benjamin Stadtmüller[2] — [1]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, 67633 Kaiserslautern, Germany — [2]Institute of Physics, University of Augsburg, 86159 Augsburg, Germany

Three-dimensional topological insulators host spin-momentum-locked surface states protected by time-reversal symmetry, giving them potential for spintronic devices. Controlling these states remains challenging but is crucial for opening gaps, shifting the Dirac point and tailoring spin textures for applications. In our work, we utilize a monolayer of the spin-crossover complex $Fe(phen)_2(SCN)_2$ on the topological insulator Bi_2Se_3 to break the time-reversal symmetry of the substrate. Employing angle-resolved photoemission spectroscopy, we trace the evolution of the electronic structure as a function of molecular coverage and temperature. Despite a conspicuous energy shift and modified dispersion, there is no clear evidence for a band gap opening after deposition of a molecular monolayer. Concurrently, additional spectral weight from molecular orbitals emerges, and thermally and optically driven spin-crossover transitions in the $Fe(phen)_2(SCN)_2$ layer induce changes in the Dirac-point energy and spectral weight. Our findings demonstrate that a spin-crossover overlayer can quantitatively alter the dispersion of topological surface states, while allowing them to exist due to strong interactions between molecules and surfaces.

TT 38.2 Tue 14:00 P2

Deciphering the complex surface of the topological phase in the polar semiconductor BiTeI — •Adrian Weindl, Christoph Setescak, and Franz J. Giessibl — Faculty of Physics, University of Regensburg, D-93053 Regensburg, Germany

BiTeI is a semiconductor consisting of polar layers that can form Rashba spin-split p-n junctions on its surface due to stacking faults. It has been shown that gentle annealing can transform the surface of BiTeI into a topological insulator with spin-polarized surface modes exhibiting linear dispersion. Previous LEED and RHEED measurements revealed that the surface undergoes a structural change from a non-centrosymmetric triple-layer structure to a quintuple-layer structure. However, the exact surface structure remains elusive. Using scanning tunneling microscopy, atomic force microscopy, and Kelvin probe force spectroscopy we study the surface before and after annealing with atomic resolution. We show that the annealing results in different surface phases that are highly sensitive to the annealing temperature: a chemically homgeneous phase at around 240°C and a inhomogeneous phase with strong charge disorder at 250°C. We determine the termination of each phase and confirm that the surface exhibits the signature of a topological surface state even in the strongly disordered phase.

TT 38.3 Tue 14:00 P2

THz-driven nonlinear dynamics studied with high-power THz sources — Atiqa Arshad[1,2], Jan-C Deinert[2], Igor Ilyakov[2], Andreas Gebauer[2], Anjan Kumar N M[1], and •Stefan Kaiser[1] — [1]TU Dresden,Germany — [2]HZDR, Dresden,Germany

THz pump-photoelectron spectroscopy (ARPES) probe is currently being implemented at the THz facility TELBE at Helmholtz-Zentrum Dresden-Rossendorf. This unique combination of high-field terahertz excitation and tr-ARPES probe will enable groundbreaking experiments on solid surfaces and interfaces. To this aim we have set up a high-repetition rate THz source driven by a 180 W laser source yielding > 50 mW THz output power. We report on the THz generation and characterization scheme as well as on first experiments. A highly promising material class to be studied with these light sources is BiTeI, a dual topological insulator that exhibits two different types of surface states on different interfaces. We present our study on the complex nonlinear dynamics, in particular THz harmonic generation in these compounds.

TT 38.4 Tue 14:00 P2

The quasi one-dimensional van der Waals material α-Bi_4Br_4 — •Jonathan K. Hofmann[1,2], Serhii Kovalchuk[1,3], Mingqian Zheng[4], Yuqi Zhang[4], Vasily Cherepanov[1], Timofey Balashov[1], Jin-Jian Zhou[4], Zhiwei Wang[4], Yugui Yao[4], Irek Morawski[3], F. Stefan Tautz[1,2], Felix Lüpke[1,5], and Bert Voigtländer[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [2]Experimentalphysik IV A, RWTH Aachen University, Germany — [3]Institute of Experimental Physics, University of Wrocław, Poland — [4]Key Laboratory of Advanced Optoelectronic Quantum Architecture and Measurement, Beijing Institute of Technology, China — [5]II. Physikalisches Institut, Universität zu Köln, Germany

α-Bi_4Br_4 is a quasi-one-dimensional material: covalently bonded Bi_4Br_4 chains are arranged in parallel, side-by-side and layer-by-layer, with van der Waals gaps in between. Bulk α-Bi_4Br_4 is higher-order topological insulator. At step edges on the (001) surface, quantum spin Hall (QSH) edge states are present. Using a scanning tunneling microscope (STM), we observe a significant shift of the chains, relative to each other, which we attribute to shear stress. Scanning tunneling spectroscopy reveals that the edge states are robust against the strain. Density functional theory confirms that a strained monolayer of Bi_4Br_4 is a QSH insulator with $\mathbb{Z}_2 = 1$. Furthermore, we use a four-tip STM to analyze the electrical transport of α-Bi_4Br_4 *in situ*.

TT 39: Focus Session: Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects I (joint session TT/DS/MA)

Nickel, a direct neighbor of copper in the periodic table, has been considered a promising candidate for high-temperature superconductivity since the early 1990s. After more than three decades of research, this prediction was confirmed with the discovery of superconductivity in nickelates, marking the beginning of the "nickel age" of superconductivity. Recent advances include Sm-based infinite-layer nickelates with transition temperatures approaching 40 K, as well as bilayer nickelates exhibiting superconductivity above 90 K under pressure and up to 60 K under compressive epitaxial strain. These results highlight the crucial roles of structural engineering, epitaxial strain, and precise synthesis control, and they open new frontiers for both fundamental understanding and materials design. This focus session aims to define key scientific challenges ahead, strengthen collaboration within Germany and Europe, and accelerate progress toward higher superconducting transition temperatures.

Coordinators: Marta Gibert (TU Wien), Mattias Hepting (MPI FKF Stuttgart), Ilya M. Eremin (Ruhr-University Bochum)

Time: Wednesday 9:30–12:45 Location: HSZ/0003

Topical Talk TT 39.1 Wed 9:30 HSZ/0003

Unconventional Superconductivity in Infinite-layer Samarium Nickelates — •Danfeng Li — City University of Hong Kong, Kowloon, Hong Kong SAR, China

Infinite-layer nickelates have emerged as a frontier platform for studying unconventional superconductivity beyond the cuprates. In this talk, I will present our recent advances on samarium-based infinite-layer nickelate thin films, which exhibit enhanced superconductivity and a mixed two- and three-dimensional superconducting character arising from strong coupling between rare-earth 5*d* and Ni 3*d* orbitals. I will further highlight our discovery of robust field-induced reentrant superconductivity in heavily Eu-doped $Sm_{0.95-x}Ca_{0.05}Eu_xNiO_2$, where superconductivity suppressed at low fields re-emerges above 6 T and persists to 45 T. This exotic high-field state results from the interplay between NiO-plane superconductivity and Eu^{2+}-sublattice ferromagnetism, revealing a unique coexistence of magnetism and superconductivity within a single material system. These findings demonstrate how rare-earth-site engineering and magnetic-field tuning provide powerful routes for realising and manipulating high-temperature ferromagnetic superconductivity.

[1] M. Yang, H. Wang, J. Tang, J. Luo et al., arXiv:2503.18346 (2025).
[2] M. Yang, J. Tang, X. Wu, H. Wang et al., arXiv:2508.14666 (2025).

Topical Talk TT 39.2 Wed 10:00 HSZ/0003

Recent insights into infinite-layer nickelate heterostructures from x-ray spectroscopy — •Eva Benckiser — Max Planck Institute for Solid State Research, Stuttgart, Germany

Nickelates have emerged as an important class of materials for studying unconventional superconductivity. However, the exact cation concentrations and oxygen stoichiometry in infinite-layer nickelates are difficult to determine due to the complex synthesis process. This has so far prevented the clear experimental identification of the nickel valence electron configuration in the superconducting phase.

In my talk, I will discuss our recent x-ray spectroscopy studies on $NdNiO_x$-$SrTiO_3$ heterostructures [1] and $PrNiO_x$ thin films [2] at various intermediate stages of topotactic reduction with $x = 2-3$. We find that even the most reduced films do not exhibit a pure Ni^{1+}-$3d^9$ configuration. The quantitative analysis shows that there is an average of 1.35 holes in the nickel $3d$ states and superconducting samples have even higher values [2]. These results challenge previous findings regarding the doping range in which superconductivity occurs in infinite-layer nickelates. Variations between samples are attributed to a complex interplay of ordered, self-doped regions, interfacial reconstructions, and disorder occurring on different length scales in both the cation and anion sublattices.

[1] R. A. Ortiz et al., Phys. Rev. Materials 9, 054801 (2025).
[2] R. Pons et al., submitted (2025).

Topical Talk TT 39.3 Wed 10:30 HSZ/0003

Theory of infinite-layer nickelate superconductors — •Karsten Held — TU Wien, Austria

The discovery of superconductivity in infinite-layer nickelates [1] marked a new age of superconductivity: the nickel age. Using density functional theory, dynamical mean-field theory and dynamical vertex approximation (DΓA [2]), we successfully predicted [3] the phase diagram T_c vs. Sr-doping of $Nd_{1-x}Sr_xNiO_2$ with –for an unconventional superconductor– unprecedented accuracy with defect free films synthesized only 3 years later [4]. Also, the normal state spin spectrum well agrees with resonant inelastic x-ray spectroscopy (RIXS) [5] and the one-particle spectrum with angular-resolved photoemission spectroscopy (ARPES) [6], which both enter into the calculation of T_c. With this excellent agreement to later experiments, we can now with some confidence calculate the phase diagram of finite-layer nickelates [7] and predict that infinite-layer nickelates have a much higher T_c under 100GPa of pressure even without any chemical doping [8].

This work has been supported by the ERC project 101201037 and the FWF project I5398.

[1] D. Li et al., Nature 572, 624 (2019).
[2] G. Rohringer et al., Rev. Mod. Phys. 90, 25003 (2018).
[3] M. Kitatani et al., npj Quantum Materials 5, 59 (2020).
[4] K. Lee et al., Nature 619, 288 (2023).
[5] L. Si et al., Phys. Rev. Res. 6, 043104(2024).
[6] P. Worm et al., Phys. Rev. B 109, 235126 (2024).
[7] A. Hausoel et al., npj Quantum Mater. 10, 69 (2025).
[8] S. Di Cataldo et al., Nature Comm. 15, 3952 (2024).

15 min. break

Topical Talk TT 39.4 Wed 11:15 HSZ/0003

Disorder and distortions: what electrons tell us about nickelate superconductivity — •Berit H. Goodge — MPI-CPfS, Dresden, Germany

Recent realizations of superconductivity in both square-planar and bilayer Ruddlesden-Popper nickelates have opened a host of opportunities to explore fundamental questions of high-temperature superconductivity, while simultaneously posing unique synthetic challenges. Despite recent breakthroughs in sample synthesis, however, the highest quality thin films still pose immense challenges for investigation of fundamental characteristics, such as the pairing symmetry of the superconducting order parameter. Systematically introducing point-like disorder with high-energy electron irradiation consistently suppresses the superconducting transition, pointing towards a sign-changing order parameter in square-planar nickelates [1]. In parallel, epitaxial stabilization of superconductivity in bilayer nickelate thin films has opened the door to investigate local atomic structure and bonding environments. Leveraging the highest accessible spatial resolution and light-element sensitivity enabled by state-of-the-art multislice electron ptychography, we survey a series of bilayer nickelate thin films spanning a full series of tensile and compressive strain. We combine these experimental with strain-decomposed DFT calculations to investigate correlations between the observed atomic structure and superconductivity [2].

[1] Ranna et al., *PRL* 135, 126501 (2025).
[2] Bhatt et al., arXiv:2501.08204 (2025).

Topical Talk TT 39.5 Wed 11:45 HSZ/0003

Superconducting gap structure and bosonic mode in $La_2PrNi_2O_7$ thin films at ambient pressure — •Hai-Hu Wen — Hankou Rd. 22, Gulou, Nanjing, China

The recent discovery of high temperature superconductivity in nickelate systems has generated tremendous interests in the community. The core issue to understand the pairing mechanism is about the superconducting gap and its symmetry. We have successfully synthesized the superconducting thin films of $La_2PrNi_2O_7$ with T_c^{onset} = 41.5 K, and measured the superconducting tunneling spectra after we expose the superconducting layer by using the tip-excavation technique. The spectrum shows a two-gap structure with Δ_1 = 9 meV, Δ_2 = 6-8 meV, and fittings based on the Dynes model indicate that the dominant gap should have an s-wave structure with low anisotropy, this allows us to select the s^{+-}-pairing symmetry among the two possibilities s^{+-} and d-wave. Furthermore, a clear bosonic mode with energy $\Omega = 30 \pm 2$ meV is observed, which further supports a sign reversal gap[1]. Our results shed new light in understanding the mystery of superconductivity in bilayer nickelate superconductors.

Collaborators: Huan Yang, Ilya M. Eremin, Shengtai Fan, Mengjun Ou, Marius Scholten, Qing Li, Zhiyuan Shang, Yi Wang, Jiasen Xu

[1] S. Fan et al., arXiv: 2506.01788

TT 39.6 Wed 12:15 HSZ/0003

Investigation of Ruddlesden-Popper nickelates and the monolayer-trilayer polymorph using Raman spectroscopy — •Vignesh Sundaramurthy[1], Abhi Suthar[1], Pascal Puphal[1,2], Hasan Yilmaz[3], Masahiko Isobe[1], Matteo Minola[1], Bernhard Keimer[1], and Matthias Hepting[1] — [1]Max-Planck-Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany — [2]2^{nd} Physics Institute, University of Stuttgart, 70569 Stuttgart, Germany — [3]University of Stuttgart, Institute for Materials Science, Materials Synthesis Group, Heisenbergstraße 3, 70569 Stuttgart, Germany

Ruddlesden-Popper nickelates have attracted intense interest following the discovery of superconductivity in several members of the series, including bilayer $La_3Ni_2O_7$, trilayer $La_4Ni_3O_{10}$, and structural polymorphs composed of monolayer-bilayer or monolayer-trilayer (ML-TL) units. In this talk, we explore the phononic and electronic Raman responses of high-quality ML-TL single crystals and contrast them with those of the other nickelate phases, using samples with optimized oxygen content.

TT 39.7 Wed 12:30 HSZ/0003

Multiorbital density wave in the trilayer nickelate $La_4Ni_3O_{10}$ — Abhi Suthar[1], Vignesh Sundaramurthy[1], Matias Bejas[2], Congcong Le[3], Pascal Puphal[1], Pablo Sosa-Lizama[1], Masahiko Isobe[1], Peter A. van Aken[1], Y. Eren Suyolcu[1], Matteo Minola[1], Andreas P. Schnyder[1], Xianxin Wu[4], Bernhard Keimer[1], Giniyat Khaliullin[1], Andres Greco[2], and •Matthias Hepting[1] — [1]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [2]UNR-CONICET, Rosario, Argentina — [3]RIKEN, Saitama, Japan — [4]Institute of Theoretical Physics, Beijing, China

Ruddlesden–Popper nickelates exhibit high-temperature superconductivity closely intertwined with charge and spin density wave order. However, fundamental questions persist regarding the orbital character and symmetry underlying the density wave instabilities. Using polarized Raman scattering on trilayer $La_4Ni_3O_{10}$, we resolve characteristic phonon anomalies and a redistribution of electronic spectral weight across the density wave transitions. Momentum-selective electronic Raman responses, combined with multiorbital model calculations, reveal a density-wave–induced gap with incoherent, non-mean-field opening and contributions from both Ni-$d_{x^2-y^2}$ and d_{z^2} states [1]. These results reconcile conflicting experimental reports of the density wave gap and underscore its multiorbital character.

[1] A. Suthar *et al.*, arXiv:2508.06440 (2025).

TT 40: Focus Session: Quantum Sensing with Solid State Spin defects II (joint session TT/HL/MA)

Time: Wednesday 9:30–10:30 Location: HSZ/0101

TT 40.1 Wed 9:30 HSZ/0101

Locally Imaging the Insulator to Metal Transition of Ca_2RuO_4 with Single Spin Magnetometry — •Hayden Binger[1], Cissy Suen[2], Young-Gwan Choi[1], Yejin Lee[1], Haolin Jin[1], Max Krautloher[2], Yuchen Zhao[1], Luke Turnbull[1], Elina Zhakina[1], Jeffrey Neethirajan[1], Lotte Boer[1], Berit Goodge[1], Piotr Surówka[3], Roderich Moessner[4], Bernhard Keimer[2], Claire Donnelly[1], and Uri Vool[1] — [1]MPI CPfS, Dresden, Germany — [2]MPI FKF, Stuttgart, Germany — [3]Wrocław University of Science and Technology, Wrocław, Poland — [4]MPI PKS, Dresden, Germany

The current-driven insulator to metal transition (IMT) in Ca_2RuO_4 is a fascinating phenomenon where increasing current driven across a sample causes a smaller voltage difference to develop. We have created devices of size 10-20 um by 10-20 um and 100 nm thick using Focused Ion Beam (FIB) milling. Through the utilization of Nitrogen Vacancies (NV), optically addressable spin-1 defects acting as a qubit at room temperature, we probe the local magnetic field at the defect via the Zeeman interaction. We are thusly able to image the local character of the insulator to metal transition in Ca_2RuO_4. At low currents we image the formation of a singular conducting channel at the edge of the device, which gradually grows throughout the entire device as more current is applied until eventually current flows evenly across the device. We explore reasons why local current channels nucleate at the edge, such as strain, defects, and crystalline lattice orientation.

TT 40.2 Wed 9:45 HSZ/0101

Topological Ambiguity in Stray Field Magnetometry — •Shirsopratim Chattopadhyay[1,2] and Aparajita Singha[1,2] — [1]IFMP, TU Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence (ct.qmat)

Inferring magnetic topology from stray field measurements is central to characterizing skyrmions, vortices, and other topological textures. Yet, the uniqueness of such reconstructions remains poorly characterized. We present a computational framework to systematically generate pairs of magnetization configurations with distinct topological charges ($|\Delta Q| = q$, where q can be set by the user) that produce nearly identical stray fields (Normalized Root Mean Square Error ~ 0.8-4 percent). Our approach uses constrained optimization with a physics informed loss to jointly evolve magnetization pairs towards field degeneracy while preserving topological distinction. Across 200 randomized trials with varied initializations, we demonstrate rapid and reliable generation of adversarial pairs spanning skyrmions, merons, fractional defects and uniform domain textures. We theoretically analyse the relation between topological charge and stray field and construct an explicit example of near identical stray field from distinct topologies. Our adversarial dataset enables rigorous assessment of magnetization reconstruction algorithms and guides the design of measurement strategies capable of resolving topological ambiguity.

TT 40.3 Wed 10:00 HSZ/0101

Towards Cryogenic Scanning Nitrogen Vacancy Magnetometry — •Lotte Boer[1], Kilian Srowik[1], Hayden Binger[1], Young-Gwan Choi[1], Ahmet Ünal[1], Edouard Lesne[1], Matheus Barbosa[2], Bernd Büchner[2], Alexey Popov[2], and Uri Vool[1] — [1]MPI CPfS, Dresden, Germany — [2]IFW Dresden, Germany

In scanning nitrogen vacancy (NV) magnetometry, an atomic force microscopy tip is replaced with a diamond pillar containing a single NV center, which acts as a highly sensitive magnetic field sensor. Scanning over a sample then allows to map the magnetic stray field. This method has been widely used at room temperature to investigate, for example, magnetic textures in thin films or local current flow patterns. However, a wide range of interesting material properties, such as emergent magnetic phases and superconductivity only occur at lower temperatures. As the NV center retains its ability to sense magnetic fields at low temperatures, we are developing a variable temperature cryogenic scanning NV system. This will not only allow for the imaging of materials at low temperatures, but also allow for the unique opportunity of mapping magnetic phase transitions in quantum materials.

Building a cryogenic NV setup presents several challenges, as the NV requires optical access for readout and microwave pulses for control, all within tight spatial confines and while preventing sample heating. In this talk, we will discuss our setup, which is in its final stages of development, and show preliminary measurement results at few Kelvin temperatures.

TT 40.4 Wed 10:15 HSZ/0101

CISS from Vibrationally Assisted Tunneling in Chiral Molecules — •Fedor Baranov, Virginia Gali, and Maxim Breitkreiz — Dahlem Center for Complex Quantum Systems, Freie Universitat Berlin, Arnimallee 14, 14195 Berlin, Germany

Chiral-induced spin selectivity (CISS) remains a puzzling phenomenon, despite extensive experimental evidence. A possible explanation emerges when recognizing that charge transport through chiral insulating molecules occurs in the tunneling regime, where even small spin-orbit coupling becomes crucial inside the barrier. This enhancement leads to a spin-dependent potential that gives different tunneling probabilities for different spin orientations. Because this tunneling alone produces extremely small currents, one has to take into account the vibrational degrees of freedom of the system that in the static limit increases the current while preserving the spin splitting nature. Together, these ingredients offer a transparent physical mechanism underlying the CISS effect.

TT 41: Topological Semimetals

Time: Wednesday 9:30–12:30 Location: HSZ/0103

TT 41.1 Wed 9:30 HSZ/0103

Pushing transport to the edge: Inducing superconductivity in WTe_2 — •Marieke Altena, Guido Wiersma, Jort Verbakel, Esra van 't Westende, Pantelis Bampoulis, Alexander Brinkman, and Chuan Li — MESA+ Institute for Nanotechnology, University of Twente, 7500 AE, Enschede, The Netherlands

WTe_2 is a type-II Weyl semimetal hosting higher-order topological states (HOTS) protected by crystal symmetries and characterized by quantum spin Hall-like spin-momentum locking. These states are of particular interest for quantum computing. Recent studies have reported anomalous edge-enhanced supercurrents in WTe_2-based Josephson junctions [1,2].

To reveal the topological nature and test the robustness of HOTS, we measured the electronic transport properties of thin, nanometer sized WTe_2 devices at low temperatures. Superconductivity was successfully induced into the WTe_2 flakes by using superconducting Nb-contacts. We observe a strong enhancement of the supercurrent at the edge of the WTe_2 flake by studying single junctions. Interestingly, the enhancement of the supercurrent at the edge is also observed at a step in the middle of the flake. The current-phase relation is also measured via superconducting quantum interference devices (SQUID), which provides the insight to its topological properties. The topological nature of these states is studied with RF Shapiro measurements and DC SQUID measurements.

[1] Choi et al., Nat. Mater. 19, 974 (2020).
[2] Endres et al., Nano Letters 23, 4654 (2023).

TT 41.2 Wed 9:45 HSZ/0103

Terahertz third-harmonic generation of lightwave-driven Weyl fermions far from equilibrium — •Patrick Pilch[1], Changqing Zhu[1], Sergey Kovalev[1,2], Renato M. A. Dantas[3,4], Amilcar Bedoya-Pinto[5,6], Stuart S. P. Parkin[5], and Zhe Wang[1] — [1]TU Dortmund University, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Germany — [3]University of Basel, Switzerland — [4]University of Minho, Portugal — [5]Max Planck Institute for Microstructure Physics, Halle, Germany — [6]University of Valencia, Spain

We report on time-resolved ultrafast terahertz third- harmonic generation spectroscopy of nonequilibrium dynamics of Weyl fermions in a nanometer thin film of the Weyl semimetal TaP [1]. Terahertz third-harmonic generation is observed at room temperature under the drive of a multicycle narrowband terahertz pulse with a peak field strength of down to tens of kV/cm. The observed terahertz third-harmonic generation exhibits a perturbative cubic power-law dependence on the terahertz drive. By varying the polarization of the drive pulse from linear to elliptical, we realize a sensitive tuning of the third harmonic yield. By carrying out theoretical analysis based on the Boltzmann transport theory, we can properly describe the experimental results and ascribe the observed THz nonlinearity to field-driven kinetics of the Weyl fermions.

[1] P. Pilch et al., *Nano Lett.* (2025), DOI: 10.1021/acs.nanolett.5c04143

TT 41.3 Wed 10:00 HSZ/0103

Quantum Geometric Origin of Intrinsic Nonlinear Hall effects — •Yannis Urich[1,2], Johannes Mitscherling[3], Laura Classen[1,2], and Andreas Schnyder[1] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart, Germany — [2]School of Natural Sciences, Technische Universität München, D-85748 Garching, Germany — [3]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, D-01187 Dresden, Germany

We decompose the intrinsic second-order nonlinear Hall effect (NLHE) of a generic multiband system into quantum geometric contributions using a fully quantum-mechanical projector formalism. Expanding the nonlinear conductivity in powers of the quasiparticle lifetime τ, we recover the established Berry curvature dipole at order τ and clarify discrepancies in prior work concerning the (interband) quantum metric dipole (also called Berry curvature polarizability) at order τ^0. Our method further reveals an additional order-τ^0 term, determined by the *intraband* quantum metric dipole (intraQMD), which originates from virtual interband transitions captured only within the fully quantum-mechanical treatment. The intraQMD is generically nonzero in systems with broken time-reversal symmetry and can be identified independently by symmetry. We highlight candidate materials expected to exhibit a large intrinsic NLHE, including the topological antiferromagnet Yb_3Pt_4. Finally, we discuss the extension of this framework to higher-order nonlinear responses, which requires a structured understanding of higher-order quantum geometry beyond Berry curvature and quantum metric.

TT 41.4 Wed 10:15 HSZ/0103

Raman spectroscopic evidence for linearly dispersed nodes and magnetic ordering in the topological semimetal $V_{1/3}NbS_2$ — •Shreenanda Ghosh[1,2], Chris Lygouras[1], Zili Feng[3], Mingxuan Fu[3], Satoru Nakatsuji[1,3], and Natalia Drichko[1] — [1]Institute for Quantum Matter and William H. Miller III Department of Physics and Astronomy, Johns Hopkins University, Baltimore, USA — [2]Institute of Physics, University of Münster, Germany — [3]Department of Physics, University of Tokyo, Japan

We report polarization-resolved magnetic and electronic Raman scattering of the intercalated transition metal dichalcogenide $V_{1/3}NbS_2$, proposed as a Weyl semimetal [1,2]. The electronic scattering reveals a linear with frequency continuum of excitations, as the signature of electronic transitions within the proposed Weyl nodes in a 2D electronic structure [3]. Additionally, two-magnon excitations of V moments are observed near 15 meV in the magnetically ordered phase below 50 K[3], which are well reproduced by calculations using spin wave exchange parameters [4] and confirm the antiferromagnetic character of the order. These magnetic and electronic scattering, observed in the same spectra, provide independent spectroscopic evidence for a collinear antiferromagnetic Weyl semimetal state in $V_{1/3}NbS_2$.

[1] M. K. Ray et al., Nat Com 16, 3532 (2025).
[2] H. Wang et al., Phys. Rev. B 107, 134436 (2023).
[3] S. Ghosh et al., arXiv:2504.04590 (2025).
[4] K. Lu et al., Phys. Rev. Mat 4, 054416 (2020).

TT 41.5 Wed 10:30 HSZ/0103

Large tunability of the magnetism in the Dirac semimetal $EuMnBi_2$ under uniaxial pressure — •Caitlin I. O'Neil[1], Hilary M.L. Noad[1], Andrew P. Mackenzie[1], Hideaki Sakai[2], and Elena Gati[1,3] — [1]MPI-CPfS, Dresden — [2]Tohoku University, Japan — [3]Goethe University Frankfurt

Uniaxial pressure provides a controlled method for breaking lattice symmetries in crystals, and it has therefore become a powerful tool for tuning quantum materials. Although uniaxial-pressure techniques have been widely used in recent years to probe the coupling between correlated electrons and the lattice [1-2], their use to investigate the interplay between topological electrons, magnetism, and the lattice has been less common. We report on the discovery of a strong uniaxial pressure response in the magnetic Dirac semimetal $EuMnBi_2$. In this material, there are layers of localised Eu^{2+} moments alternating with Bi square nets that host Dirac fermions. By measuring the AC Young's modulus [3], we map out the phase diagram as a function of [1 0 0] uniaxial pressure and magnetic field, revealing a strong sensitivity of the Eu^{2+} magnetic order to strain, including the observation of multiple magnetic phases. We suggest that the pronounced tunability of the Eu^{2+} order arises from its coupling to a low-energy electronic structure that is sensitive to symmetry-breaking strains.

Work is supported by the DFG through TRR 288-422213477.

[1] Gati *et al.*, Sci. Adv. **2**, e1601646 (2016)
[2] Noad *et al.*, Science **382**, 447 (2023)
[3] O'Neil *et al.*, RSI **95**, 073909 (2024)

15 min. break

TT 41.6 Wed 11:00 HSZ/0103

Novel difference-frequency quantum oscillations in $MoSi_2$ — •Ivan Volkau[1], Nico Huber[2], Louw Feenstra[1], Andreas Bauer[1,4], Christian Pfleiderer[1,3,4], and Marc A. Wilde[1,4] — [1]Technical University of Munich (TUM) — [2]Cornell University — [3]MCQST, Munich — [4]TUM Zentrum für Quantum Engineering

Recently, we established temperature-stable quantum oscillations of the quasiparticle lifetime (QPLOs) in CoSi (space group $P2_13$) [1]. QPLOs may shed new light on scattering processes in materials, since they arise in transport properties at finite coupling between semi-classical Onsager orbits. $MoSi_2$ (space group *I4/mmm*) exhibits a difference frequency in its SdH spectra, composed of distinct low- and high-temperature (LT and HT) components. The temperature stability and the absence in thermodynamic properties of the HT component is consistent with the theoretical framework of QPLOs [2]. Conversely, the LT component cannot be attributed to QPLOs, as it is observed in both SdH and dHvA measurements. Furthermore, its phase shift of approximately $0.75(10)\pi$ relative to the HT component is inconsistent with standard non-Onsager mechanisms, such as magnetic breakdown, magnetic interaction, or chemical potential oscillations [3]. In this work, we present a detailed study of quantum oscillations in $MoSi_2$, analyzing the interplay between these components to clarify the nature of the scattering mechanisms involved.

[1] Huber et al., Nature **621**, 276 (2023)
[2] Leeb et al., PRB **108**, 054202 (2023)
[3] Leeb et al., APR, Vl4, Is4 2400134 (2025)

TT 41.7 Wed 11:15 HSZ/0103

Probing the Fermi Surface of $NdAgSb_2$ through Large Linear Magnetoresistance and Quantum Oscillations — •Aarti Gautam[1], Haribrahma Singh[1], Prabuddha Kant Mishra[3], Rie. Y Umetsu[4], and Ashok Kumar Ganguli[1,2] — [1]Indian Institute of Technology Delhi, Hauz Khas New Delhi — [2]Indian Institute of Science Education and Research, Berhampur — [3]Institute of Low Temperature and Structure Research, Polish Academy of Sciences, ul. Okolna 2, 50-422 Wroclaw, Poland — [4]Institute for Materials Research, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan

We present a comprehensive study of the magnetic, transport, and magnetotransport properties of single-crystalline $NdAgSb_2$. The compound exhibits anisotropic magnetic behavior, with an antiferromagnetic ground state for fields applied in the ab plane and de Haas van Alphen oscillations observed along the c axis. Magnetotransport measurements reveal a large linear magnetoresistance (450 % at 2 K under 9 T), indicative of a clean-limit electronic structure with suppressed scattering. Notably, both de Haas van Alphen and Shubnikov de Haas quantum oscillations are observed simultaneously, enabling a detailed mapping of the Fermi surface. Analysis of the oscillation frequencies, effective masses, and Berry phases provides insight into the low-energy electronic states governed by the two-dimensional Sb square-net topology, highlighting $NdAgSb_2$ as a model system to explore the interplay of anisotropic magnetism, high-mobility carriers, and quantum oscillations in layered rare-earth pnictides.

TT 41.8 Wed 11:30 HSZ/0103

Topological Dirac Semimetal Carbon Nanoscroll — •Tzu-Ching Hsu[1], Jhih-Shih You[1], Hsiu-Chuan Hsu[2], and Ion Cosma Fulga[3] — [1]Department of Physics, National Taiwan Normal University, Taipei, Taiwan, — [2]Graduate Institute of Applied Physics, National Chengchi University, Taipei, Taiwan — [3]Institute for Theoretical Solid State Physics, IFW Dresden, Dresden, Germany

Carbon nanoscrolls (CNS), rolled-up structures formed from single-layer graphene, have recently attracted significant attention owing to their distinctive geometry. In this work, we theoretically investigate the topological properties of a series of CNS under different axial magnetic fields and various edge alignment conditions, within the large-radius approximation. As a function of magnetic field strength and the number of turns in the scroll, these systems host topologically protected Dirac cones, which survive even when chiral symmetry is broken. Furthermore, the number of Dirac cones, their real-space probability density, and the magnetic flux at which they occur can be controlled deterministically, being dictated by the system's symmetries. Our results establish a foundation for further studies of the fundamental physics and potential applications of CNS and other two-dimensional materials with similar geometries.

TT 41.9 Wed 11:45 HSZ/0103

End spin formation in capped carbon nanotubes — •István Markó[1], Dominik Szombathy[1,2], Cătălin P. Moca[4,2], and Gergely Zaránd[1,3] — [1]Budapest University of Technology and Economics, Budapest, Hungary — [2]Nokia Bell Labs Budapest site, Hungary — [3]HUN-REN–BME Quantum Dynamics and Correlations, Budapest, Hungary — [4]University of Oradea, Oradea, Romania

Semiconducting open carbon nanotubes (CNTs) have been shown to exhibit topological bound states within the spectral gap [1], giving rise to spin formation at the ends of the nanotube [2]. However, the production of open-ended CNTs is difficult. Here, we investigate the electronic properties of capped topological

CNTs using exact diagonalization and Chebyshev expansion methods to identify local resonances and bound states in the density of states at the end of long tubes [3]. While capping removes topological states, non-topological bound states and resonances localized on the pentagons appear, presumably related to Euler topology. We observe an abundance of local resonances and bound states, and about 20% of the investigated stable caps are predicted to produce end spins [4]. We identify a specific CNT of chirality (6,5) which produces well-defined end spins. This type of CNT can be produced with ultra-high purity (>95%) [5], and is an excellent candidate for a geometrically controlled spin qubit.

[1] W. Izumida, et al. Phys. Rev. B 93, 195442 (2016).
[2] C. P. Moca, et al. Phys. Rev. Lett. 125, 056401 (2020).
[3] A. Weiße, et al. Rev. Mod. Phys. 78, 275 (2006).
[4] I. Markó, et al. unpublished
[5] S. Shiina, et al. ACS Nano 18, 23979 (2024)

TT 41.10 Wed 12:00 HSZ/0103

Anomalous Fractional Chiral Currents in Step Edges of Weyl Semimetals — •Oskar Schweizer[1], Virginia Gali[1], Piet Brouwer[1], Gal Lemut[1], Adam Yanis Chaou[2], and Maxim Breitkreiz[1] — [1]Dahlem Center for Complex Quantum Systems and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — [2]Donostia International Physics Center (DIPC), 20018 Donostia-San Sebastián, Spain

Bulk-boundary correspondence predicts surface states in Weyl semimetals (WSM) only when the 3d bulk Weyl-node separation projects nontrivially onto a given 2d surface. However recent experiments report states on surfaces where no such protected modes are expected, localized instead to 1d step-edge defects. We study such WSM surfaces with step edges and find chiral currents bound to the steps, even though the surface itself hosts no protected modes. Remarkably, these currents can take fractional, non-integer values determined solely by the bulk Weyl-node separation.

TT 41.11 Wed 12:15 HSZ/0103

Correlated Hopf Insulators — •Konstantinos Ladovrechis[1] and Shouvik Sur[2] — [1]Ruhr Universität Bochum, Germany — [2]Rice University, USA

Hopf insulators represent an exceptional class of topological matter, unanticipated by the periodic table of topological invariants. These systems point to the existence of previously unexplored states of matter with unconventional topology. In this work, we take a step toward exploring this direction by investigating correlation-driven instabilities of Hopf insulators. Organizing our analysis around the topological quantum critical point that separates the Hopf insulating phase from a trivial insulator, we demonstrate the emergence of unconventional Weyl semimetallic and topological insulating states. Notably, upon doping, the Weyl semimetal supports non-reciprocal superconductivity and a Bogoliubov-Fermi surface, potentially providing a novel framework for realizing the superconducting diode effect. Finally, we highlight the interconnectedness of the effective descriptions of correlated Hopf insulators, two-dimensional quadratic band-touching semimetals, and Luttinger semimetals.

TT 42: Other Transport Topics

Time: Wednesday 9:30–12:45 Location: HSZ/0105

TT 42.1 Wed 9:30 HSZ/0105

Enhancement of the thermopower of Anderson impurity by Van Hove singularities in graphene nanoribbons — •Damian Krychowski and Krzysztof Wójcik — Institute of Molecular Physics, Polish Academy of Sciences, M. Smoluchowskiego 17, 60-179 Poznań, Poland

We present results from the numerical renormalization group theory of spin-1/2 ad-atom coupled to contacts made of zigzag graphene nanoribbons (ZGNRs). We propose tuning ZGNRs with a transverse electric field [1] and back gates such that they exhibit one of their asymmetric power-law Van Hove singularities at the Fermi level. We demonstrate that, under these conditions, the local spectral density of the ad-atom spin exhibits a sharp and asymmetric pseudo-gap despite complete Kondo screening. This ensures weak charge conductance and a large Seebeck coefficient at low and moderate temperatures, leading to a high figure of merit over a wide temperature range and impurity energy level. A similar enhancement of the Seebeck coefficient is observed in magic-angle twisted bilayer graphene with a highly particle-hole asymmetric band, though it occurs at a different energy scale [2]. At a set temperature, the sign of thermopower of Kondo-correlated system can be further tuned by dragging the singularity through the Fermi level with gate voltage.

[1] Y.-W. Son, M. L. Cohen and S. G. Louie, Nature 347, 444 (2006).
[2] A. K. Paul et al., Nat. Phys. 18, 691 (2022).

TT 42.2 Wed 9:45 HSZ/0105

Dynamical current as a spin-state discriminator in open-shell GNR's — •Nico Leumer[1], Geza Giedke[2], and Thomas Frederiksen[2] — [1]Wrocław Tech — [2]Donostia International Physics Center

The recent advances of surface synthesis unlocked the potential of open-shell physics in graphene nanoribbons (GNRs) which ever since have gained significant attention. Normally chemically unstable, these structures feature unpaired, localized p_Z-electrons pinned at zero energy, giving rise to the unique phenomenon of π-magnetism. At half-filling certain GNRs host quasi degenerate spin singlets/triplets states with a vanishing energy gap for long ribbons and without significantly increasing the gap conventional current-based measurements hardly distinguish these spin textures.

In our setup charge current $I(t)$ discriminates between the responsible states –even for a vanishing gap– by means of a Spin-Pauli blockade (SPB). We discuss how our setup preserves the states, how their distinct spatial profile causes different charging energies and such that a variation of the reservoirs chemical potentials allow the isolation of singlet/triplet signals.

Rather than considering only ensembles of measurements or repetitions, our setup allows for single-shot experiments simulated by Monte-Carlo trajectories. From relative frequencies, we estimate overhaul time-scale $\Delta t = 6\hbar/\Gamma$ for a successful identification of the spin. For experiments on shorter time scales, we report on the fidelity and the necessary time for a confident identification of the state.

TT 42.3 Wed 10:00 HSZ/0105

Single Spin-Flip Dynamics in the Ising Model — •Luca Cervellera, Fred Hucht, and Björn Sothmann — University of Duisburg-Essen, Duisburg, Germany

We investigate the real-time spin-flip dynamics of the 1D Ising model by means of waiting time distributions between subsequent spin flips. At large temperatures the waiting time distribution shows an exponential decay due to thermal excitation and relaxation of spins. At low temperatures, the waiting time distribution is dominated by an algebraic decay caused by domain wall motion. The latter can be suppressed by an external magnetic field. Our results are relevant to understand the dynamics of dimer flipping on the Si(001) surface [1].

[1] C. Brand et al., Phys. Rev. Lett. **130**, 126203 (2023).

TT 42.4 Wed 10:15 HSZ/0105

Universal relations between thermoelectrics and noise in mesoscopic transport across a tunnel junction — •Andrei Pavlov[1] and Mikhail Kiselev[2] — [1]TKM, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]The Abdus Salam International Centre for Theoretical Physics, Strada Costiera 11, I-34151 Trieste, Italy

We develop a unified theory of weakly probed differential observables for currents and noise in transport experiments. Our findings uncover a set of universal transport relations between thermoelectric and noise properties of a system probed through a tunnel contact, with the Wiedemann-Franz law being just one example of such universality between charge and heat currents. We apply this theory to various quantum systems, including multichannel Kondo, quantum Hall and Sachdev-Ye-Kitaev quantum dots, resonant impurity and two-stage Kondo models, and demonstrate that each of the microscopic theories is characterized by a set of universal relations connecting conductance and thermoelectrics with noise. Violations of these relations indicate additional energy scales emerging in a system.

TT 42.5 Wed 10:30 HSZ/0105

Relaxation to persistent and oscillating currents in simply and doubly frustrated spin systems coupled to fermionic baths — •Nikodem Szpak[1], Gernot Schaller[2], Ralf Schützhold[2,3], and Jürgen König[1] — [1]Fakultät für Physik and CENIDE, Universität Duisburg-Essen, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [3]Institut für Theoretische Physik, Technische Universität Dresden, Germany

We study relaxation dynamics in a strongly-interacting three and four-site Fermi-Hubbard system (quantum dots) coupled to environment represented by fermionic baths. We analyze the simply frustrated (trimer) and doubly frustrated (tetrahedron) spin geometries to observe the relaxation to steady states containing persistent or oscillating spin currents. Due to high sensitivity of these results to the coherence of the final state, we can test several variants of the Lindblad master equations, derived under different assumptions and parameter regimes: local and global, secular and coherent.

[1] E. Kleinherbers, N. Szpak, J. König, and R. Schützhold, Phys. Rev. B 101, 125131 (2020)

[2] G. Schaller, F. Queisser, N. Szpak, J. König, and R. Schützhold, Phys. Rev. B 105, 115139 (2022)
[3] N. Szpak, G. Schaller, R. Schützhold and J. König, Phys. Rev. B 110, 115131 (2024)

TT 42.6 Wed 10:45 HSZ/0105

Fluctuation Spectroscopy and Filament Simulations on HfO_2 RRAM devices — •Demian Ranftl[1], Yingxin Li[2], Tristan Stadler[1], Eszter Piros[2], Philipp Schreyer[2], Taewook Kim[2], Lambert Alff[2], and Jens Müller[1] — [1]Institute of Physics, Goethe University, Frankfurt am Main, Germany — [2]Institute of Materials Science, TU Darmstadt, Darmstadt, Germany

Low-frequency noise spectroscopy plays a crucial role in understanding resistive switching mechanisms and filament dynamics in RRAM devices [1]. In this work, we compare the noise characteristics of undoped [2] and La-doped [3] HfO_2-based devices across multiple resistance states and during DC cycling. Measurements are complemented by phenomenological simulations that assume various states of a stable filament with differing amounts of surrounding defects. The results provide new insights into the roles of filament geometry and defect densities on resistance and noise behaviour. We identify multi-stage resistance-noise scaling relationships, highlighting the competition between trap numbers and system size. These findings offer deeper insight into switching dynamics and the role of doping in modulating noise sources, contributing to the optimisation of RRAM configurations for neuromorphic applications.

[1] J. Müller, Contemporary Physics **29** (2025)
[2] P. Schreyer, N. Kaiser *et al.*, ACS Appl. Mater. Interfaces (2025)
[3] T. Kim, M. Major *et al.*, Adv. Electron. Mater. (2025)

15 min. break

TT 42.7 Wed 11:15 HSZ/0105

Symmetry breaking in the non-degenerate parametric oscilator — •Jonathan Schluck, Steven Kim, and Fabian Hassler — Institute for Quantum Information, RWTH Aachen University, 52074 Aachen, Germany

Two harmonic oscillators that are parametrically driven at the sum of their natural frequencies exhibit an instability once the driving strength exceeds the damping. Close to and beyond this instability threshold, nonlinearities must be taken into account. As a consequence of the instability, the system develops a separation of time scales, which can be used to derive an effective Liouvillian describing the long-time dynamics. The effective model possesses a U(1)-symmetry akin to that of a laser. Above the transition, a symmetry-broken state with a fixed phase exhibits an extended lifetime, indicating the symmetry breaking. The phase coherence of this state increases with increasing photon number, following the conventional Schawlow-Townes limit. We propose a measure of symmetry breaking that compares the photon lifetime to the dephasing time in the lasing regime.

TT 42.8 Wed 11:30 HSZ/0105

Reconfigurable Optoelectronics at the Single-Molecule Level — •Atif Ghafoor — Department of Physics, Nanoscience Center, University of Jyväskylä, Jyväskylä, Finland.

Controlling exciton and its coupling at the single-molecule scale is a fundamental challenge for nanoscale optoelectronics and quantum technologies. The ability to precisely reposition individual atom within a single-molecule to alter transition dipole moment, thereby enabling on-demand switching of light emission, remains an unrealized yet transformative goal in single-molecule optoelectronics. Here, by displacing the central metal atom of a planar phthalocyanine molecule adsorbed on decoupling layer, we demonstrate active control over its transition dipole moment, leading to suppression or enhancement of light emission via scanning tunneling microscopy-induced luminescence. Through this atomic-scale control, we designed a tunable homogenous dimer in three distinct optical states: a non-emissive state, a single-molecule-like emissive state, and a coupled state (subradiant and superradiant modes) directly revealing intermolecular dipole-dipole coupling. Furthermore, we realized a heterodimer, in which resonant energy transfer can be switched on or off simply by controlling the dipole of the acceptor molecule. Our strategy for manipulating transition dipole moment and optical emission, not only enables deeper exploration of plasmon-exciton coupling, tunable dipole-dipole interaction, and tunable energy transfer dynamics at the single-molecule level but also stimulates the development of single-molecule quantum engineering and atomically reconfigurable optoelectronic devices.

TT 42.9 Wed 11:45 HSZ/0105

Negative electronic friction and non-Markovianity in charge transport through molecular nanojunctions — •Riley Preston[1], Samuel Rudge[1], Daniel Kosov[2], and Michael Thoss[1] — [1]Institute of Physics, University of Freiburg — [2]College of Science and Engineering, James Cook University

The electronic friction approach is a popular mixed quantum-classical method for modeling the dynamics of atoms and molecules at metal or semiconductor surfaces. If the electrons are far from equilibrium, such as in molecular nanojunctions at high bias voltages, the electronic friction coefficient can become negative, meaning it acts to amplify the nuclear vibrations in the molecular bridge rather than dampen them, triggering bond rupture and a loss of device functionality. The physicality of negative electronic frictions has long been debated, owing to the hierarchy of underlying assumptions upon which the electronic friction method is built. We investigate the emergence of negative electronic friction in a donor-acceptor model of a molecule in a molecular nanojunction. We observe that negative electronic frictions arise predictably at high bias voltage according to the geometry of the donor and acceptor on the molecular bridge, resulting in large vibrational excitations that are validated by comparison to numerically exact quantum data calculated with the hierarchical equations of motion approach. However, we also show that the same physical conditions that give rise to negative electronic friction are also suggestive of non-Markovian dynamics, challenging the underlying assumptions of the electronic friction approach.

TT 42.10 Wed 12:00 HSZ/0105

Vibrational Instabilities in Molecular Nanojunctions - The Role of Anharmonic Nuclear Potentials — •Martin Mäck, Samuel Rudge, Riley Preston, and Michael Thoss — Institute of Physics, University of Freiburg

Current-induced vibrational excitation is a key factor determining the stability of molecular nanojunctions. Beyond conventional Joule heating, a different mechanism caused by nonconservative current-induced forces has been reported for models with multiple vibrational modes, leading to vibrational instabilities already at low bias voltages [1].

So far, this mechanism has only been investigated for harmonic nuclear potentials [1,2]. A natural question, is whether this effect can also be observed in more realistic models with anharmonic potentials and if it has a measurable impact on observables such as the dissociation probability of the junction. In this contribution, we apply a mixed quantum-classical approach based on electronic friction and Langevin dynamics [2,3] to different anharmonic model systems, studying the influence of anharmonicity on the reported instability and the dissociation dynamics of the junction. The results show that, in our models, anharmonic nuclear potentials destroy the mechanism leading to vibrational instabilities.

[1] J.-T. Lü, M. Brandbyge, P. Hedegård, T.Todorov, D. Dundas, Phys. Rev. B **85**, 245444 (2012)
[2] M. Mäck, M. Thoss, S. Rudge, Phys. Rev. B **112**, 075430 (2025)
[3] R. J. Preston and D. S. Kosov, J. Chem. Phys. **158**, 224106 (2023)

TT 42.11 Wed 12:15 HSZ/0105

Thermodynamic and kinetic uncertainty relations in topological surface states — •Phillip Mercebach[1], Pablo Burset[1], and Sun-Yong Hwang[2] — [1]Department of Theoretical Condensed Matter Physics and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049 Madrid, Spain — [2]Theoretische Physik, Universitat Duisburg-Essen and CENIDE, D-47048 Duisburg, Germany

Strong fluctuations in nanoscale devices can hinder output precision, while the unavoidable entropy production is detrimental to performance. Device operation can be optimized to achieve a strong output signal while minimizing noise, entropy, and frenesy. However, there are fundamental constraints between the output and these drawbacks: the thermodynamic uncertainty relation (TUR) quantifies the trade-off between signal-to-noise ratio (SNR) and entropy, while the kinetic uncertainty relation (KUR) describes the trade-off between SNR and frenesy. Both relations are especially interesting as quantum coherent processes can yield output precisions surpassing classical limits. Here, we study TUR and KUR in a ballistic junction comprised of a 3D topological insulator (3DTI) in proximity to a ferromagnet. The 3DTI surface states, in combination with the ferromagnet, enable near-Carnot efficiency, indicating low entropy production [1]. We demonstrate that the SNR in this device becomes very high at optimum temperatures and voltage bias, where the thermal and shot noises are rather suppressed.

[1] P. Mercebach et. al., arXiv:2508.20969

TT 42.12 Wed 12:30 HSZ/0105

Electromagnetic chiral anisotropy of the semiconducting $LaRhC_2$-enantiomorphs — •Volodymyr Levytskyi[1], Ulrich Burkhardt[2], Markus König[2], Eteri Svanidze[2], Yuri Grin[2], and Roman Gumeniuk[1] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg, Freiberg, Germany — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden, Germany

In past decades, the majority of research is focused on chiral crystalline solids due to their non-trivial spin and charge transport properties. However, the preparation of mono-chiral samples is a complicated task – perhaps explaining why the influence of chirality on electrical properties has remained almost unexplored. EBSD (electron backscatter diffraction) -based enantiomorph distribution maps allow the extraction and shaping of suitable microdevices from polycrystalline material by the FIB (focused ion beam) micropreparation method. Here, we present results on the electrical transport studied on the mono-chiral, crystallographically oriented, single-crystalline $LaRhC_2$ (space groups $P4_1$ or $P4_3$) microdevices. Significant anisotropy of the electrical resistivity is observed for each enantiomorph, both parallel to and normal to the fourfold screw axis. The different linear coefficients of the longitudinal magnetoresistivity probed

along the fourfold screw axis for the nonmagnetic right-handed (4_1-axis) and left-handed (4_3-axis) $LaRhC_2$ crystals in the oriented magnetic field parallel and antiparallel to the current flow direction (dc regime), confirm the electromagnetic chiral anisotropy (eMChA) – a rarely studied effect.

TT 43: Superconducting Electronics: Qubits

Time: Wednesday 9:30–12:45 Location: CHE/0089

TT 43.1 Wed 9:30 CHE/0089

Analysis of Flux Noise in Charge Qubits — •Daniel Kruti and Roman-Pascal Riwar — Peter Grünberg Institute, Theoretical Nanoelectronics, Jülich Research Centre, Jülich, D-52425, Germany & Cologne University

Improving the lifetime of quantum information stored in superconducting qubits is a focal point of contemporary research. However, the modelling of time-dependent flux noise has long been based on simplified lumped-element approaches, neglecting details of the device layout and flux distribution. Building on a recently developed quantum geometric description of Faraday's law of induction, we provide an in-depth analysis of charge qubit relaxation and decoherence rates for various flux noise sources, such as surface spins and the surrounding qubit control hardware. Contrary to standard circuit theory, our treatment reveals that a circuit does not require flux-tunability (e.g. a dc-SQUID) in order to be affected by flux noise, as flux-induced relaxation persists in the single junction limit. We link relaxation and dephasing by a geometry-dependent form factor, allowing experimental 1/f flux noise spectra to be used for quantitative estimates. These suggest that, while surface spins are likely negligible for current qubit performances, far-field flux sources due to the surrounding hardware can, in principle, contribute significantly.

TT 43.2 Wed 9:45 CHE/0089

Observation of two-level systems in superconducting titanium-aluminum-nitride films — •Marius Frohn[1,2], Florian Mezger[1], Maximilian Kristen[1], Jan Nicolas Voss[1], Hannes Rotzinger[1,2], and Alexey Ustinov[1,2] — [1]Physikalisches Institut (PHI), Karlsruhe Institute for Technology (KIT), Germany — [2]Institute for Quantum Materials and Technologies (IQMT), Karlsruhe Institute for Technology (KIT), Germany

Thin films of disordered superconductors are currently the subject of extensive study due to their potential applications in modern quantum circuits and kinetic inductance detectors. While many materials are possible candidates, those with low microwave loss and a high degree of disorder are especially interesting for high impedance circuits. The disordered microscopic structure also favors the presence of intrinsic material defects, some of which behave as two-level systems (TLS)[1]. Found in dielectrics such as surface oxides or tunneling barriers, TLS are a significant source of electromagnetic loss, which limits the coherence of superconducting qubits. It has been recently proposed [2], that applied direct-currents in the disordered superconductors are influencing the observable TLS coupling, e.g. to a microwave resonator. We present microwave spectroscopy measurements of ultra-compact, high impedance resonators made from titanium-aluminium-nitride films. By applying electric fields, we observe TLS strongly interacting with the resonator modes.

[1] M. Kristen et al., Phys. Rev. Lett. 132, 217002 (2024)
[2] T. Liu et al., Phys. Rev. B 111, L180502 (2025)

TT 43.3 Wed 10:00 CHE/0089

Embedding Superconducting Quantum Circuits in a Millimeter-Wave Environment — •Jakob Lenschen[1], Sergei Masis[1], Jürgen Lisenfeld[1], Hannes Rotzinger[1,2], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut (PHI), Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany — [2]Institut für Quantenmaterialien and Technologie (IQMT), Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany

Superconducting mm-wave quantum circuits operating at around 100 GHz offer many interesting new possibilities. Compared to microwave implementations, the higher photon energy and wider bandwidth enhance resilience to thermal fluctuations, and speed up qubit manipulations. However, mm-wave measurements at ultra-low temperatures are largely unexplored, and technical challenges demand alternative approaches [1]. The coherence and energy relaxation of superconducting quantum circuits is sensitive to a variety of loss mechanisms, e.g. interference with parasitic modes in the sample box and within the chip. Particular attention is required for mm-waves, as their wavelength is comparable to the dimensions of the dielectric substrate and many other structures in a conventional sample box. We have developed several approaches for coupling superconducting quantum circuits to waveguides, utilizing machined ridge gap waveguides and other techniques. In this presentation, we will discuss embedded superconducting mm-wave quantum chips, parasitic modes, and ways to inhibit or channel them out. We will compare our simulations with the experimental results.

[1] Lenschen et al., arXiv:2411.15058 (2024)

TT 43.4 Wed 10:15 CHE/0089

Niobium-based Josephson junctions for superconducting mm-wave qubits — •Urs Strobel[1], Benedict Rothmund[1], Jakob Lenschen[1], Jonas Kaemmerer[1], Lucas Radke[1], Sergei Masis[1], Jinji Luo-Hofmann[3], Danny Reuter[3], Hannes Rotzinger[1,2], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut (PHI), KIT, 76131 Karlsruhe, Germany — [2]Institut for Quantum Materials and Technologies (IQMT), KIT, 76131 Karlsruhe, Germany — [3]Fraunhofer-Institut für Elektronische Nanosysteme (ENAS), Chemnitz, Germany

Superconducting quantum circuits operating at millimeter-wave frequencies are an exciting area of research and offer the potential to maintain functionality at temperatures considerably higher than their widely studied centimeter-wave counterparts. The reduced wavelength allows for a smaller circuit footprint and faster qubit manipulation. Implementing such millimeter-wave qubits requires a superconductor with an energy gap above 100 GHz, which renders aluminum unsuitable. However, other conventional superconductors with larger gaps, such as niobium, are available with the technology to produce submicrometer Josephson junctions, key elements for superconducting quantum circuits.

To reduce dielectric losses, we use the low-loss substrate to eliminate extra dielectric layers present in classical niobium-based junction techniques [1]. We will present the concept, design constraints, and low-temperature characteristics. (2024)

[1] Patent pending DPO:02025132612.6 (2025)

TT 43.5 Wed 10:30 CHE/0089

fluxonium qubits inductively coupled to granular aluminum based readout resonators — •li-wei chang, asen Lyubenov georgiev, fabian kaap, christoph kissling, victor gaydamachenko, sergey lotkhov, mark bieler, and lukas grünhaupt — Physikalisch-Technische Bundesanstalt, Braunschweig, Germany

The fluxonium qubit is a specific type of superconducting qubit, which has garnered significant interest due to its coherence time in the milli-second range, high gate fidelities on the order of 99.9%, and a large anharmonicity up to several GHz. Recent years have also seen a surge in material studies related to this type of qubit, with a particular focus on high kinetic inductance materials such as granular aluminum (grAl). Three basic components form a fluxonium qubit: a Josephson junction, a capacitor, and a so-called superinductor with an impedance larger than the resistance quantum $R_Q = \frac{h}{4e^2}$. To enable dispersive readout, we employ a high-quality granular aluminum based readout resonator which is inductively coupled to the qubit through a shared inductor. Here, we present our methodology of qubit design, fabrication process and first experimental results.

TT 43.6 Wed 10:45 CHE/0089

Low-crosstalk modular flip-chip architecture with superconducting kinetic-inductively coupled flux-qubit-resonator circuits — •Sören Ihssen[1], Simon Geisert[1], Gabriel Jauma[2,3], Patrick Winkel[1,4,5], Martin Spiecker[1], Nicolas Zapata[1], Manuel Pino[2,7], Juan Jose Garcia-Ripoll[2], and Ioan M. Pop[1,6,8] — [1]IQMT, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Institute of Fundamental Physics IFF-CSIC, Calle Serrano 113b, 28006 Madrid, Spain — [3]Applied Physics Department, Salamanca University, Salamanca 37008, Spain — [4]Departments of Applied Physics and Physics, Yale University, New Haven, CT 06520, USA — [5]Yale Quantum Institute, Yale University, New Haven, CT 06520, USA — [6]PHI, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [7]Nanotechnology Group, USAL-Nanolab, Salamanca University, Salamanca 37008, Spain — [8]Physics Institute 1, Stuttgart University, 70569 Stuttgart, Germany

We introduce a flip-chip architecture for arrays of coupled superconducting qubits in which each circuit component is placed inside its own microwave enclosure. Unlike conventional flip-chip designs, our qubit chips are electrically floating, enabling straightforward modular assembly of capacitively coupled elements while strongly suppressing microwave crosstalk. We demonstrate the architecture using a chain of three nearest-neighbor coupled generalized flux qubits, where the central qubit serves as a frequency-tunable coupler. This system achieves a transverse coupling on/off ratio of 50, zz-crosstalk of 0.7 kHz between resonant qubits, and >60 dB isolation between outer enclosures.

15 min. break

TT 43.7 Wed 11:15 CHE/0089

Investigation of tunable interactions between quarton flux qubits — •Hossam Tohamy[1], Alex Kreuzer[1], Thilo Krumrey[1], Hannes Rotzinger[1,2], and Alexey V. Ustinov[1,2] — [1]Physikalisches Institut (PHI), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]Institute for Quantum Materials and Technologies (IQMT), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Tunable qubits are useful in superconducting quantum processors because they enable high-performance quantum gates. Although transmon-based multiqubit systems are widely used in recent architectures, the quarton flux qubit [1] emerges as a promising alternative, offering a positive anharmonicity that is three to five times larger than in typical transmons. In this work, we present an experimental investigation of quarton flux qubits in a capacitively coupled multiqubit architecture. The qubit inductances are realized using a novel stacked-junction fabrication technology [2]. We performed microwave spectroscopy and time-domain measurements on coupled qubits, demonstrating tunable capacitive coupling between the qubits. We benchmarked the measured coupling strengths against analytical models and RF simulations and found good agreement.

[1] F. Yan et al., arXiv:2006.04130 (2020).
[2] A. Kreuzer et al., arXiv:2503.11437 (2025).

TT 43.8 Wed 11:30 CHE/0089

Improving performance of planar tantalum resonators and transmon qubits on silicon using advanced deposition techniques — Maciej W. Olszewski[1], Lingda Kong[2], •Simon Reinhardt[2], Daniel Tong[2], Shilling Du[3], Gabriele Di Gianluca[4], Haoran Lu[2], Saswata Roy[1], Aleksandra Biedron[5], David A. Muller[2], and Valla Fatemi[2] — [1]Department of Physics, Cornell University, USA — [2]School of Applied and Engineering Physics, Cornell University, USA — [3]Cornell NanoScale Facility, USA — [4]Department of Physics, University of Florida, USA — [5]NY Creates, USA

The cubic phase of tantalum is a very promising material for superconducting transmon qubits, due to its self-limiting surface oxide, low bulk losses, and low kinetic inductance.

We present a novel method of growing high-crystallinity tantalum films on silicon with magnetron sputtering, using a significantly lower substrate temperature than found in literature. Using coplanar waveguide resonators, we measure the losses and microwave performance of our films, achieving single photon quality factors above four million for resonators with gap size of 3-μm. We present first results on transmon qubits based on these low loss tantalum films.

Funding: This prototype was primarily supported by the Microelectronics Commons Program, a DoW initiative, under award number N00164-23-9-G061. Funding for shared facilities used in this prototype was provided by the Microelectronics Commons Program, a DoW initiative, under award number N00164-23-9-G061.

TT 43.9 Wed 11:45 CHE/0089

Microwave pulse shape optimization for enhanced spin excitation in a ^{31}P:^{28}Si ensemble coupled to a superconducting resonator — Patricia Oehrl[1,2], •Ana Strinic[1,2], Tahereh Sadat Parvini[1,2], and Hans Huebl[1,2,3] — [1]Walther-Meissner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]School of Natural Sciences, Technical University of Munich, Garching, Germany — [3]Munich Center for Quantum Science and Technology, Munich, Germany

Phosphorus donors in silicon are considered as promising candidates for the realization of microwave quantum memories due to their electron spin transitions in the GHz regime with exceptionally long coherence times [1]. Here, we investigate the transduction of pulsed coherent microwave signals to spin excitations of a spin ensemble. This effectively pulsed electron spin resonance experiment uses a hybrid system consisting of a superconducting lumped-element microwave resonator coupled to a spin ensemble of phosphorus donors in isotopically engineered silicon. By modeling the system using an input-output formalism, we identify optimal pulse shapes and coupling parameters for enabling this excitation transfer. The understanding and optimization is of importance for the implementation of efficient quantum state storage protocols, which are of relevance for microwave quantum memory applications as well as quantum sensing.

[1] M. Steger et al., Science 336, 1280 (2012)

TT 43.10 Wed 12:00 CHE/0089

Quantum dynamics of two XY interacting PT-symmetric non-Hermitian qubits: enhancement of quantum annealing — •Yana Komissarova, Mikhail V. Fistul, and Ilya M. Eremin — Institut für Theoretische Physik III, Ruhr-Universität Bochum, Bochum 44801, Germany

Quantum information processing devices enable the realization of analog quantum simulations, such as quantum annealing, and offer a promising route toward solving complex computational and combinatorial optimization problems. In this work, we introduce a new type of quantum information platform based on a network of interacting parity-time (PT) symmetric non-Hermitian qubits. The quantum dynamics of individual PT-symmetric non-Hermitian qubits have already been demonstrated experimentally using several approaches, including dilation schemes with digital coupling to an auxiliary qubit. These experiments carried out on a variety of platforms, such as NV centers, superconducting qubits, and superconducting and trapped-ion qutrits, have revealed exceptional points of different orders, as well as PT-symmetry-preserving and symmetry-breaking quantum states. A key next step is the investigation of coherent quantum dynamics in systems of interacting PT-symmetric non-Hermitian qubits. Here, we study both time-independent and time-dependent Hamiltonians relevant for quantum annealing in an exemplary two-qubit non-Hermitian network based on the XY model. We analyze the system in both PT-symmetric and PT-broken regimes to identify conditions that maximize the probability of reaching the ground state after quantum annealing.

TT 43.11 Wed 12:15 CHE/0089

Strongly interacting phases of spins and bosons in circuit QED — •Adrian Paul Misselwitz[1,2,3], Jacquelin Luneau[1,2,3], Enrico Di Benedetto[4], and Peter Rabl[1,2,3] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany — [4]Università degli Studi di Palermo, Dipartimento di Fisica e Chimica–Emilio Segrè, Via Archirafi 36, I-90123 Palermo, Italy

The scalability of superconducting circuit hardware is a promising route for the implementation and exploration of complex many-body systems. In this work, we study emerging phases of matter in a waveguide QED framework, arising from the interplay of competing forces of atom-bound state localization and Kerr-type photon-photon interactions. In addition, we extend our analysis to 1D flatband systems, map out the phase space and characterize the flatband states, which take on a unique form due to the nonlinear photonic dynamics of circuit QED.

TT 43.12 Wed 12:30 CHE/0089

Light-controlled transport across impurities in cavity quantum materials — Lukas Krieger[1], •Debashish Mondal[1,2], Ahana Chakraborty[3], and Peter P. Orth[1,2] — [1]Department of Physics, Saarland University, Campus, 66123 Saarbrücken, Germany — [2]Center for Quantum Technologies (QuTe), Saarland University, Campus, 66123 Saarbrücken, Germany — [3]Department of Physics and Astronomy, Louisiana State University, Baton Rouge, Louisiana 70803, USA

We investigate quantum materials placed inside optical cavities in the deep-strong and ultra-strong light-matter coupling regimes. In these regimes, standard perturbative techniques and aprroximation from quantum electrodynamics usch as rotating-wave approximation become unreliable. To address this challenge, we employ the asymptotic decoupling (AD) transformation, a unitary approach that shifts the minimal-coupling interaction to the renormalization of electronic mass and shift of the electronic position.

We examine how strong light-matter coupling affects electron scattering at the impurity site in a one dimensional system. We are analyzing these effects using both low-order perturbation theory and Green-function-based methods to capture higher-order scattering contributions. This work aims to build a framework for understanding scattering phenomena in cavity-embedded quantum materials and to guide future simulations and analytical studies in non-perturbative coupling regimes.

TT 44: Nonequilibrium Quantum Systems I (joint session TT/DY)

Time: Wednesday 9:30–12:45 Location: CHE/0091

TT 44.1 Wed 9:30 CHE/0091

Quantum geometric force in nonlinear phononics — •Sota Kitamura and Takahiro Morimoto — University of Tokyo, Tokyo, Japan

When phonons are resonantly excited by intense laser fields, nonlinear effects can dynamically alter the crystal structure. The field of controlling material properties through such processes is referred to as nonlinear phononics. In conventional theoretical frameworks of nonlinear phononics, the electron dynamics are typically assumed to be adiabatic. However, this assumption generally breaks down under strong driving, and nonadiabatic corrections become essential.

Using nonequilibrium Green function methods, we investigate the electron

dynamics under resonant phonon excitation beyond the adiabatic approximation, thereby exploring nonadiabatic effects appearing in the phonon equations of motion. Our analysis reveals that quantum geometric contributions originating from the electronic Berry curvature give rise to unconventional forces on phonons. These quantum geometric corrections are then applied to the dynamical control of crystal chirality, i.e., right- or left-handedness of chiral crystals, using a minimal tight-binding model coupled to the Peierls phonon.

TT 44.2 Wed 9:45 CHE/0091

Macroscopic mechanical torque for lattice and electronic chirality measurement — •Nikolai Peshcherenko[1], Ning Mao[1], Claudia Felser[1], and Yang Zhang[2,3] — [1]Max Planck Institute for Chemical Physics of Solids, 01187, Dresden, Germany — [2]Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA — [3]Min H. Kao Department of Electrical Engineering and Computer Science, University of Tennessee, Knoxville, Tennessee 37996, USA

The concept of chirality is known to be critical for a number of phenomena related either to a structural asymmetry or topological electronic band crossings. In the present work we develop a robust chirality probe of TR-symmetric systems with mechanical torque measurement. Namely, we show that driving a system out of equilibrium with temperature gradient (or electric field to excite electrons) would result in uncompensated angular momentum and mechanical torque. Calculations are made for both phonons (insulating case) and electrons (metallic case) carrying angular momentum. For phonons, our theoretical findings stand in reasonable agreement with a recent experiment [1]. For electronic subsystem, we discuss both cases of structural and topological electronic chirality probe.

[1] H. Zhang, N. Peshcherenko, F. Yang, T. Ward, P.Raghuvanshi, L.Lindsay, C.Felser, Y.Zhang, J.-Q. Yan, H.Miao, Nat.Phys.1 (2025)

TT 44.3 Wed 10:00 CHE/0091

Hybrid quantum–classical matrix-product state and Lanczos methods for electron–phonon systems with strong electronic correlations: Application to disordered systems coupled to Einstein phonons — •Heiko Georg Menzler[1], Suman Mondal[2], and Fabian Heidrich-Meisner[1] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden

We present two quantum-classical hybrid methods for simulating the time-dependence of electron-phonon systems that treat electronic correlations numerically exactly and optical-phonon degrees of freedom classically. These are a time-dependent Lanczos and a matrix-product state method, each combined with the multi-trajectory Ehrenfest approach. Due to the approximations, reliable results are expected for the adiabatic regime of small phonon frequencies. We discuss the convergence properties of both methods for a system of interacting spinless fermions in one dimension and provide a benchmark for the Holstein chain. As a first application, we study the decay of charge density wave order in a system of interacting spinless fermions coupled to Einstein oscillators and in the presence of quenched disorder. We investigate the dependence of the relaxation dynamics on the electron-phonon coupling strength and provide numerical evidence that the coupling of strongly disordered systems to classical oscillators leads to delocalization, thus destabilizing the (finite-size) many-body localization in this system.

This research is supported by the DFG (Deutsche Forschungsgemeinschaft) via SFB 1073 and FOR 5522.

TT 44.4 Wed 10:15 CHE/0091

Frozen non-equilibrium dynamics of exciton Mott insulators in moiré superlattices — Shibin Deng[1], •Jonas Reimann[2], Heonjoon Park[3], Jonas M. Peterson[1], Ammon Fischer[2], Xiaodong Xu[3], Dante M. Kennes[2,4], and Libai Huang[1] — [1]Department of Chemistry, Purdue University, West Lafayette, IN 47907, USA — [2]Max Planck Institute for the Structure and Dynamics of Matter, Center for Free Electron Laser Science, 22761 Hamburg, Germany — [3]Department of Physics, University of Washington, Seattle, WA 98195, USA — [4]Institut für Theorie der Statistischen Physik, RWTH Aachen University, 52056 Aachen, Germany

Moiré superlattices, such as those formed from transition metal dichalcogenide heterostructures, have emerged as an exciting platform for exploring quantum many-body physics. A key open question is the coherence and dynamics of the quantum phases arising from photoexcited moiré excitons, particularly amid dissipation. Here we use transient photoluminescence and ultrafast reflectance microscopy to image non-equilibrium exciton phase transitions. Counterintuitively, experimental results and theoretical simulations indicate that strong long-range dipolar repulsion freezes the motion of the Mott insulator phase for over 70 ns. In mixed electron-exciton lattices, reduced dipolar interactions lead to diminished freezing dynamics. These findings challenge the prevailing notion that repulsion disperses particles, whereas attraction binds them. This talk focuses on the theoretical efforts that support the experimental data.

TT 44.5 Wed 10:30 CHE/0091

Cavity-induced Eliashberg effect: superconductivity vs charge density wave — •Md Mursalin Islam[1,2], Michele Pini[1,2], Rafael Flores- Calderón[2], and Francesco Piazza[1,2] — [1]Theoretical Physics III, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Nothnitzer Straße 38, 01187 Dresden, Germany

Recent experiments have shown that non-equilibrium effects can play a key role in cavity-based control of material phases, notably in systems with charge-density-wave order. Motivated by this, we extend the theory of the Eliashberg effect, originally developed for superconducting phases, to charge-density-wave phases. Starting from a minimal electronic model where superconductivity and charge-density-wave order are equivalent at equilibrium, we introduce coupling to cavity photons, which are in turn coupled to an environment at a temperature different from the one of the electronic environment. This drives the system into a non-thermal steady state, which breaks the equivalence between superconductivity and charge-density-wave order. In the superconducting case, we recover the known behavior: a shift from continuous to discontinuous phase transitions with bistability. In contrast, the charge-density-wave case displays richer behavior: tuning the cavity frequency induces both continuous and discontinuous transitions, two distinct ordered phases, and a bistable regime ending at a critical point. These findings demonstrate that the scope of cavity-based non-thermal control of quantum materials is broader than at thermal equilibrium, and strongly depends on the targeted phases.

TT 44.6 Wed 10:45 CHE/0091

Quantum Monte Carlo Nonequilibrium work estimator of Rényi negativites — •Jannis Kastell and David Luitz — Universität Bonn, Bonn, Germany

We develop a Quantum Monte Carlo method for the calculation of Rényi generalizations of the logarithmic negativity, an entanglement measure for mixed states. Extending previous works using the replica trick and nonequilibrium-work-based estimators of Rényi entanglement entropy, we adapt this framework to the moments of the partially transposed reduced density matrix at finite temperature. Using the stochastic series expansion (SSE) method, we compute these moments in bi- and tri-partitioned systems. We apply this approach to the spin-1/2 isotropic Heisenberg antiferromagnet on a 3D simple cubic lattice, analysing the scaling of the higher order moments with subsystem size for both contiguous and disjoint partitions. Our results demonstrate that this approach provides an efficient and scalable method for estimating mixed-state entanglement measures in large quantum many-body systems.

15 min. break

TT 44.7 Wed 11:15 CHE/0091

Enhancing quantum metric using periodic driving — •Dhruv Tiwari, Roderich Moessner, and Johannes S. Hofmann — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

The advent of periodically driven systems has revolutionized modern condensed matter physics by offering two transformative opportunities. First, they enable the realization of nonequilibrium analogs of well-established equilibrium phases under highly tunable conditions. Second, they facilitate the emergence of novel phases with no equilibrium counterparts. In this work, we focus on the former, leveraging the tunable parameters of periodically driven systems to enhance the quantum metric in flat-band models. The quantum metric, a fundamental geometric property of the band structure, plays a crucial role in stabilizing various correlated phases. Here, we present results demonstrating that an appropriately chosen periodic drive can amplify the quantum metric and modify density-density interactions. Using both numerical and analytical techniques, we map out the phase diagram of the resulting model.

TT 44.8 Wed 11:30 CHE/0091

Scattering in periodic fields: Floquet resonances — •Sebastian Eggert, Christoph Dauer, and Axel Pelster — University of Kaiserslautern-Landau (RPTU)

An alternative mechanism of tuning many-body interactions in atomic systems is proposed, which is based on dynamically creating Floquet bound states using time-periodic fields. By developing a Floquet-scattering theory we show that sharp Floquet resonances occur at which the effective interaction can be tuned to very large attractive or repulsive values. The resulting predictions explain recent experimental data and provide additional tuning possibilities. Analytic predictions are given for adjusting amplitude, frequency and mean of the applied oscillating field in order to to accurately choose location and width of scattering resonances over a wide range. This paves the road to a versatile toolbox of tailored interactions in setups with multiple atomic species.

TT 44.9 Wed 11:45 CHE/0091

A comparative study of perturbative and nonequilibrium Green's function approaches for Floquet sidebands in periodically driven quantum systems — •Karun Gadge[1], Marco Merboldt[2], Wiebke Bennecke[2], Jan Philipp Bange[2], Marcel Reutzel[3], Stefan Mathias[2], Michael A Sentef[4],

Michael Schüler[5], and Salvatore R Manmana[1] — [1]Institute for Theoretical Physics, Georg-August-University Göttingen, Friedrich-Hund-Platz 1, Göttingen, Germany — [2]I. Physikalisches Institut, Georg-August-University Göttingen, Friedrich-Hund-Platz 1, Göttingen, Germany — [3]Fachbereich Physik, Philipps-University Marburg, Marburg, Germany — [4]Institute for Theoretical Physics and Bremen Center for Computational Materials Science, University of Bremen, Bremen, Germany — [5]Laboratory for Materials Simulations, Paul Scherrer Institute, Villigen PSI, Switzerland

We compare two complementary theoretical approaches to compute and interpret Floquet sidebands in periodically driven quantum materials: a first-order perturbative approach (PB1) and time-dependent nonequilibrium Green's functions (tdNEGF). Using graphene as a model Dirac system, we disentangle in pump-probe setups Floquet-dressed initial states, Volkov-dressed final states (also known as laser-assisted photoelectric effect, LAPE), and their interference. We quantify how photoemission matrix elements, polarization, incidence angle, and near-surface screening shape the momentum-resolved sideband intensity observed in tr-ARPES.

TT 44.10 Wed 12:00 CHE/0091

Towards Floquet-GW: interacting electrons in time-periodic potentials — •Ayan Pal[1,2], Erik G C P Van Loon[1,2], and Ferdi Aryasetiawan[1,3] — [1]Division of Mathematical Physics, Lund University, Professorsgatan 1, Lund, Sweden — [2]NanoLund, Lund University, Professorsgatan 1, Lund, Sweden — [3]LINXS Institute of advanced Neutron and X-ray Science, Lund, Sweden

The Floquet theory of time-periodic systems provides a middle ground between equilibrium and far-from-equilibrium physics, making it ideal for studying nonequilibrium steady states. We employ this framework to interacting electrons exposed to spatially and time-periodic potentials by combining Floquet theory with RPA and GW. This is applied to both the homogeneous electron gas and lattice Hamiltonians, allowing us to resolve the interplay between periodic driving, electronic correlations, and collective charge excitations. We compute Floquet-induced Greens function, dielectric function, and screened interaction; and demonstrate the formation of Bloch-Floquet sidebands in the electronic spectral function and in direct and inverse photoemission spectra. The periodic modulation further induces plasmonic sidebands and generates additional Floquet-umklapp regions for the electron-hole continuum. Our analysis highlights how the structure of the travelling drive - frequency, amplitude, and momentum controls the redistribution of spectral weight and the renormalisation of collective modes. This framework provides a route for predicting the plasmonic, dielectric, and optical response properties of weakly to moderately correlated materials under periodic laser driving.

TT 44.11 Wed 12:15 CHE/0091

Emergent Floquet Fermi Surfaces from Disorder — Inti Sodemann Villadiego, Akihiro Ozawa, and •Felix Frederking — Institut für Theoretische Physik, Universität Leipzig, Brüderstraße 16, 04103 Leipzig, Germany

We investigate the non-equilibrium steady states of periodically driven fermions coupled to a fermionic heat bath and in the presence of disorder (i.e. random impurities). In the absence of disorder, the steady state occupation would be a "stair-case" version of the Fermi-Dirac distribution, which is smooth at finite temperatures. Remarkably, however, we have found that disorder induces non-analyticities in the occupation of states that behave as emergent Fermi surfaces. We will discuss the physical phenomena arising from these non-equilibrium emergent Fermi surfaces and make the case for the feasibility of their detection in ulta-clean 2D materials subjected to low frequency radiation.

TT 44.12 Wed 12:30 CHE/0091

Emergent Fermi surfaces from non-equilibrium heat baths: exact results from Keldysh formalism — •Akihiro Ozawa and Inti Sodemann Villadiego — Institut für Theoretische Physik, Universität Leipzig, 04103, Leipzig, Germany

Recent studies have shown that periodically driven fermions coupled to a boson bath display non-analyticities in their occupation functions of momentum that behave like emergent Fermi surfaces. Remarkably, we have found that analogous non-equilibrium emergent Fermi surfaces can arise when the system is coupled to two baths at different temperatures, even without external periodic driving. The mechanism driving the formation of these non-equilibrium Fermi surfaces, is a kind of transfer from non-analyticities from the density of states into the occupation of states which is only allowed away from equilibrium, in the absence of detailed balance in the scattering rates. We demonstrate that this result is exact at weak coupling using the Keldysh formalism and propose a numerical scheme to investigate the fate of these non-analyticities at finite coupling.

TT 45: Many-body Systems: Equilibration, Chaos, and Localization (joint session DY/TT)

Time: Wednesday 9:30–12:45 Location: HÜL/S186

TT 45.1 Wed 9:30 HÜL/S186

Compression of Floquet random circuits — •Francesca De Franco[1,2], David Luitz[3], Dante Kennes[4], Matteo Rizzi[1,5], and Markus Schmitt[1,2] — [1]FZ Juelich, Institute of Quantum Control (PGI-8) — [2]University of Regensburg — [3]University of Bonn — [4]RWTH Aachen University — [5]University of Cologne

Current quantum computing hardware suffers from significant dissipation due to the coupling to the environment. This limits the depth of unitary quantum circuits which can be applied with high fidelity and hence the physical timescales reachable by digital quantum simulation. Here, we show that the reachable timescale in practice depends strongly on the physics of the many-body system under investigation: For systems deep in a many-body localized phase, we can find shallow circuit representations of the evolution operator U to late times, while in a chaotic regime this is not possible. The associated compressibility of the late time evolution operator is hence associated with the accessibility of long times on noisy quantum hardware. Moreover, we compare the performance of these compressed, variationally obtained circuits to tensor-network simulations, which allow us to compute quantum-information-spreading diagnostics such as entanglement entropy and out-of-time-ordered correlators.

TT 45.2 Wed 9:45 HÜL/S186

Spectral pairing statistics in Floquet time crystals — Alexander-Georg Penner[1], •Harald Schmid[1,2,3], Leonid I. Glazman[4], and Felix von Oppen[1] — [1]Dahlem Center for Complex Quantum and Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — [2]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany — [4]Department of Physics, Yale University, New Haven, Connecticut 06520, USA

Floquet time crystals are characterized by the subharmonic behavior of temporal correlation functions. Studying the paradigmatic time crystal based on the disordered Floquet quantum Ising model, we show that its temporal spin correlations are directly related to spectral characteristics and that this relation provides analytical expressions for the correlation function of finite chains, which compare favorably with numerical simulations. Specifically, we show that the disorder-averaged temporal spin correlations are proportional to the Fourier transform of the splitting distribution of the pairs of eigenvalues of the Floquet operator, which differ by pi to exponential accuracy in the chain length. We find that the splittings are well described by a log-normal distribution, implying that the temporal spin correlations are characterized by two parameters. We discuss possible implications for the phase diagram of Floquet time crystals.

TT 45.3 Wed 10:00 HÜL/S186

Spin-Spin Correlations and Multifractality in 1D disordered $SU(2)$-Invariant Heisenberg Spin Chains — •Debasmita Giri, Julian Siegl, and John Schliemann — Institute for Theoretical Physics, University of Regensburg, Regensburg, Germany

Disorder and interactions in one-dimensional quantum spin chains give rise to rich non-ergodic phenomena that lie beyond the conventional eigenstate thermalization hypothesis (ETH). In the presence of sufficiently strong quenched disorder, many-body localization (MBL) can emerge: transport is frozen, entanglement growth is logarithmically slow, and local operators retain memory of their initial conditions even at infinite temperature. On the contrary, studies on models with non-Abelian symmetries have demonstrated that continuous symmetries, such as $SU(2)$, can obstruct the construction of local integrals of motion and thus hinder full localization. We investigate spin correlations in one-dimensional $SU(2)$-invariant Heisenberg chains with exchange disorder for spin lengths $S = 1/2$ and $S = 1$. In the weak-disorder regime, the eigenmodes of the spin-spin correlation matrix are delocalized, consistent with ergodic behavior. Under strong disorder, the system enters a quasi-localized multifractal phase characterized by exponentially decaying, dimer-like spin correlations. Finite-size scaling of the inverse participation ratios of the correlation-matrix eigenmodes yields a correlation dimension, $D_2 \approx 0.37 - 0.39$, confirming the presence of a multifractal regime that is distinct from both the ergodic limit ($D_2 = 1$) and the fully localized limit ($D_2 = 0$).

TT 45.4 Wed 10:15 HÜL/S186

Timescales for Deep and Full Thermalization — •Tabea Herrmann[1], Felix Fritzsch[2], and Arnd Bäcker[1] — [1]TU Dresden, Institut für Theoretische Physik, Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Isolated quantum systems typically approach thermal equilibrium as described by the Eigenstate Thermalization Hypothesis (ETH). Going beyond this involves either higher order correlators (full ETH) or the approach of moments of the reduced density matrix towards thermal equilibrium (deep thermalization). In this talk we compare these two types of thermalization using extensive numerical studies within a paradigmatic model for chaotic many-body quantum dynamics. For this we find exponential relaxation for both types: For deep thermalization all moments relax with the same rate, which approximately equals the relaxation rate of two-point correlation functions within full ETH. In contrast, all higher order correlation functions approach equilibrium twice as fast.

TT 45.5 Wed 10:30 HÜL/S186

Free Cumulants and Full Eigenstate Thermalization from Boundary Scrambling — •Felix Fritzsch, Gabriel O. Alves, Michael A. Rampp, and Pieter W. Claeys — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Out-of-time-order correlation functions (OTOCs) represent important probes of quantum information dynamics and scrambling. We introduce a solvable many-body quantum circuit model, which we term boundary scrambling, for which the full dynamics of OTOCs is analytically tractable. These dynamics support a decomposition into free cumulants and unify recent extensions of the eigenstate thermalization hypothesis (full ETH) with predictions from random quantum circuit models. We moreover obtain exact expressions for higher-order correlations between matrix elements as predicted by the full ETH. The solvability is enabled by the identification of a higher-order Markovian influence matrix, capturing the effect of the full system on a local subsystem.

TT 45.6 Wed 10:45 HÜL/S186

Mechanism of Eigenstate Thermalization Breakdown — •Rafał Świetek[1,2,3] and Lev Vidmar[2,3] — [1]Institut für Theoretische Physik, Georg-August-Universität Göttingen, D-37077 Göttingen, Germany — [2]Department of Theoretical Physics, J. Stefan Institute, SI-1000 Ljubljana, Slovenia — [3]Department of Physics, Faculty of Mathematics and Physics, University of Ljubljana, SI-1000 Ljubljana, Slovenia

Establishing a common framework for ergodicity-breaking transitions has many potential applications and provides insight into the nature of non-ergodic phases. In this work, we show that the softening of fluctuations within the recently established fading ergodicity framework can be derived directly from the emergence of the Fermi Golden Rule (FGR), ultimately classifying fading ergodicity as manifestation of FGR physics in quantum many-body systems. We show that this framework identifies the width of the local density of states and the fractal nature of eigenstates in the unperturbed basis as building blocks for fading ergodicity. Furthermore, we argue that our theory can be also applied to integrability-breaking transitions, where the critical point drifts exponentially with system size to a singular point, providing a common framework for ergodicity breaking in RMT models and integrability-breaking in local Hamiltonians.

15 min. break

TT 45.7 Wed 11:15 HÜL/S186

Entanglement in bipartite systems with symmetry: coupled chaotic kicked Bose-Hubbard systems — •Jan Himmelsbach[1], Maximilian F.I. Kieler[1,2], and Arnd Bäcker[1] — [1]TU Dresden, Institut für Theoretische Physik, Dresden, Germany — [2]CESAM research unit, University of Liège, B-4000 Liège, Belgium

We study the eigenstate entanglement of a time-periodically driven Bose-Hubbard system in a bipartite setting with a tunable coupling between two subsystems. By incorporating the symmetry of the particle conservation and employing perturbation theory we find that the entanglement transition for varying coupling strength is described by a universal transition parameter. It turns out that the entanglement transition is governed by localization for the particle conservation symmetry and a thermalizing process between the subsystems.

TT 45.8 Wed 11:30 HÜL/S186

Dynamical Pictures for Growth of Entanglement and Decay of Correlators in U(1) Conserving Random Circuits — •Marco Lastres[1,2], Olexei I. Motrunich[3], and Sanjay Moudgalya[1,2] — [1]Technical University of Munich, School of Natural Sciences, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany — [3]Department of Physics, Caltech, Pasadena, CA, USA

We study the dynamics of random circuit models with a global $U(1)$ charge conservation law. Prior work showed that systems without conservation laws exhibit linear growth of entanglement, linked to domain wall dynamics in an effective ferromagnetic model. In contrast, rigorous upper bounds for $U(1)$-conserving systems indicate that diffusive charge transport constrains Rényi entropies to grow only diffusively as $\sqrt{t}$. We study the second Rényi entropy in $U(1)$-conserving random circuits by mapping its dynamics onto the low-energy physics of an effective interacting Hamiltonian. This approach explicitly demonstrates the microscopic mechanism which produces diffusive growth of entanglement in the effective replica model. We also show that the same effective model naturally captures the recently discovered subexponential decay of non-hydrodynamic correlations through a closely related mechanism. Further, we demonstrate that in a different regime this model can also describe the dynamics of entanglement in noisy free-fermion systems, which also exhibit diffusive entanglement growth, but through a different mechanism. Finally, we discuss extensions to other continuous symmetries and to higher Rényi entropies.

TT 45.9 Wed 11:45 HÜL/S186

Correspondence principle, dissipation, and Ginibre ensemble — •David Villaseñor, Hua Yan, Matic Orel, and Marko Robnik — CAMTP - Center for Applied Mathematics and Theoretical Physics, University of Maribor, Mladinska 3, SI-2000 Maribor, Slovenia, European Union

The correspondence between quantum and classical behavior has been essential since the advent of quantum mechanics. This principle serves as a cornerstone for understanding quantum chaos, which has garnered increased attention due to its strong impact in various theoretical and experimental fields. When dissipation is considered, quantum chaos takes concepts from isolated quantum chaos to link classical chaotic motion with spectral correlations of Ginibre ensembles. This correspondence was first identified in periodically kicked systems with damping, but it has been shown to break down in dissipative atom-photon systems [Phys. Rev. Lett. 133, 240404 (2024)]. In this contribution, we revisit the original kicked model and perform a systematic exploration across a broad parameter space, reaching a genuine semiclassical limit. Our results demonstrate that the correspondence principle, as defined through this spectral connection, fails even in this prototypical system. These findings provide conclusive evidence that Ginibre spectral correlations are neither a robust nor a universal diagnostic of dissipative quantum chaos.

TT 45.10 Wed 12:00 HÜL/S186

Quantum Mpemba effect from Stark localization — •Nico Albert[1], Masudul Haque[1], and Shovan Dutta[2] — [1]TU Dresden, Dresden, Germany — [2]Raman Research Institute, Bangalore, India

In the Mpemba effect a system prepared at a higher temperature cools down faster to a target equilibrium state than the same system prepared at a lower temperature. We investigate how quantum effects can influence the occurence of such an effect. As an example we consider a bosonic chain subject to a suitable onsite potential that is dissipatively cooled to its ground state, and find that Stark localization significantly enhances the Mpemba effect compared to analogous classical systems.

TT 45.11 Wed 12:15 HÜL/S186

Robustness of interference-caged QMBS under real-space local perturbations: analysis through the Fock-space local interference pattern — •Tao-Lin Tan[1] and Yi-Ping Huang[1,2,3] — [1]Department of Physics, National Tsing Hua University, Hsinchu 30013, Taiwan — [2]Physics Division, National Center for Theoretical Sciences, Taipei 10617, Taiwan — [3]Institute of Physics, Academia Sinica, Taipei 115, Taiwan

Quantum many-body scars (QMBS) represent a notable violation of the eigenstate thermalization hypothesis (ETH), hosting non-thermal eigenstates embedded in an otherwise thermal spectrum. Despite recent progress, a systematic understanding of their stability under real-space local (r-local) perturbations remains lacking. Building on recent insights of interference-caged quantum many-body scars (ICQMBS), protected by exact many-body destructive interference on Fock-space graphs, we develop an interference-based diagnostic to assess the robustness of ICQMBS in various lattice Hamiltonians. Applying this framework to quantum link models (QLM) and quantum dimer models (QDM), we analyze how r-local perturbations deform the underlying Fock-space local (f-local) interference structure, thereby identifying heuristic mechanisms that stabilize or destabilize ICQMBS. Our results broaden the applicability of the interference-based perspective beyond previously studied models and provide practical criteria for evaluating the persistence of ICQMBS in experimentally relevant Hamiltonians.

TT 45.12 Wed 12:30 HÜL/S186

Scrambling and Scarring in Topological Materials — •Nicholas Sedlmayr, Dominik Szpara, and Szczepan Głodzik — Institute of Physics, M. Curie-Skłodowska University, 20-031 Lublin, Poland

Topological insulators and superconductors have recently attracted considerable attention, and many different theoretical tools have been used to gain insight into their properties. Here we investigate how perturbations can spread through exemplary one-dimensional topological insulators and superconductors using out-of-time ordered correlators. Out-of-time ordered correlators are often used to consider how information becomes scrambled during quantum dynamics. The wavefront of the out-of-time ordered correlator can be ballistic regardless of the underlying system dynamics, and here we confirm that for topological free fermion systems the wavefront spreads linearly at a characteristic butterfly velocity. We pay special attention to the topologically protected edge states, finding that information can become trapped in the edge states and essentially decoupled from the bulk, surviving for relatively long times - a form of scar-

ring. We further investigate what happens due to the chiral and helical edge modes of two dimensional topological models. The information travels around the edge, carried by the edge mode, but again is not scrambled over very long time scales.

TT 46: Spin Transport and Orbitronics, Spin-Hall Effects I (joint session MA/TT)

Time: Wednesday 9:30–12:45 Location: POT/0112

Invited Talk TT 46.1 Wed 9:30 POT/0112

Exploring the interplay between spin and chirality — •Angela Wittmann — Johannes Gutenberg University Mainz, Germany

Chirality is omnipresent in nature, bridging magnetic and molecular spin phenomena. At the core of this connection lies the chiral-induced spin selectivity (CISS) effect, describing the highly efficient generation of spin polarized currents in chiral molecules. Despite extensive experimental evidence, the underlying mechanisms of CISS remain debated. Here, we explore how chirality is directly linked to the intrinsic magnetic moments in molecules and how molecular design can be harnessed to control spin phenomena at hybrid chiral molecule magnetic interfaces [1]. Our findings pave a pathway towards functional "chiralitronic" devices - turning a fundamental puzzle into a technological opportunity.

[1] A. Moharana, AW et al., Sci. Adv.11, eado4285 (2025)

TT 46.2 Wed 10:00 POT/0112

Chiral Molecule-Induced Magnetic Anisotropies — •Simon Sochiera[1], Ashish Moharana[1], Yael Kapon[2], Fabian Kammerbauer[1], Shira Yochelis[2], Mathias Kläui[1], Yossi Paltiel[2], and Angela Wittmann[1] — [1]Johannes Gutenberg University, Mainz, Germany — [2]Hebrew University of Jerusalem, Jerusalem, Israel

The chiral-induced spin selectivity effect promises novel spintronic devices. Despite numerous interdisciplinary experiments revealing its implications and trends, this phenomenon challenges our theoretical understanding of the interplay between spin and chirality, particularly regarding apparent time-reversal symmetry breaking. This symmetry breaking can be observed by measuring a magnetic thin film's anisotropy upon chiral-molecule adsorption. We quantify this phenomenon by measuring the magnetic anisotropy through electrical magnetotransport measurements. Upon chiral-molecule adsorption, we observe a 35% change in out-of-plane hard-axis anisotropy. This approach enables sensitive probing of magnetic property changes induced by different chiral molecular systems on various conductive or insulating magnetic thin films. Correlating molecular properties, such as spin-orbit coupling, with their impact on magnetic anisotropy will be crucial for understanding the fundamental mechanisms of chiral-induced spin selectivity and for facilitating the design of spintronic devices that require a precisely tuned anisotropy.

TT 46.3 Wed 10:15 POT/0112

Generation, Transmission, and Conversion of Orbital Torque by an Antiferromagnetic Insulator — •Shilei Ding[1,2], Paul Noël[2], Gunasheel Kauwtilyaa Krishnaswamy[2], Niccolò Davitti[2], Giacomo Sala[2], Marzia Fantauzzi[3], Antonella Rossi[2,3], and Pietro Gambardella[2] — [1]School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371, Singapore — [2]Department of Materials, ETH Zürich, 8093 Zürich, Switzerland — [3]Dipartimento di Scienze Chimiche e Geologiche, Università degli Studi di Cagliari, Campus di Monserrato S.S. 554, Italy

Orbital currents and orbital torques have recently emerged as powerful tools for controlling magnetization, yet their transport has been studied almost exclusively in metals. We report the first demonstration of orbital generation, transport, and conversion through an insulating antiferromagnet CoO. By inserting CoO between Cu* and Co, we show that orbital transport is preserved and the orbital-torque efficiency is strongly enhanced. Temperature-dependent measurements indicate that orbital transport above the Néel temperature is mediated by thermal fluctuations, while antiferromagnetic order and exchange bias provide additional transport channels at low temperature. These results identify insulating antiferromagnets as effective mediators of orbital angular momentum and highlight transition-metal oxides with unquenched orbital moments as promising materials for efficient spin-orbitronic technologies.

TT 46.4 Wed 10:30 POT/0112

Modern theory of the Orbital Hall effect from Wannier Representation — •Mirco Sastges[1,2], Insu Baek[3], Hojun Lee[3], Hyun-Woo Lee[3], Yuriy Mokrousov[1,2], and Dongwook Go[4] — [1]Peter Grüunberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany — [3]Department of Physics, Pohang University of Science and Technology, Pohang, Kyungbuk 37673, South Korea — [4]Department of Physics, Korea University, Seoul 02841, South Korea

In the field of orbital dynamics and orbital transport a particularly important quantity is the so-called orbital Hall conductivity (OHC), which is expressed in terms of operators of velocity and orbital angular momentum (OAM). To overcome the difficulties in treating the unbounded position operator, very often the so-called atom-centered approximation (ACA) is used. However, while being very practical, this approach captures only some local contributions to the OAM operator. Here, we will report on developing a new approach to quantify the OAM operator in the basis of Wannier functions, which is based on the modern theory of orbital magnetization. This method allows us to capture both local and itinerant contributions to the OHC. By performing first principles calculations for selected transition metals we show that a significant correction to the OHC due to non-local contributions arises, while the local effects are captured in accordance to the ACA. Our approach is very promising since it improves our understanding of OAM and allows for a precise estimation of the OHC.

TT 46.5 Wed 10:45 POT/0112

Chirality-induced orbital Edelstein effect in an analytically solvable model — •Lennart Schimpf, Börge Göbel, and Ingrid Mertig — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg

Chirality-induced spin selectivity (CISS), a phenomenon wherein chiral structures selectively determine the spin polarization of electron currents flowing through the material, has garnered significant attention due to its potential applications in areas such as spintronics, enantioseparation, and catalysis. The underlying physical effect is the Edelstein effect that converts charge to angular momentum. Besides a spin contribution, there exists a contribution based on the orbital angular momentum but the precise mechanism for its generation remains yet to be understood. Here, we introduce the minimal model for explaining the phenomenon based on the orbital Edelstein effect [1]. We consider nonlocal intersite contributions to the current-induced orbital angular momentum and reveal the underlying mechanism by analytically calculating the Edelstein susceptibilities in a tight-binding and Boltzmann approach. While the orbital angular momentum is directly generated by the chirality of the crystal, the spin contribution of each spin-split band pair relies on spin-orbit coupling. Using tellurium as an example, we show that the orbital contribution surpasses the spin contribution by orders of magnitude.

[1] B.Göbel, L. Schimpf, I. Mertig, Phys. Rev. Res. 7, 033180 (2025)

15 min break

TT 46.6 Wed 11:15 POT/0112

Spin-charge and Orbital-charge Interconversion on SrTiO3-based Two-dimensional Electron Gases: A Semiclassical Approach — •Le Viet Duc Pham and Annika Johansson — Max Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle (Saale), Germany

Two-dimensional electron gases (2DEGs) at SrTiO3-based oxide interfaces display large, gate-tunable Rashba-like spin-orbit coupling (SOC) that enables spin-charge interconversion via the spin Edelstein effect [1, 2]. It has also been demonstrated that the orbital Edelstein effect, i.e, current-induced orbital magnetization, is larger than the spin Edelstein effect by more than one order of magnitude [3]. Yet, most transport studies assume a constant relaxation time [1, 3], potentially underestimating the role of anisotropic relaxation times and scattering-in contributions. Here, we systematically study charge-spin and charge-orbital conversion in SrTiO3-based 2DEGs, combining the Boltzmann semiclassical transport theory and various ansatzes for the scattering terms, such as constant relaxation time, momentum relaxation time, as well as scattering on various impurity potentials. Comparing different scattering approaches, we gain insights into the influence of impurity scattering on charge-spin and charge-orbital interconversion phenomena.

[1] Vaz, Diogo C., et al. Nature Materials 18.11 (2019): 1187-1193. [2] Caviglia, A. D., et al. Physical Review Letters 104.12 (2010): 126803. [3] Johansson, Annika, et al. Physical Review Research 3.1 (2021): 013275.

TT 46.7 Wed 11:30 POT/0112

Quantum geometry for orbital magnetization and spintronics from parallel transport of Bloch states — •Johannes Mitscherling, Jan Priessnitz, and Libor Šmejkal — Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

Quantum geometry emerges as a unifying, quantitative guiding principle for the linear and nonlinear response functions of quantum matter. Going beyond current-current responses [1,2], we identify the generator of parallel transport of Bloch states, given by the commutator of the band projector and its momentum derivative, as a further essential building block of quantum geometry [3]. I

will show that orbital magnetism arises from the non-commutativity of adiabatic transport in orthogonal directions. We will see that the spin Berry curvature and the spin quantum metric, which control the linear spin conductivity, are not fundamentally geometric but yield three geometric contributions of distinct physical origin. Our theory enables efficient numerical and analytical evaluations for general Bloch Hamiltonians with an arbitrary number of potentially degenerate bands. I will exemplify the results in application to altermagnets [4] and p-wave magnets [5].

[1] Avdoshkin*, Mitscherling*, and Moore, PRL 135, 066901 (2025). [2] Mitscherling*, Avdoshkin*, and Moore, PRB 112, 085104 (2025). [3] Mitscherling and Šmejkal, to be submitted. [4] Šmejkal, Sinova, and T. Jungwirth, PRX 12, 031042 (2022). [5] Birk Hellenes, Jungwirth, Jaeschke-Ubiergo, Chakraborty, Sinova, and Šmejkal, arXiv:2309.01607v3.

TT 46.8 Wed 11:45 POT/0112

Signatures of magnon dispersion in spin transport — •Sebastian Sailler, Denise Reustlen, Michaela Lammel, Sebastian T. B. Goennenwein, and Richard Schlitz — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

The spin Hall magnetoresistance (SMR) provides electrical access to the magnetization of a magnetically ordered material. It recently became clear that changes in the net magnetization due to magnon creation and annihilation can be observed in the SMR. However, the number of magnons - and thus the magnetization - can also be modified by changing the energy of the system. In this work, we experimentally demonstrate that the changes of magnon occupation due to magnetic fields and crystal orientation sensitively modify the SMR response. Higher magnetic fields reduce the magnon population by pushing the magnon manifold to higher energies, leading to an increase of magnetization and thus the SMR. In turn, the influence of the anisotropic magnon gap in yttrium iron garnet films leads to a crystal orientation dependence of the SMR. The magnetic field and orientation dependence can be rationalized in terms of the changing magnon occupation. Our results showcase that magnetoresistive effects not only probe the properties of the static magnetization, but also reveal information about the dynamics, i.e., the magnons.

TT 46.9 Wed 12:00 POT/0112

Non-reciprocal spin-orbital-charge interconversion via magnon transport in nonlocal devices — •Jose Omar Ledesma-Martin[1], Sachin Krishnia[1], Edgar Galindez-Ruales[1], Duc Tran[1], Marcel Gasser[1], Dongwook Go[1,2], Gerhard Jakob[1], Yuriy Mokrousov[1,2], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg University Mainz, Mainz, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany

In magnetic systems, angular momentum is carried by electrons' spin and orbital angular momentum. We use devices based on Pt nanowires on insulating magnets to study angular-momentum transport mediated by magnons, enabling angular-momentum information to propagate without charge flow. In these systems, magnons are generated by spin accumulation from the Spin Hall Effect (SHE) and detected via the inverse Spin Hall Effect (iSHE). In conventional Pt-YIG nonlocal geometries, this spin-charge interconversion is fully reciprocal: interchanging the injector and detector yields equal efficiencies. We further confirm that this power-to-power efficiency remains reciprocal when the thickness of one Pt wire is varied. However, when Ru is used as a source and detector of orbital currents via the orbital Hall effect (OHE) and inverse OHE, the reciprocity is broken. In our devices, the combined SHE + OHE-driven magnon generation, followed by detection through the iSHE, becomes ~35% more efficient than the reverse process, demonstrating nonreciprocity in the system. (1)

(1) J.O. Ledesma-Martin, Nano Lett. 2025, 25, 8, 3247-3252

TT 46.10 Wed 12:15 POT/0112

Giant orbital magnetoresistance in orbital magnets — •Sachin Krishnia[1], Christin Schmitt[1], Edgar Galindez Ruales[1], Takashi Kikkawa[2], Timo Kuschel[1], Eiji Saitoh[2], Olena Gomonay[1], Yuriy Mokrousov[1], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg-University Mainz, Mainz, Germany — [2]Department of Applied Physics, The University of Tokyo, Tokyo, Japan

Generation and transport of large orbital angular momentum (OAM) currents have recently emerged as a key research area in the field of orbitronics. In contrast to spin currents, whose generation depends on weak spin-orbit coupling, OAM currents arise directly from the coupling between crystal momentum and electronic OAM even in light and environmentally friendly materials (Cu, Al, Cr)[1]. A major challenge has been to exploit these giant orbital currents in magnetic systems, where static magnetization is dominated by spin. We show that this limitation can be overcome by employing magnetic materials in which OAM contributes significantly to the static magnetization. Using these orbital magnets, we demonstrate two orders of enhancement of orbital Hall magnetoresistance, compared to the spin counterpart. This enhancement originates from the interaction of the dynamic OAM generated in light metals with the static orbital moments of the orbital magnet. Our results establish a pathway to harness giant OAM currents for device functionalities that cannot be achieved with conventional spin-dominated magnets[2]. [1] S. Ding et al, PRL 125, 177201 (2020). [2] C. Schmitt, S. Krishnia et al. (under review).

TT 46.11 Wed 12:30 POT/0112

Spin-Current Sensitivity in $CuSeO_3$ Across the Antiferromagnetic Transition — •Ankita Nayak[1], Mathew James[1], Maxim Mostovoy[2], and Aisha Aqeel[1] — [1]University of Augsburg, 86135Augsburg, Germany — [2]Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG Groningen, The Netherlands

Antiferromagnets are promising materials for next-generation spintronics due to their robustness against magnetic fields and ultrafast dynamics. Spin Hall magnetoresistance (SMR) provides a sensitive method to probe spin transport at normal-metal–antiferromagnetic-insulator interfaces. In antiferromagnets, SMR can detect Néel-vector reorientation, spin-flop behaviour, and short-range correlations above the ordering temperature, as shown in systems such as NiO and α-Fe_2O_3.

Here, we use SMR in a Pt/$CuSeO_3$ bilayer to investigate spin transport in the unconventional antiferromagnet $CuSeO_3$. An AC current in the Pt Hall bar generates a transverse spin accumulation, whose interface reflection modulates the Pt resistance and enables electrical detection of the magnetic state.

$CuSeO_3$ consists of Cu(1) spin dimers and Cu(2) spins that order antiferromagnetically below 8 K. SMR measurements between 5 and 100 K with magnetic-field rotation in three planes reveal clear SMR signals, including a finite response above the Néel temperature, indicating persistent spin correlations. The plane-dependent SMR amplitude also reflects the intrinsic magnetic anisotropy of $CuSeO_3$.

TT 47: Frustrated Magnets II (joint session MA/TT)

Time: Wednesday 9:30–12:45 Location: POT/0361

TT 47.1 Wed 9:30 POT/0361

Finite-size spectral signatures of order by quantum disorder: A perspective from Anderson's tower of states — •Subhankar Khatua[1], Griffin C. Howson[2], Michel J. P. Gingras[2], and Jeffrey G. Rau[3] — [1]IFW Dresden, Germany — [2]University of Waterloo, Canada — [3]University of Windsor, Canada

In frustrated magnetic systems with a subextensive number of classical ground states, quantum zero-point fluctuations can select a unique long-range ordered state, a celebrated phenomenon referred to as order by quantum disorder (ObQD). While ObQD is well understood in the semiclassical, large spin length limit, its behavior in quantum spin-1/2 systems is less clear. As exact analytical solutions are scarce for frustrated systems, numerical approaches are essential. We show that ObQD can be identified from exact diagonalization (ED) calculations through an analysis akin to the Anderson tower of states associated with spontaneous symmetry breaking. By defining an effective quantum rotor model, we describe the competition between ObQD-induced localization of the rotor and its tunneling between symmetry-related ground states, identifying the crossover lengthscale from the finite-size regime where the rotor is delocalized, to the infinite system-size limit where it becomes localized. This rotor model relates the characteristic splittings in the ED energy spectrum to the ObQD selection energy scale, providing an estimate that can be compared to spin wave calculations. We demonstrate the general applicability of this approach in one-, two- and three-dimensional frustrated spin models that exhibit ObQD.

TT 47.2 Wed 9:45 POT/0361

Magnetic resonance experiments on the quantum spin liquid candidate $YbCuSe_2$ — Madhurima Biswas[1], •Marlis Schuller[3], Khokan Bhattacharya[1], Yoshifumi Tokiwa[2], Mamoun Hemmida[3], Hans-Albrecht Krug von Nidda[3], Norbert Büttgen[3], István Kézsmárki[3], and Mayukh Majumder[1] — [1]Department of Physics, Shiv Nadar Institution of Eminence, IN — [2]Advanced Science Research Center, Japan Atomic Energy Agency, JPN — [3]EPV, Institut of Physics, University of Augsburg, DE

Frustrated magnetism in triangular-lattice delafossites offers a fertile route to realising quantum spin liquids (QSL) beyond conventional ordered phases. Among these materials a new candidate, $YbCuSe_2$, stands out as a QSL candidate from the present study. Magnetisation and ESR measurements on high-quality single crystals of $YbCuSe_2$ reveal easy-plane anisotropy. Furthermore, heat-capacity measurements down to 400 mK and μSR measurements down to 30 mK show no signatures of long-range magnetic ordering, establishing this

compound as a promising QSL candidate. To probe the low-energy spin dynamics, we performed ^{63}Cu (I = 3/2) NMR measurements down to 20 mK. We document in-plane and out-of-plane spin-lattice relaxation T_1 as a function of temperature in an applied field of approximately 4 T. A dynamical phase separation was observed below 0.7 K, where one phase corresponds to the disorder-induced state, whereas the temperature evolution of the relaxation rate of the other phase exhibits a power-law divergence indicative of some quantum-critical spin fluctuations due to the proximity to a field-induced ordered state.

TT 47.3 Wed 10:00 POT/0361

Fluctuation driven phases in the triangular lattice — •P. Peter Stavropoulos[1], Roser Valentí[1], and Johannes Knolle[2] — [1]Goethe University, Frankfurt, Germany — [2]Technical University of Munich, Garching, Germany

The triangular lattice has proven to be a model platform of frustrated magnetism, with a rich landscape of emergent phases. It is also an experimentally accessible platform, with many family of materials showing quasi-2D triangular arrangements of magnetic ions. Motivated by this, we revisit magnetic exchange models on the triangular lattice. We discuss phases that are stabilized by order by disorder mechanisms, and comment on their observable signatures.

TT 47.4 Wed 10:15 POT/0361

Frustrated spin-1/2 chains in a correlated metal Ti4MnBi2 — •Xiyang Li and Meng Lyu — No.8, 3rd South Street, Zhongguancun, Haidian District, Beijing, China, 100190

Electronic correlations lead to heavy quasiparticles in three-dimensional(3D) metals, and their collapse can destabilize magnetic moments. It is an open question whether there is an analogous instability in one-dimensional (1D) systems, unanswered due to the lack of metallic spin chain materials. We report neutron scattering measurements and density matrix renormalization group calculations establishing spinons in the correlated metal Ti4MnBi2, confirming that its magnetism is 1D. Ti4MnBi2 is inherently frustrated, forming near a quantum critical point that separates different phases at temperature T = 0. One-dimensional magnetism dominates at the lowest T, and is barely affected by weak interchain coupling. Ti4MnBi2 is a previously unrecognized metallic spin chain in which 3D conduction electrons become strongly correlated due to their coupling to 1D magnetic moments.

TT 47.5 Wed 10:30 POT/0361

Low-temperature spin-freezing in frustrated zirconates $Tb_2Zr_{2-x}Ti_xO_7$ — •Frederik Leon Carstens[1], Sujata Singh[2], C. S. Yadav[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Germany — [2]School of Physical Sciences, IIT Mandi, India

We report on magnetic studies of polycrystalline $Tb_2Zr_{1-x}Ti_xO_7$ (x = 0, 0.5). The zironates possess significant cationic disorder due to similar radii of the cations which introduces magnetic frustration. The materials are investigated by means of low-temperature ac and dc magnetization measurements in magnetic fields up to 7 T and down to 400 mK. Long-range magnetic order is not found down to T = 400 mK. However, in small magnetic fields, we observe a low-temperature spin-frozen state below T = 1.4 K and a slow spin relaxation regime which is significantly enhanced in static magnetic fields, e.g. to 15 K at B = 2 T. A similar behavior has been previously reported for the related rare-earth zirconate $Ho_2Zr_2O_7$ and in the hafnate $Tb_2Hf_2O_7$ [1,2].

[1] A. Elghandour et al., Phys. Rev. B **110**, 064408 (2024)
[2] V. K. Anand et al., Phys. Rev. B **97**, 094402 (2018)

TT 47.6 Wed 10:45 POT/0361

Magnetization plateaus, spin-canted orders and field-induced transitions in a spin-1/2 Heisenberg antiferromagnet on a distorted diamond-decorated honeycomb lattice — •Katarina Karlova and Jozef Strecka — Pavol Jozef Safarik University in Kosice, Slovakia

We investigate the spin-1/2 Heisenberg antiferromagnet on a distorted diamond-decorated honeycomb lattice in an external magnetic field. Using density-matrix renormalization group, sign-problem-free quantum Monte Carlo, exact diagonalization, and an effective lattice-gas approach based on localized-magnon physics, we determine the ground-state phase diagram and analyze the finite-temperature magnetization process.

The model hosts a rich variety of frustration-induced quantum phases, including Lieb-Mattis ferrimagnetic states, spin-canted regimes, monomer-dimer and dimer-tetramer phases, and dimensional-crossover states with 0D or 1D character. Depending on the lattice distortion, we identify robust magnetization plateaus at 0, 1/4, 1/2, and 3/4 of the saturation value, originating from competing local singlet clusters, composite spins, and flat-band localized magnons. Finite-temperature QMC data show how thermal fluctuations progressively smear the plateau structure, while the effective lattice-gas description reliably captures the corresponding low-temperature trends.

Funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V04-00403.

15 min break

TT 47.7 Wed 11:15 POT/0361

Effect of Ca-doping on the exotic quantum spin liquid states of Y3Cu2Sb3O14 — •Muhammad Usama Akbar[1], Hans-Albrecht Krug von Nidda[1], Mamoun Hemmida[1], Avinash Mahajan[2], and Saikat Nandi[2] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, D-86135 Augsburg, Germany — [2]Department of Physics, Indian Institute of Technology, Mumbai, 400076, India

The three-dimensional spin S = 1/2 compound Y3Cu2Sb3O14 was recently identified as a promising candidate for novel quantum spin liquid (QSL) behavior, with two inequivalent Cu2+ sites in edge-sharing triangles and no long-range order observed in multiple experiments [1]. NMR detects a transition near 120 K, associated with partial singlet formation, while muSR and DFT indicate frustrated antiferromagnetic interactions around both Cu+2 sites. ESR shows a Lorentzian line (g = 2.16) above 120 K that splits into two components on cooling, with only a part of spins being ESR-active. In the current work, we extend this investigation to Ca-doped Y3-xCaxCu2Sb3O14 (x = 0.05, 0.10, 0.25), to examine how chemical substitution at the Y site influences the spin dynamics of the compound.

[1] S. Nandi et al. (2025), arXiv:2509.15835 [cond- mat.str-el]

TT 47.8 Wed 11:30 POT/0361

Synthesis and H-T phase diagram of $Cu_2(OH)_3HCOO$ — •Issei Niwata[1,2], Kaushick K. Parui[1], Maxim Avdeev[3], Anton A. Kulbakov[1], Dmytro S. Inosov[1], and Darren C. Peets[1] — [1]TU Dresden, Dresden, Germany — [2]Hokkaido University, Sapporo, Japan — [3]ANSTO, Sydney, Australia

$Cu_2(OH)_3X$ (X = monovalent anion) consists of quasi one-dimensional (1D) ferromagnetic (FM) and antiferromagnetic (AFM) chains which alternate to form two-dimensional triangular layers, which are stacked along the c axis. As the interchain interactions are frustrated and interlayer interactions are weak, the system can be regarded as weakly coupled 1D FM and AFM chains. In bulk measurements, these compounds typically show AFM behavior with a Néel temperature (T_N) below 10 K. Because of the coexistence of FM and AFM chains, exotic magnetic excitations are expected. As a matter of fact, for $X = Br^-$, inelastic neutron scattering revealed magnon excitations and a gapped spinon continuum in the same energy range. In addition, for $X = NO_3^-$, the realization of a Tomonaga-Luttinger-liquid state in the AFM chain was suggested in magnetic fields around 20 T, where the magnetization shows a half saturation indicating full polarization of the FM chains. Recently, we grew single crystals of the $X = HCOO^-$ compound. Magnetization measurements showed T_N = 5.4 K and a half saturation below 5 T, much lower than $X = NO_3^-$. This suggests that we can explore the excitation structure in relatively low magnetic fields. I will discuss the phase diagram obtained by physical properties measurements.

TT 47.9 Wed 11:45 POT/0361

***H*–*T* Phase Diagram of the Frustrated Quantum Magnet Antlerite, $Cu_3SO_4(OH)_4$** — •Darren C. Peets[1], Nikolai S. Pavlovskii[1], Roman Gumeniuk[2], Sergey Granovsky[1], and Dmytro S. Inosov[1] — [1]IFMP, TU Dresden, Germany — [2]IEP, TU Bergakademie Freiberg, Germany

The magnetic copper sites in antlerite, $Cu_3SO_4(OH)_4$, are arranged in three-leg triangular-lattice ladders, a unique magnetic lattice. In the ground state, the outer legs are ferromagnetic and antialigned, while the central leg is antiferromagnetic. This material has four distinct magnetic states in zero field alone, and we show that the phase diagram in applied fields is also remarkably rich.

TT 47.10 Wed 12:00 POT/0361

Magnetic structure of a geometrically frustrated Mn3V2Ge3O12 garnet oxide — •Sagar Mal Kumawat[1], Tsai-Ling Liu[1], Chin-Wei Wang[2], Jia-Xiang Hsu[1,3], En-Pei Liu[3], Wei-Tin Chen[3,4,5], and Chien-Lung Huang[1] — [1]Department of Physics and Center for Quantum Frontiers of Research & Technology (QFort), National Cheng Kung University, Tainan 701, Taiwan — [2]National Synchrotron Radiation Research Center, Hsinchu 30076, Taiwan — [3]Center for Condensed Matter Sciences, National Taiwan University, Taipei 10617, Taiwan — [4]Center of Atomic Initiative for New Materials, National Taiwan University, Taipei 10617, Taiwan — [5]Taiwan Consortium of Emergent Crystalline Materials, National Science and Technology Council, Taipei 10622, Taiwan

We investigated the low-temperature magnetic structure and thermodynamic properties of Mn3V2Ge3O12 (MVGO) using neutron diffraction, magnetic, and heat capacity measurements. MVGO crystallizes in a cubic Ia-3d structure with a minor MnV2O4 impurity. Two successive transitions at TN1 = 4 K and TN2 = 2.4 K indicate noncollinear antiferromagnetic ordering of the frustrated V3+ and Mn2+ sublattices. Field-dependent heat capacity shows suppression of the TN1 anomaly and a shift of TN2, consistent with magnetic frustration and spin reorientation. The total magnetic entropy reaches approximately 51 J/mol K above 20 K, accounting for ~81% of the theoretical entropy for the full spin system. Temperature-dependent measurements reveal noncollinear antiferromagnetic order below TN2, with peak broadening up to TN1 indicating strong spin frustration.

TT 47.11 Wed 12:15 POT/0361

Crystallographic and magnetic structure of Pr_2PdSi_3: a single crystal neutron diffraction study — •Matthias Frontzek — Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

The intermetallic compound series R_2PdSi_3 (R = rare earth metal) exhibits intriguing magnetic properties, including giant magnetoresistance, pronounced anisotropy in its electronic behavior, and a generic field-induced phase. The magnetic structures are complex, with large magnetic unit cells arising from the delicate interplay between competing crystal electric-field effects, magnetic exchange interactions, and geometric frustration. Recently, the discovery of a Skyrmion lattice in Gd_2PdSi_3 has renewed interest in the magnetic properties of this series.

In our contribution, we present a detailed neutron single crystal diffraction study using the WAND^2 diffractometer at the High-Flux Isotope Reactor (HFIR) at ORNL. In heavy rare earth members, Pd/Si ordering lowers the symmetry from hexagonal to monoclinic; in contrast, the Pr_2PdSi_3 compound adopts an orthorhombic structure with a $2*a, 2*b, 4*c$ unit cell relative to the primitive hexagonal cell. Magnetic order setting in at T_N = 2.1K is preceded by broad diffuse scattering around the nuclear reflections, and below T_N a long-wavelength spin-density wave is observed coinciding with the short-range order evidenced by the diffuse scattering.

TT 47.12 Wed 12:30 POT/0361

Dynamical heterogeneity and fractal subdiffusive transport in spin-ice — •Malte Bieringer[1], Gianluca Teza[1,2], Claudio Castelnovo[3], and Roderich Moessner[1] — [1]Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, 01187 Dresden, Germany — [2]Department of Physics, University of Trieste, Strada Costiera 11, 34136 Trieste, Italy — [3]TCM Group, Cavendish Laboratory, University of Cambridge, Cambridge CB3 0HE, UK

Spin ice is a paradigmatic model that, despite its simplicity, enables the exploration of rich and robust emergent phenomena in topological magnets. Here we uncover a novel set of spin-ice phenomenology typically associated with vitrification processes in disordered systems.

We identify a pronounced peak in dynamical heterogeneity in a classical spin-ice model on the three-dimensional pyrochlore lattice, in the complete absence of disorder and - remarkably - in thermal equilibrium. At low temperatures, additional dynamical constraints emerge that confine the motion of magnetic monopole excitations to three-dimensional percolation clusters. This gives rise to ergodic subdiffusion, opposing conventional emergent hydrodynamics. The observed dynamical heterogeneity arises without disorder or ergodicity breaking, distinguishing it from conventional glasses and systems with Hilbert space fragmentation, suggesting a generic feature of topological magnets hosting deconfined quasiparticles.

Our results motivate the search for materials and artificial spin-ice realizations of this physics and propose higher-order dynamical correlations as a distinctive experimental signature of topological magnetism.

TT 48: 2D Materials: Electronic structure, excitations, etc. II (joint session O/HL/TT)

Time: Wednesday 10:30–12:30 Location: TRE/MATH

TT 48.1 Wed 10:30 TRE/MATH

Polarons in epitaxial single-layer $MnBr_2$ — •Affan Safeer, Oktay Güleryüz, Guangyao Miao, Wouter Jolie, Thomas Michely, and Jeison Fischer — II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany

We investigate polaron formation in insulating single-layer $MnBr_2$ grown by molecular beam epitaxy on three different substrates: graphene on Ir(110), graphene on Ir(111), and Au(111). The polaron number densities and species depend strongly on the underlying substrate, underscoring the crucial role of the substrate. Our findings show that modeling of polarons in such single-layer insulators in contact with conducting substrates must explicitly include the substrate. For $MnBr_2$ grown on graphene/Ir(110), we identify four distinct polaron species, three of which closely resemble those reported for $CoCl_2$ on graphite. These polarons can be created, converted, and laterally manipulated by the STM tip when a tunneling current flows at suitable bias voltages. For graphene on Ir(110) as a substrate, mobile polarons in $MnBr_2$ are guided by the periodic potential imposed by the super-moiré pattern arising from the interaction of $MnBr_2$ with graphene and Ir(110).

TT 48.2 Wed 10:45 TRE/MATH

Chirality in the Kagome Metal CsV_3Sb_5 — •Tom P. Lammerskötter[1], H.J. Elmers[2], G. Schönhense[2], O. Tkach[2], Y. Lytvynenko[2], H. Agarwal[2], S. Chernov[3], M. Hoesch[3], D. Kutnyakhov[3], M. Scholz[3], K. Rossnagel[4], A. Gloskovskii[3], C. Schlueter[3], A. Winkelmann[5], A. Haghighirad[6], M. Schmitt[7], T. Lee[7], R. Claessen[8], M. Le Tacon[6], J Demsar[2], and O. Fedchenko[1] — [1]Goethe-Universität Frankfurt (Germany) — [2]JGU Mainz (Germany) — [3]DESY Hamburg (Germany) — [4]Universität zu Kiel (Germany) — [5]AGH University of Krakow (Poland) — [6]KIT Karlsruhe (Germany) — [7]DIAMOND (UK) — [8]Universität Würzburg (Germany)

Kagome metals AV_3Sb_5 (A = Cs, K, Rb) exhibit flat bands, Dirac points, and van Hove singularities that drive unconventional charge-density-wave (CDW) order and topological states. We study chirality in CsV_3Sb_5 using angle-resolved photoemission spectroscopy (ARPES) and x-ray photoelectron diffraction (XPD) with circularly polarized photons. XPD reveals a local crystal chirality in the CDW phase. ARPES shows pronounced magnetic circular dichroism (MCD), demonstrating a chiral electronic structure and indicating orbital moments possibly linked to loop-current order. To probe orbital-moment coupling, we study Nb-doped CsV_3Sb_5, where band broadening and enhanced Dirac-like gaps occur. In the CDW phase, the strongly increased MCD indicates time-reversal-symmetry breaking and couples to the three van Hove singularities at the M points.

TT 48.3 Wed 11:00 TRE/MATH

Ab initio and group theory ananlysis of monolayer BiTeI — •Josep Mas-Garcia, Jorge Cervantes-Villanueva, Alejandro Molina-Sánchez, and Alberto García-Cristóbal — ICMUV - University of Valencia - Spain

Monolayer BiTeI is a prototypical polar semiconductor whose remarkable Rashba spin splitting, rooted in strong spin-orbit coupling and non-centrosymmetric structure, offers a fertile landscape for advancing two-dimensional spintronics. This work presents and ab initio and group-theoretical analysis of BiTeI. Employing fully relativistic density functional theory and GW calculations, we obtain electronic structures that serve as benchmarks for the group-theory based Hamiltonian model. Leveraging the systematic method of invariants, we construct symmetry-constrained k-p Hamiltonians near the Γ point. Our implementation of the method of invariants enables precise fitting of the Hamiltoninan eigenvalues to ab initio band dispersions for the obtention of the parameters, and yields a highly compact analytic model that reproduces Rashba splitting and symmetry-dependent features. This framework facilitates straightforward evaluation of key physical quantities, such as effective masses or spin textures, and perturbative responses including electric and magnetic fields and strain effects within a unified and transparent formalism. Moreover our methodology establishes a versatile template for the symmetry-guided modeling of nonmagnetic semiconductors with strong spin-orbit coupling.

TT 48.4 Wed 11:15 TRE/MATH

Production of Interstitials in 2D Transition-Metal Dichalcogenides (TMDs) by Ion Irradiation: ab-initio Simulations — •Silvan Kretschmer[1], Joel Davidsson[2], and Kristian S. Thygesen[1] — [1]CAMD, Technical University of Denmark — [2]Department of Physics, Linköping University, Sweden

Defects critically shape the properties of two-dimensional (2D) materials and can be purposefully introduced to tune magnetic, electronic, and optical behavior. Low-energy ion irradiation has recently emerged as an effective route for generating specific defect types via direct implantation [1,2].

First-principles simulations are essential for understanding irradiation-induced defect formation [3], but DFT-based molecular dynamics (MD) is computationally costly and limits broad exploration of materials and irradiation conditions. Machine-learning (ML) interatomic potentials provide a high-accuracy, low-cost alternative, enabling efficient screening of large datasets such as the Impurities in 2D Materials Database [4].

Here, we benchmark a ML potential against ab-initio MD, emphasizing accurate treatment of the short interatomic distances occurring during ion impacts. We apply the fine-tuned ML to study interstitial defect formation in TMDs under low-energy ion irradiation, providing defect formation probabilities and identifying suitable ion-beam parameters for targeted defect engineering in 2D materials.

[1] 10.1038/s41699-022-00318-4 [2] 10.1021/acsnano.4c03475
[3] 10.1103/PhysRevMaterials.8.114003 [4] 10.11583/DTU.19692238

TT 48.5 Wed 11:30 TRE/MATH

Long-living metastable electronic states in substituted 1T-TaS_2 — •Gaël Reecht[1], Jesumony Jayabalan[1], Ričards Knipšis[2], Florian Diekmann[3], Friedemann Queisser[2], Ping Zhou[1], Walter Schnelle[4], Kai Rossnagel[3,5], Ralf Schützhold[2], Manuel Gruber[1], and Uwe Bovensiepen[1] — [1]University Duisburg-Essen, Germany — [2]HZ Dresden-Rossendorf, Germany — [3]CAU of Kiel, Germany — [4]MPI for Chemical Physics of Solids, Dresden, Germany — [5]DESY, Hamburg, Germany

$1T$-TaS_2 is a prototypical correlated material whose low-temperature phase exhibits a commensurate charge density wave forming Star-of-David (SOD) clusters. Each SOD hosts a single electron close to E_F and, due to strong on-site Coulomb repulsion, the system enters a Mott insulating state. Adding or removing an electron creates doublon or holon excitations, which typically relax within few femtoseconds [1]. Here, we manipulate the lifetime of the quasiparticle excitations by substituting some Ta with an electron richer element. Using LT-scanning tunnelling microscopy and spectroscopy (STM/STS) and time-resolved photoemission spectroscopy, we observe metastable doublons with lifetimes ranging from fs to hours. STM/STS further shows that these excitations are locally confined. The experimental observations are corroborated by a theoretical description based on a Fermi-Hubbard model. The disorder induced by the random substitution leads to a spatial localization of holon and doublon wavefunctions at the origin of the long lifetimes observed experimentally.

[1] M. Ligges et *al.*, Phys. Rev. Lett., **120**, 166401 (2018)

TT 48.6 Wed 11:45 TRE/MATH

Fingerprints of Excitonic Collective Modes in the Two-Dimensional Electron Gas — •Jakob Wolff[1,2,3], Silvana Botti[2,3], Lucia Reining[4,3], and Matteo Gatti[4,3,5] — [1]Institut für Festkörpertheorie- und Optik, Friedrich-Schiller-Universität Jena, Germany — [2]Research Center Future Energy Materials and Systems, University Alliance Ruhr and Interdisciplinary Centre for Advanced Materials Simulation, Faculty of Physics and Astronomy, Ruhr University Bochum, Germany — [3]European Theoretical Spectroscopy Facility (ETSF) — [4]LSI, CNRS, CEA/DRF/IRAMIS, École polytechnique, Institut Polytechnique de Paris, France — [5]Synchrotron SOLEIL, Gif-sur-Yvette, France

We investigate the collective charge excitations of the two-dimensional homogeneous electron gas in the low density regime within the framework of time-dependent density functional theory. We show that beyond the well-known plasmons new collective excitonic modes emerge, which leave characteristic fingerprints in experimentally accessible quantities, such as asymmetric peak structures in the loss function and enhanced Friedel oscillations. Further, at sufficiently low densities the collective modes become imaginary, indicating an instability towards the formation of a charge-density-wave phase with excitonic origin.

TT 48.7 Wed 12:00 TRE/MATH

Moir'e modulated quantum spin liquid candidate 1T-TaSe2 — Ziying Wang, Adolfo O. Fumega, Ana Vera Montoto, Mohammad Amini, Büsra Gamze Arslan, Ales Cahlik, Yuxiao Ding, Jose L. Lado, •Robert Drost, and Peter Liljeroth — Aalto University, Department of Applied Physics

Quantum spin liquids continue to fascinate with their highly entangled quantum states and promises of fractional many-body excitations. Yet there are few tools to probe these materials, and none sensitive enough for applications in 2D materials. This seriously hampers the study of monolayer QSL candidates such as α-RuCl3 and 1T-TaSe2. Scanning tunneling microscopy and spectroscopy may overcome this challenge, as they can access the fundamental excitations of 2D samples through inelastic tunneling spectroscopy. These low-energy excitations can be compared against theoretical models and provide fingerprints of QSL states. We employ this approach against the quantum spin liquid candidate 1T-TaSe2. We observe the emergence of a root 3 reconstruction driven by the substrate, equivalent spectroscopy across all spin sites, and the coexistence of zero and finite energy excitations. These observations are consistent with a QSL ground state. Our results demonstrate that IETS provides a powerful route to obtain atomic-scale insight into the magnetic excitations of two-dimensional materials. Spectral fingerprints may help to identify exotic phases of matter that are otherwise difficult to detect.

TT 48.8 Wed 12:15 TRE/MATH

Long-Range Interactions in Twisted Bilayer Materials with Machine Learning for the Electronic Density — •Zekun Lou[1], Alan Lewis[2], and Mariana Rossi[1] — [1]MPI for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Department of Chemistry, University of York, York, U.K.

Moiré superlattices in twisted bilayer (TB) 2D materials exhibit extraordinary quantum phenomena, but first-principles understanding remains limited by computational costs. While most machine learning (ML) methods for density functional theory (DFT) acceleration are based on the locality assumption, we demonstrate that accurate moiré electronic structure prediction requires long-range encoding due to charge rearrangement, orbital hybridisation, and moiré potential modulation. Using long-range representations [1] for electronic-density prediction [2,3], we achieve low-energy band-structure predictions with <15 meV errors across twisted bilayer graphene (TBG), hBN, and transition-metal dichalcogenides (TMDCs), while ~100 times faster than DFT. Descriptor requirements are material-dependent: homoatomic systems (e.g., TBG) are well-described by local descriptors, while hBN and TMDCs require long-range encoding. We summarise the physical implications of these findings that marry machine learning and the fundamental physics that governs the electronic density of twisted bilayer materials.

[1] A. Grisafi, M. Ceriotti, JCP 151, 204105 (2019)
[2] A. Lewis, A. Grisafi, M. Ceriotti, M. Rossi, JCTC 17, 7203 (2021)
[3] A. Grisafi, A. Lewis, M. Rossi, M. Ceriotti, JCTC 19, 4451 (2023)

TT 49: Correlated Electrons: Charge Order

Time: Wednesday 10:45–12:45 Location: HSZ/0101

TT 49.1 Wed 10:45 HSZ/0101

Charge density wave and superconductivity interplay in 2H-$TaSe_2$ — •Yuliia Tymoshenko[1], Amir-Abbas Haghighirad[1], Rolf Heid[1], Gaston Garbarino[2], Luigi Paolasini[2], and Frank Weber[1] — [1]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [2]European Synchrotron Radiation Facility, 71 avenue des Martyrs, CS 40220, Grenoble 38043, France

The suppression of an ordered state is often discussed as a pathway to enhancing superconducting (SC) transition temperatures. Transition-metal dichalcogenides (TMDs), where both charge-density-wave (CDW) order and superconductivity arise from electron-phonon coupling, offer an ideal platform to study this interplay.

We performed high-pressure single-crystal X-ray diffraction (XRD) and inelastic X-ray scattering (IXS) on 2H-$TaSe_2$ and traced the evolution of its CDW superstructure and soft phonon mode over a broad temperature-pressure range. Our measurements show that the suppression of CDW order remains continuous down to low temperatures, demonstrating the persistence of a second-order phase transition, which is a necessary prerequisite for a CDW-related quantum-critical scenario. These findings refine the understanding of how CDW order collapses under pressure and how this behavior relates to the reported maximum superconducting transition temperature near 20 GPa.

Overall, 2H-$TaSe_2$ emerges as a controlled model system for investigating the interplay between CDW order, lattice dynamics, and superconductivity.

TT 49.2 Wed 11:00 HSZ/0101

Dynamics of CDW puddles in bulk 2H-$NbSe_2$ — •Shreya Kumbhakar[1,2], Marina Esposito[3], Anjan Kumar N M[1], Sushmita Chandra[4], Claudia Felser[4], Kornelius Nielsch[1,2], Nicola Poccia[2,3], Stefan Kaiser[1], and Golam Haider[2] — [1]TU Dresden — [2]IFW Dresden — [3]U. Naples — [4]MPI CPfS

In complex materials, incommensurate charge-density-wave (CDW) is often formed from local commensurate domains or puddles. Measuring the dynamics of these puddles, we probe the effect of lattice pinning, electronic correlations and disorder on emergent phases. Raman scattering reveals a Fano lineshape of the CDW amplitude mode, indicating strong coupling between the interlayer shear vibration and the CDW order. Time-resolved reflectivity shows a coherent overdamped oscillation below the CDW transition temperature, indicating a new low-frequency hybrid phonon-CDW amplitude mode around 0.15 THz. This we identify as the CDW puddle emerging from the strong Fano coupling. Our measurements further reveal a transition at 14 K, pointing to a possible crossover of the dominant commensuration order of these puddles. These results highlight how the layered structure affects the CDW order, which is crucial for the design and understanding of novel vdW heterostructures.

TT 49.3 Wed 11:15 HSZ/0101

Electronic band gap tuning of interchain phonon transport in $Ta_2Ni(S_xSe_{1-x})_5$ — Yuan-Shan Zhang[1], Masahiko Isobe[1], Hidenori Takagi[1,2,3], and •Dennis Huang[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Germany — [3]National Institute for Materials Science, Tsukuba, Japan

The dual electronic and structural characters of the 326 K transition in the quasi-one-dimensional compound Ta_2NiSe_5 continues to inspire heated discussion as to the origin of its primary driving force. The current state of affairs may be best summarized as a three-party debate, in which electron-hole interactions (excitonic insulator), electron-lattice coupling (hybridization gap), and "instrinsic" lattice effects are all championed to play some role. The isostructural compound Ta_2NiS_5 should serve as a valuable foil for better understanding Ta_2NiSe_5, as substitution of Se for S enlarges the single-particle electronic band gap, which diminishes the role of electronic degrees of freedom and greatly reduces the transition temperature. Here, we report thermal transport measurements that probe the interchain phonon conductivity of $Ta_2Ni(S_xSe_{1-x})_5$. A soft-phonon anomaly observed in the Se-rich compounds is absent in the S-rich compounds, implying the crucial role of electronic (excitonic and hybridization-gap) fluctuations that couple to the lattice and boost the structural transition temperature.

TT 49.4 Wed 11:30 HSZ/0101

Doping tunable charge density waves in misfit layer compounds — •Hugo Le Du[1], Ludovica Zullo[2], Justine Cordiez[3], Robin Salvatore[1], Daniel Schmieg[1], Giovanni Marini[4], François Debbontridder[1], Marie Hervé[1], Shunsuke Sasaki[3], Florent Pawula[3], Etienne Janod[3], Matteo Calandra[4], Laurent Cario[3], and Tristan Cren[1] — [1]Institut des Nanosciences de Paris, Sorbonne Université, Paris, France — [2]Julius-Maximilians-Universität Würzburg, Würzburg, Germany — [3]Institut des Matériaux de Nantes, Nantes, France — [4]University of Trento, Italy

Misfit layer compounds are van der Waals heterostructures formed by stacking transition metal dichalcogenide (TMD) and monochalcogenide layers. Theoretically, charge transfer from monochalcogenide to TMD layers results in significant doping. Adjusting the monochalcogenide composition enables precise control over TMD doping levels. We show via scanning tunneling microscopy (STM) that in $(La_xPb_{1-x}Se)1.14(NbSe_2)_2$, the $NbSe_2$ Fermi level shifts from 0.0 eV to 0.3 eV by varying La content. Combining STM with DFT calculations, we demonstrate that $NbSe_2$ transitions from the conventional 3×3 CDW state to alternative configurations at higher doping. Superconducting properties also change, offering a novel platform to explore the interplay between superconductivity and charge density waves.

TT 49.5 Wed 11:45 HSZ/0101

Coherent amplitude response in the excitonic insulator $Ta_2Pd_3Te_5$ — •Anjan Kumar Naralapura Manohara[1], Shuhan Wang[1], Snehashish Chatterjee[2], Chandra Shekhar[2], Claudia Felser[2], and Stefan Kaiser[1] — [1]Institute of Solid State and Materials Physics, TU dresden — [2]Topological Quantum Chemistry Group, Max Planck Institute for Chemical Physics of Solids, Dresden

The excitonic insulator represents a fascinating electronic phase in which bound electron-hole pairs condense into a macroscopic quantum state. The layered compound $Ta_2Pd_3Te_5$ has recently emerged as a compelling platform for exploring this elusive phase. A hallmark of such condensate is the presence of collective excitations analogous to the Higgs (amplitude) and Goldstone (phase) modes in superconductors. In this work, we present the experimental fingerprint of a coherent amplitude response in the excitonic insulator phase of $Ta_2Pd_3Te_5$. Through non-degenerate pump-probe spectroscopy, we identify three low frequency A1g phonons that show strong coupling to the excitonic condensate. We characterise these modes as a function of temperature and excitation fluence to reveal their link to the emergence and dynamics of the excitonic condensate.

TT 49.6 Wed 12:00 HSZ/0101

Doping-tunable charge ordering in semiconducting single-layer Cr_2Se_3 — •Sisheng Duan and Miguel Ugeda — Donostia International Physics Center, Paseo Manuel de Lardizábal 4, 20018 San Sebastián, Spain

The charge density wave (CDW), a charge ordering phase, offers a valuable framework for exploring electron-electron interactions, electron-phonon coupling, and quantum phase transitions. In CDW materials, carrier density substantially influences the ground state, typically altered through foreign ion doping and investigated at macro- or mesoscopic scales via photoemission or transport techniques. However, atomic-scale visualization, particularly in doped CDW systems without foreign ions, remains rare. Here, we present real-space observation of doping-tunable granular charge ordering using scanning tunneling microscopy in semiconducting single-layer Cr_2Se_3, a group VIB transition metal chalcogenide. Observations of lattice distortion, bandgap modulation at the Fermi energy, and STM contrast inversion at low temperatures indicate a charge ordering origin. The semiconducting nature of Cr_2Se_3 enables charge ordering modulation through doping: Hole doping suppresses it, whereas electron doping alters the pattern, yielding a periodic $3\sqrt{3} \times 3\sqrt{3}$ CDW phase. This tunable charge ordering in a group VIB TMC advances the understanding of charge doping and ordering interactions in two-dimensional materials.

TT 49.7 Wed 12:15 HSZ/0101

On the origin of charge density waves as an emergent phenomenon from the electron-phonon interactions in $ZrTe_3$ — •Raghottam M Sattigeri[1,2], Niccolò Mignani[1], Claudia Dallera[1], Ettore Carpene[1], Simona Achilli[2], and Alberto Crepaldi[1] — [1]Physics Department, Politecnico di Milano, Milan, Italy — [2]Physics Department, University of Milan, Milan, Italy

Charge density ordering is not elusive in electronic structures which are highly anisotropic, thus indicating a strong electron-phonon (e-ph) interaction which drives such phenomenon. There has been an active debate on the origin of such ordering in two-dimensional transition metal dichalcogenides, however, similar investigations for bulk materials are scarce. It is evident from experiments that, quasi one-dimensional crystal structure $ZrTe_3$ exhibits stable modulations with long-range ordering which facilitates the system to host charge density waves (CDW). We address and investigate thoroughly the origin of CDW in bulk $ZrTe_3$ using density functional theory based first-principles calculations. We analyze the role of electronic instability and e-ph coupling, respectively, as possible mechanisms for the formation of CDW. From our calculations we were able to identify a peak in the the Lindhard response function and strong e-ph interactions suggesting that, both, the electronic and phononic contributions have a role in the process of CDW ordering in $ZrTe_3$.

TT 49.8 Wed 12:30 HSZ/0101

Controlling metastable charge-ordered states in δ-$Ag_{2/3}V_2O_5$ — •Masahiko Isobe[1], Taisei Kubo[2], Naoyuki Katayama[2], and Robert E. Dinnebier[1] — [1]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — [2]Department of Applied Physics, Nagoya University, Nagoya 464-8603, Japan

Vanadium bronzes have attracted much interest as a playground of various quantum phenomena. They are essentially mixed valent oxides where metallic conductivity and novel phenomena with spin, charge and orbital degrees of freedom can be exhibited. Recently we have investigated the delta-phase of vanadium bronze, focusing on the phase transition in δ-$Ag_{2/3}V_2O_5$ which shows characteristic super-cooling effects. The structure consists of double trellis layer formed by edge/corner-shared VO_6 octahedra and Ag ions located between the layers. We have observed the phase transition at around 230 K accompanied by jumps of magnetic susceptibility and resistivity. Structural analysis of the low-temperature triclinic phase reveals that Ag ion order and Vanadium dimer formation. Below the transition temperature the magnetic susceptibility shows a broad maximum around 110 K followed by spin gap behavior. We conclude that the phase transition in δ-$Ag_{2/3}V_2O_5$ is a charge order into V^{4+} and V^{5+} induced by Ag ion order. The V^{4+} ions form dimers with the spin-gapped ground state. Also it can be super-cooled down to the lowest temperature by rapid cooling.

TT 50: German-French Focus Session: Superconducting Junctions and Quantum Circuits

Superconducting junctions are important building blocks for various applications including qubits. The importance of superconductivity to probe macroscopic quantum physics has been underlined by the Nobel prize in physics 2025. Current research activities in the field of superconducting quantum circuits bridge from fundamental symmetry aspects of superconductivity to material science for improved performance of superconducting electronics. Beyond these activities, superconductivity has developed as a tool to probe also unconventional normal conducting properties. The scope of this focus session is to showcase recent activities in this field in France and Germany and to tighten the interaction between the very active research communities in both countries.

Coordinators: Clemens Winkelmann (CEA/UGA Grenoble), Guillaume Weick (University of Strasbourg), Elke Scheer (University of Konstanz).

Time: Wednesday 15:00–18:30 Location: HSZ/0003

Topical Talk TT 50.1 Wed 15:00 HSZ/0003

Josephson Quantum Tunneling at Odd Parity — Manuel Houzet[1], •Julia S. Meyer[1], and Yuli V. Nazarov[2] — [1]Univ. Grenoble Alpes, France — [2]Delft University of Technology, The Netherlands

When a Josephson junction is embedded in an electromagnetic circuit, the superconducting phase difference across the junction becomes a quantum-fluctuating variable. The resulting quantum mechanics of the Josephson effect is the core ingredient for quantum technologies with superconducting circuits. On a microscopic level, the Josephson effect is related to Andreev bound states in the junction and depends on their occupation. When a single quasiparticle is trapped in an Andreev bound state–a situation known as quasiparticle poisoning–the junction is in the odd-parity sector. Because of parity conservation, such a poisoned state may exhibit a long lifetime. Our work opens a new avenue in this field by showing that the Josephson quantum mechanics in the odd-parity sector differs fundamentally from the conventional behavior in the

even-parity sector. We uncover a rich phenomenology that contrasts with the naïve expectation of a simple supercurrent quench, which prevailed so far. Covering several representative cases, we predict a variety of novel effects that can be probed in upcoming experiments. Hybrid superconductor-semiconductor-superconductor junctions, that have been intensively studied in recent years both with nanowires and two-dimensional electron gases, provide a promising platform for observing these phenomena.

Topical Talk TT 50.2 Wed 15:30 HSZ/0003

Superconducting qubits and amplifiers resilient to Tesla-scale magnetic fields — •Ioan Pop — KIT, Karlsruhe, Germany

Superconducting qubits with quantum non-demolition readout and active feedback can act as information engines to probe and control microscopic degrees of freedom, both engineered and environmental. However, performing such experiments in magnetic fields above tens of mT poses a significant challenge for conventional superconducting qubits. We demonstrate a fluxonium qubit with a granular aluminum nanojunction (gralmonium) that maintains spectral stability and coherence above 1 T [1]. This robust performance enables exploration of spin environment dynamics and supports hybrid quantum architectures integrating superconducting qubits with spin systems [2].

[1] Günzler & Beck et al., Nature Comm. 16, 9564 (2025)
[2] Günzler et al., Phys. Rev. B 112, 115424 (2025)

Topical Talk TT 50.3 Wed 16:00 HSZ/0003

Josephson metamaterials as near-quantum-limited microwave amplifiers — •Nicolas Roch — Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Neel, 38000 Grenoble, France

Josephson meta-materials have recently emerged as a highly promising platform for superconducting quantum science and technology. Their unique potential lies in the ability to engineer these materials at sub-wavelength scales, allowing for complete control over wave dispersion and nonlinear interaction. In this seminar, I will demonstrate how Josephson meta-materials can be utilized as microwave amplifiers with added noise that approaches the quantum limit. These materials are already widely used in experiments ranging from quantum information processing with superconducting qubits to dark matter detection. In the second part, I will present a recent experiment demonstrating a microwave amplifier that exhibits intrinsic isolation and can be used to read out a superconducting qubit without the need for magnetic isolators.

This research is conducted in collaboration with the company Silent Waves.

15 min. break

Topical Talk TT 50.4 Wed 16:45 HSZ/0003

Second Order Topological Insulators probed with mesoscopic physics — •Sophie Gueron — Laboratoire de Physique des Solides Universite Paris-Saclay France

Second Order Topological Insulators (SOTIs) are a new family of materials, predicted to be insulating in the bulk and surfaces, and perfectly conducting along dimensional crystal hinges. Similarly to Quantum Spin Hall edges states in 2D Topological Insulators, the hinge states are expected to carry current with no dissipation and no backscattering, due to their unique spin-momentum-locked configuration, also called helicity. I will present various mesoscopic physics experiments that have uncovered the special properties of SOTIs. Firstly, experiments with superconducting contacts have led to the discovery that Bismuth was a Second Order Topological Insulator, by providing evidence of hinge states and their topological character. We have also recently extended our experiments to new SOTI materials and to non- superconducting contacts, as well as to the investigation of the current-induced spin polarization due to spin-momentum locking in the hinge states. Finally, I will present a new detection scheme to explore orbital currents in 2D materials, that has the potential to reveal persistent currents circulating at the hinges of a mesoscopic SOTI crystal.

This work is a collaborative work conducted in the Mesoscopic Physics group at Laboratoire de Physique des Solides

Topical Talk TT 50.5 Wed 17:15 HSZ/0003

Proximity superconductivity in chiral Kagome antiferromagnets — •Piet Brouwer, Adam Chaou, Gal Lemut, and Felix von Oppen — Freie Universität Berlin, Dahlem Center for Complex Quantum Systems, Fachbereich Physik, and Halle-Berlin- Regensburg Cluster of Excellence CCE, Arnimallee 14, 14195 Berlin

Recent experiments on the chiral Kagome antiferromagnet Mn_3Ge have provided strong evidence of proximity-induced spin-polarized superconductivity. We introduce and explore a minimal model which exhibits a rich phase diagram as a function of chemical potential and spin canting. We find a valley-singlet superconducting phase for chemical potentials and canting consistent with the experimental system. This phase transitions into a Chern insulator at larger canting and gives way to topological superconducting phases with Chern numbers $C_{\mathrm{BdG}} = \pm 1, \pm 3$ at other chemical potentials. Our results show that proximity-induced superconductivity in Kagome antiferromagnets is a promising route towards superconductivity with spin-polarized Cooper pairs.

TT 50.6 Wed 17:45 HSZ/0003

Spectroscopy of a nanowire fluxonium — •Hugues Pothier[1], Joan Caceres[1], Diego Sanz[1], Jon Ortuzar[1], Emmanuel Flurin[1], Jesper Nygard[2], Cristian Urbina[1], and Marcelo Goffman[1] — [1]Quantronics group, SPEC (CNRS UMR 3680), CEA-Paris Saclay, University Paris-Saclay, 91191 Gif-sur-Yvette, France — [2]Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, Universitetsparken 5, 2100 Copenhagen, Denmark

We fabricated a fluxonium qubit [1] in which the Josephson junction is replaced with a semiconducting nanowire weak link. The Josephson effect in the nanowire is associated with Andreev bound states, which themselves have been shown to behave as qubits [2-4]. Through precise analysis of the spectroscopy data, we searched for evidence of strongly transmitted channels [5] and for an hybridization of the two types of qubits.

[1] V.E.Manucharyan, J.Koch, M.H.Devoret, Science 326, 113 (2009).
[2] C. Janvier et al., Science 349, 1199 (2015).
[3] M. Hays et al., Phys. Rev. Lett. 121, 047001 (2018).
[4] M. Hays et al., Science 373, 430 (2021).
[5] M. Pita-Vidal et al., Phys. Rev. Applied 14, 064038 (2020).

TT 50.7 Wed 18:00 HSZ/0003

Multiterminal Josephson Junctions: non-hermiticity, topology and reflectionless modes — •David Christian Ohnmacht, Wilhelm Valentin, Weisbrich Hannes, and Belzig Wolfgang — Universität Konstanz, Konstanz, Germany

In multiterminal Josephson junctions (MTJJs), the Andreev bound state energies depend on multiple phase differences, enabling band structure engineering. MTJJs are predicted to host non-trivial topological phases and associated Weyl nodes in the synthetic Brillouin zone spanned by these superconducting phases [1]. In [2], spectroscopic measurements were performed on four-terminal Josephson junctions with phase control of all three superconducting phase differences, unveiling the presence of a tri-Andreev molecule, compatible with a topologically non-trivial model. We predict that such MTJJs, in the presence of additional normal leads, host non-trivial non-Hermitian topology, leading to spectral topology in the form of point gaps and Weyl disks [3]. Additionally, we predict that reflectionless scattering modes in MTJJs are a source of topological phase boundaries [4]. Our work provides an effective bulk boundary correspondence by demonstrating a relationship between unity transmission modes and boundaries between topologically trivial and non-trivial regions, like in quantum Hall systems.

[1] R.-P. Riwar et. al., Nature Commun. 7, 1 (2016)
[2] T. Antonelli et. al., Phys. Rev. X 15, 031066 (2025)
[3] D. C. Ohnmacht et. al., Phys. Rev. Lett. 134, 156601 (2025)
[4] D. C. Ohnmacht et. al., arXiv:2503.10874 (2025)

TT 50.8 Wed 18:15 HSZ/0003

From Shapiro steps to photon-assisted tunneling in microwave-driven atomic-scale Josephson junctions with a single (magnetic) adatom — •Martina Trahms[1,2], Bharti Mahendru[1], Clemens B. Winkelmann[2], and Katharina J. Franke[1,3] — [1]Fachbereich Physik, Freie Universität Berlin, Berlin, Germany — [2]Univ. Grenoble Alpes/CEA/Grenoble-INP/IRIG-Pheliqs, Grenoble, France — [3]Fachbereich Physik and Halle-Berlin-Regensburg Cluster of Excellence CCE, Freie Universität Berlin, Berlin, Germany

Understanding Josephson junctions (JJs) on the atomic scale yields insights for the prospect of superconducting circuits in future technological applications. We form JJs between a superconducting tip and sample in a scanning tunneling microscope (STM). The phase dynamics of the JJ such as dissipation and coherence of the tunneling processes are investigated by high-frequency (HF) irradiation. Shapiro steps indicate coherent Cooper-pair tunneling while incoherent tunneling processes are described by photon-assisted tunneling. With increasing HF irradiation amplitude, the STM JJs transition from the coherent to the incoherent tunneling regime due to the increase of thermal fluctuations. Introducing a magnetic adatom into the junction reduces the Josephson coupling and increases the quasiparticle tunneling rate which leads to a suppression of coherence. We highlight the presence of phase coherence in atomic scale JJs and ascribe the transition from coherent to incoherent Cooper-pair tunneling processes to the interplay of thermal fluctuations and the Josephson coupling strength.

TT 51: Correlated Electrons: Method Development II

Time: Wednesday 15:00–18:15 Location: HSZ/0101

TT 51.1 Wed 15:00 HSZ/0101

Towards accurate low energy models — •Jonas Profe[1], Jaksa Vucicevic[2], P. Peter Stavropoulos[1], Malte Rösner[3], Roser Valenti[1], and Lennart Klebl[4] — [1]Institute for Theoretical Physics, Goethe University Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt a.M., Germany — [2]Scientific Computing Laboratory, Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia — [3]Institute for Molecules and Materials, Radboud University, Nijmegen, The Netherlands — [4]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany

Effective low-energy models are a central cornerstone for understanding emergent phenomena in quantum materials. These models, often containing only a small subset of the original degrees of freedom, capture the low temperature dynamics while being tractable to a variety of numerical and analytical techniques enabling quantitative results even in the strongly correlated limit. As such, a faithful method to derive such low-energy models is essential. In this talk, we will introduce an exact framework for deriving effective models and extract known approaches from it. We further introduce conditions under which an effective model is guaranteed to capture the effective dynamics of the material. Within this framework, we then discuss what material classes display relevant corrections beyond standard downfolding approaches and we explain the physical origin of these corrections.

TT 51.2 Wed 15:15 HSZ/0101

Study of a two-dimensional Rydberg array in a cavity with neural quantum states — •Noe Salmeron[1], Marin Bukov[2], and Markus Schmitt[1,3] — [1]University of Regensburg, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]Institute of Quantum Control (PGI-8), Forschungszentrum Jülich, Germany

Recent advances in cold atom manipulation enable the study of many-body systems where both short-range interactions between neighboring atoms and long-range interactions mediated by photons coexist. Such a combination of interactions makes a theoretical approach challenging beyond mean-field methods. In this work, we develop numerical techniques to investigate one of the simplest model capturing these features: a two dimensional lattice of Rydberg atoms coupled to a single photon mode. We use neural quantum states coupled with stochastic reconfiguration to obtain the ground state on lattices with hundreds of sites. We adapt a neural network architecture commonly used for spin models, to incorporate the additional photon mode. This allows us to capture spin-spin and spin-photon correlations and we explore how the fully correlated ground states deviate from mean field theory. The resulting method provides a scalable approach for investigating the ground state properties of such systems.

TT 51.3 Wed 15:30 HSZ/0101

Understanding discrepancies in noncovalent interaction energies from wavefunction theories for large molecules — •Andreas Irmler, Tobias Schaefer, Alejandro Gallo, and Andreas Grueneis — TU Wien, Vienna, Austria

Recent advances in combining quantum-mechanical methods with machine learning have generated excitement for large-scale molecular simulations. Yet the reliability of these approaches depends on the benchmark accuracy expected from high-level quantum reference methods. Discrepancies have been reported between two widely trusted references - diffusion quantum Monte Carlo and coupled-cluster theory - for large noncovalent complexes, posing a puzzle for the accuracy required to support QM/ML modeling. In this talk, I analyze these discrepancies, identify their origin, and present modifications to the coupled-cluster ansatz that restore reliable, high-accuracy interaction energies for molecules on the hundred-atom scale, paving the way toward more accurate predictive simulations.

TT 51.4 Wed 15:45 HSZ/0101

Embedded Impurity Models with Quantitative Predictive Accuracy: Beyond Mean Field Baths and cRPA — •Kevin Ackermann and Maurits W. Haverkort — Institute for Theoretical Physics, Heidelberg, Germany

Ab-initio embedded impurity approaches, such as DFT+DMFT, are powerful tools for studying correlated materials. However, the interface between the mean-field bath and the many-body impurity presents persistent challenges, particularly in the consistent determination of the screened Coulomb interaction, and the associated double-counting correction.

We address these challenges in the context of transition metal complexes, where an accurate description of the correlated d-electron physics is essential. We present a systematic investigation of electronic g-factors and d-d excitations – sensitive probes of the low-energy electronic structure. Our analysis reveals that achieving quantitative agreement with experimental data requires two components: (1) extending the correlated active space beyond the metal d-orbitals to include relevant ligand states, and (2) incorporating vertex corrections in the calculation of the screened interaction. Only the combination of both yields results consistent with experiment, establishing a clear path toward predictive accuracy in embedded impurity models for coordination complexes.

TT 51.5 Wed 16:00 HSZ/0101

SOLAX: An Open Source Python Package for Neural Network Configuration Interaction — Pavlo Bilous[2], Louis Thirion[1], •Max Kroesbergen[1], Paul Fadler[3], and Philipp Hansmann[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Max Planck Institute for the Science of Light, Erlangen — [3]Universität Bremen

We present a modular Python library, SOLAX [1], designed for configuration interaction (CI) calculations of fermionic quantum many-body systems in high dimensional Hilbert spaces. The provided classes allow convenient encoding of states and operators in second quantization. The JAX-based GPU-accelerated back-end efficiently performs the operations necessary to determine many-body eigenstates in finite-size Hilbert spaces. Along with its core functionalities, SOLAX integrates neural-network (NN) support for the CI calculation of otherwise prohibitively large expansions in Slater determinant basis sets. We show how a NN can be used in CI calculations to identify a priori unknown subsets of the most important Slater determinants and iteratively obtain high-quality approximate many-body eigenstates. Applications involve the paradigmatic Single Anderson Impurity Model in a solid-state physics context [2], as well as computation of molecular ground- [3,4] and excited states [5] in Quantum Chemistry.

[1] L.Thirion, P.Hansmann, P.Bilous, 10.21468/SciPostPhysCodeb.51,
[2] P. Bilous *et al.*, 10.1103/PhysRevB.111.035124
[3] Y.L.A. Schmerwitz *et al.*, 10.1021/acs.jctc.4c01479
[4] L. Thirion *et al.*, arXiv:2510.27665
[5] G. Levi *et al.*, arXiv:2510.26751

TT 51.6 Wed 16:15 HSZ/0101

Finite Temperature Neural Quantum States — •Atiye Abedinnia[1,2,3], Anka Van de Walle[1,3,4], and Annabelle Bohrdt[1,2,3] — [1]Ludwig-Maximilians-University Munich, Theresienstr. 37, Munich D-80333, Germany — [2]University of Regensburg, Universitätsstr. 31, Regensburg D-93053, Germany — [3]Munich Center for Quantum Science and Technology, Schellingstr. 4, Munich D-80799, Germany — [4]Department of Physics and Astronomy, Ghent University, 9000 Gent, Belgium

Finite-temperature effects play an important role in the design and optimization of quantum devices, as decoherence and noise often originate from thermal fluctuations. At finite temperatures, quantum systems are described by a statistical ensemble of states rather than a single pure state. Simulating such thermal states requires constructing the thermal density matrix, which suffers from significant computational challenges due to the exponential growth of the Hilbert space with system size. In this work, we propose using neural quantum states (NQS), leveraging the expressivity and scalability of transformer-based architectures to address the challenges of thermal equilibrium density matrix representation.

15 min. break

TT 51.7 Wed 16:45 HSZ/0101

Tensor Network Python (TeNPy) version 2: status and prospects — •Johannes Hauschild[1,2], Jakob Unfried[1,2], Nico Kirchner[1,2], Ludwig Zweng[1,2], and Frank Pollmann[1,2] — [1]Department of Physics, NAT school, Technical University Munich, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST),80799 Munich, Germany

TeNPy is an established python library for the simulation of strongly correlated quantum systems with tensor networks. We report on the implementation of a new linear algebra package for the library to make it more versatile. One the one hand, it allows to switch between CPU and GPU devices, providing siginificant speedup in certain cases. On the other hand, one can toggle between different symmetry backends. Backends for none or abelian symmetries have been ported from TeNPy version 1 and available with a minimal overhead. Moreover, a new symmetry backend based on fusion trees has been implemented, which can handle general fusion categories. As such, it can be used to conserve non-abelian symmetries like SU(2), SU(n), but also to implement fermions in PEPS, or models based on anyons, e.g., the Fibonaccy chain.

TT 51.8 Wed 17:00 HSZ/0101

Holographic Representation of One-Dimensional Many-Body Quantum States via Isometric Tensor Networks — Kaito Kobayashi[1], •Benjamin Sappler[2,3], and Frank Pollmann[2,3] — [1]Department of Applied Physics, the University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan — [2]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany

Isometric tensor network states (isoTNS) allow for efficient and accurate simulations of higher-dimensional quantum systems by enforcing an isometric structure. We bring this idea back to one dimension by introducing a holographic isoTNS ansatz: a (1+1)-dimensional lattice of isometric tensors where the horizontal axis encodes physical space and an auxiliary "holographic" axis boosts expressivity. We investigate this ansatz and benchmark it in comparison to matrix product states (MPS). We show that randomly initialized holographic isoTNS typically display volume-law entanglement even at modest bond dimension. We further demonstrate that holographic isoTNS can faithfully represent arbitrary fermionic Gaussian states, Clifford states, and certain short-time-evolved states under local evolution. Finally, we implement a time-evolving block decimation (TEBD) algorithm on holographic isoTNS. While the method remains efficient, error accumulation suppresses entanglement and leads to rapid deviations from exact dynamics. Overall, holographic isoTNS broaden the reach of tensor-network methods, opening new avenues to study volume-law physics.

TT 51.9 Wed 17:15 HSZ/0101

A Quasiparticle Excitation Ansatz for 2D Isometric Tensor Network States — •Lukas Wittmann[1,2], Johannes Hauschild[1,2], and Frank Pollmann[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany

Isometric tensor network states (isoTNS) in 2D were introduced as a subclass of projected entangled pair states (PEPS) with additional isometry conditions that allow for an efficient evaluation of local expectation values [1]. Based on a formulation in a finite 45 °-rotated square lattice [2], we introduce an ansatz for quasiparticles in the tangent space of an isoTNS [3,4], generalizing the ideas from 1D matrix product states (MPS) [5,6] and infinite PEPS [7]. We show that this ansatz can faithfully represent low-energy excitations with standing waves of spin flips, crucial for the dynamical structure factor, and discuss an algorithm to variationally optimize them.

[1] M.P. Zaletel, F. Pollmann, Phys. Rev. Lett. 124, 037201 (2020)
[2] B. Sappler et al., arXiv:2507.08080
[3] L. Wittmann, Master's Thesis,
https://github.com/lukasjwittmann/iso_tns-public
[4] L. Wittmann, J. Hauschild, F. Pollmann, in preparation
[5] J. Haegeman et al., Phys. Rev. B 88, 075133 (2013)
[6] M. Van Damme et al., Phys. Rev. B 104, 115142 (2021)
[7] L. Vanderstraeten et al., Phys. Rev. B 92, 201111 (2015)

TT 51.10 Wed 17:30 HSZ/0101

Finite-temperature DMRG calculations for big spin systems using matrix product states — •Lukas Horstmann and Jürgen Schnack — University of Bielefeld, Bielefeld, Germany

Nowadays DMRG is a well established method for calculating ground states. Over time and with the introduction of Matrix Product State (MPS) more and more applications were discovered. On of these is using imaginary time-evolution to calculate finite-temperature states. For this application there already exist a few different methods to achieve it: Time Evolution Block Decimation(TEBD), Time Dependent Variational Principle (TDVP) both with purification and Minimally Entangled Typical Thermal States (METTS) using a sampling approach. These methods perform differently based on the model. Here we will discuss in which scenarios which method is performing best in a one-dimensional model. The focus will be on the aspects of runtime and accuracy for temperatures down to T = 0.5, with the prospect to use it to simulate magnetic observables in real quantum systems.

TT 51.11 Wed 17:45 HSZ/0101

Renormalised Interactions via Composite Fields — •Oleksandr Sulyma[1], Jan von Delft[2], and Benedikt Schneider[2] — [1]Institute for Theoretical Physics, University of Cologne, Cologne, Germany — [2]Arnold Sommerfeld Center for Theoretical Physics, Center for NanoScience, and Munich Center for Quantum Science and Technology, Ludwig-Maximilians-University of Munich, Munich, Germany

The renormalised interactions of particles in quantum many-body systems and general field theories are described by the one-particle-irreducible vertices. The numerical calculation and treatment of these objects have proven to be challenging because of their high dimensionality and complicated frequency and momentum structure. To address these problems, multiple solutions have been proposed: a frequency parametrisation using asymptotic classes; the single-boson exchange (SBE) formalism, which uses only physical correlation functions, thereby avoiding vertex divergencies in the parquet formalism; and symmetric estimators which avoid the amputation of Green's functions, to name a few. We present a unified framework based on the inverse Legendre transform of the composite field effective action that generalises asymptotic classes, symmetric improved estimators, the SBE and the parquet formalism. We demonstrate that these representations of the four-point vertex correspond to different choices of composite fields and naturally extend to more general theories and any-order vertices via simple tree diagrams.

TT 51.12 Wed 18:00 HSZ/0101

The TRIQS arbirary X-Crossing Approximation impurity solver (triqs_xca) — •Hugo U. R. Strand[1], Paco Rilloraza[2], Zhen Huang[3], Nils Wentzell[4], Denis Golež[5], and Jason Kaye[4] — [1]Örebro University, Örebro, Sweden — [2]New York University, New York, USA — [3]University of California, Berkeley, USA — [4]Flatiron Institute, Simons Foundation, New York, USA — [5]Jožef Stefan Institute, Ljubljana, Solvenia

The triqs_xca solver is the latest quantum impurity solver addition to the Toolbox for Research on Interacting Quantum Systems (TRIQS) based on the bold hybridization expansion, a.k.a. the X:th order Crossing Approximation (XCA). Using the sum-of-exponentials trick we acheive parametrically better computational complexity compared to direct integration and the Discrete Lehmann Representation (DLR) is employed for fast convolutions as well as for representing response functions. The solver is open source and distributed as part of the TRIQS project, see github.com/TRIQS/xca.

TT 52: Heavy Fermions

Time: Wednesday 15:00–16:30 Location: HSZ/0103

TT 52.1 Wed 15:00 HSZ/0103

High-field muon spin resonance/rotation (μSR) studies on $CeRh_2As_2$ — •Seunghyun Khim[1], Oliver Stockert[1], Andrin Doll[2], and Robert Scheuermann[2] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Paul Scherrer Institute, Villigen, Switzerland

The heavy-fermion $CeRh_2As_2$ with $T_c = 0.35$ K exhibits unique two-phase superconductivity under a c-axis magnetic field. In the superconducting (SC) state, a field-induced transition at $H^* = 4$ T separates a low-field even-parity (SC1) phase from a high-field odd-parity (SC2) phase. In addition, an unusual ordering of the Ce-4f moments emerges below $T_0 = 0.55$ K, which is suppressed with increasing c-axis field. The T_0 phase boundary smoothly extends into the SC2 phase and persists to zero temperature at approximately 7 T. Previous zero-field μSR studies have identified that an internal field develops spontaneously below T_0 and becomes nearly saturated below T_c, suggesting a possible correlation between the magnetic order and superconductivity. Here, we present following high-field μSR measurements up to 7.5 T. Temperature-dependent measurements at 2 T show that the internal field is fully established below 0.3 K, coinciding with the onset of the SC1 phase. Furthermore, field-dependent measurements at 20 mK reveal that the internal field begins to be suppressed above 4 T and then vanishes entirely at around 7 T. These observations propose that the magnetic order in the T_0 phase is locked in exclusively within the SC1 phase, reflecting an intricate coupling between the magnetic and SC order parameters.

TT 52.2 Wed 15:15 HSZ/0103

Coupled magnetic and quadrupolar order in tetragonal $CeRh_2As_2$ evidenced by the basal-plane anisotropy — •Konstantin Semeniuk[1,2], Burkhard Schmidt[2], Seunghyun Khim[2], and Elena Hassinger[1,2] — [1]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

Unconventional superconductivity in Ce-based Kondo-lattice materials has been known to emerge exclusively in the vicinity of weak dipolar magnetic orders, while higher-order multipolar orders are only known to occur in a few Pr-based unconventional superconductors and possibly URu_2Si_2. Moreover, for tetragonal Ce-based compounds, quadrupolar orders are disfavoured by a two-fold degenerate ground state of the crystal electric field scheme, in contrast to a four-fold degenerate one in cubic systems. The multiphase superconductor $CeRh_2As_2$ appears to be a notable exception from both of these trends by possibly hosting coupled magnetic and quadrupolar orders. In this talk, we explain how such a scenario can be realised [1,2] and show that the field-temperature phase diagram of $CeRh_2As_2$ has a pronounced basal-plane anisotropy, which effectively proves the existence of higher-order multipolar ordering and raises questions regarding its role in the superconducting pairing.

[1] D. Hafner et al., Phys. Rev. X, 12, 011023 (2022).
[2] B. Schmidt, P. Thalmeier, Phys. Rev. B 110, 075154 (2024).

TT 52.3 Wed 15:30 HSZ/0103

Pressure evolution of coplanar antiferromagnetism in heavy-fermion $Ce_2CoAl_7Ge_4$ — •Mukkattu O. Ajeesh[1,2], Allen O. Scheie[1], Yu Liu[1], Lucas Keller[3], Sean M. Thomas[1], Priscila F. S. Rosa[1], and Eric D. Bauer[1] — [1]Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — [2]Department of Physics, Indian Institute of Technology Palakkad, Kerala 678623, India — [3]Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, Villigen CH-5232, Switzerland

$Ce_2MAl_7Ge_4$ (M = Co, Ir, Ni, or Pd) compounds are heavy-fermion materials that exhibit a variety of ground states ranging from magnetism to non-Fermi-liquid behavior. The Co, Ir, and Ni members undergo magnetic ordering with decreasing transition temperatures across the series. In contrast, the Pd compound shows no magnetic order down to 0.4 K and exhibits non-Fermi-liquid behavior, indicating proximity to a magnetic quantum critical point. Among these materials, $Ce_2CoAl_7Ge_4$ orders antiferromagnetically below T_N = 1.9 K and displays heavy-fermion behavior below 15 K. We investigated the magnetic structure of its antiferromagnetic phase along with the evolution of the magnetic transition under external pressure. Resistivity and ac calorimetry measurements under hydrostatic pressure reveal that T_N is suppressed to 1 K at $p \approx 1$ GPa, above which the transition abruptly disappears in a first order-like fashion. These results highlight that transition metal substitution is not merely a lattice volume effect akin to applied pressure; instead, carrier doping and anisotropic changes in lattice parameters likely play important role.

TT 52.4 Wed 15:45 HSZ/0103

Tuning the ground state of CePdAl by hydrogenation — Hailiang Xia, Jitong Song, He Sun, Zhaotong Zhuang, Junsen Xiang, Shuai Zhang, and •Peijie Sun — Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

CePdAl is an antiferromagnetic heavy-fermion compound crystallizing in a geometrically frustrated Kagome lattice. We have succeeded in hydrogen doping the bulk single-crystalline CePdAl by an ionic liquid gating technique, resulting in a large lattice expansion of the c axis by more than 20%. The hydrogen-doped sample $CePdAlH_x$ is stable in air, and can be subject to various ex-situ transport, magnetic and thermodynamic measurements down to very low temperatures. Hydrogen distribution in CePdAl significantly alters the crystal electric field, reducing the Ising-like magnetic anisotropy, and the antiferromagentic transition temperature T_N is reduced from 2.7 K to 1.1 K. Intriguingly, the Kondo effect remains almost intact. We discuss the results in view of a local and anisotropic negative pressure effect realized by hydrogenation.

TT 52.5 Wed 16:00 HSZ/0103

Intertwined magnetic and superconducting orders in Ce_3PtIn_{11} — Jan Fikáček[1], Sarah R. Dunsiger[2], Andrea D. Bianchi[3], Manuel Brando[4], Laurent Nicolai[5], Aki Pulkkinen[5], and •Jeroen Custers[1] — [1]Charles University, Faculty of Mathematics and Physics, Dept. Condensed Matter Physics, Prague, Czech Republic — [2]Centre for Molecular and Materials Science, TRIUMF, Vancouver, Canada — [3]Département de Physique, Université de Montréal, Montréal, Canada — [4]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [5]New Technologies Research Centre, University of West Bohemia, Pilsen, Czech Republic

The heavy fermion compound Ce_3PtIn_{11} exhibits intriguing low-temperature properties. At ambient pressure, it undergoes two successive antiferromagnetic (AFM) transitions at T_{N1} = 2.2 K and T_N = 2.0 K. Superconductivity (SC) emerges below T_c = 0.32 K (J. Prokleška *et al.*, Phys. Rev. B **92,** 161114(R) (2015)). The coexistence of AFM and SC has been proposed, attributed to the presence of two inequivalent Ce sites whose distinct local environments may stabilize either magnetic or superconducting order. In this work, we focus on the superconducting state, presenting specific heat measurements and recent muon spin rotation experiments performed at ambient pressure down to 20 mK, complemented by band-structure calculations. Together, these results reveal signatures of an unconventional SC state coexisting with magnetism.

Work is supported by the Czech Ministry for Education, Youth and Sports program INTERCOST (Grant No. LUC24139).

TT 52.6 Wed 16:15 HSZ/0103

Coupling between Kondo effect and in-plane strain in $YbRh_2Si_2$ — •Soumendra Nath Panja, Jacques G Pontanel, Julian Kaiser, Anton Jesche, and Philipp Gegenwart — Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany

We study symmetry-resolved elastoresistance in the tetragonal Kondo lattice $YbRh_2Si_2$ down to 2 K and in fields up to 14 T. By measuring longitudinal and transverse electrical transport response under applied in-plane uniaxial strain along [100] and [110], we extract the A_{1g}, B_{1g}, and B_{2g} elastoresistive responses. This is complemented by high-resolution in-plane thermal-expansion measurements utilizing a novel sample-mounting strategy for thin crystals in the capacitive dilatometer. Our results establish a thermodynamic link to the strain-dependent electronic behavior and highlight how Kondo hybridization couples to in-plane strain in this heavy-fermion system.

TT 53: Nonequilibrium Quantum Systems II (joint session TT/DY)

Time: Wednesday 15:00–17:30 Location: HSZ/0105

TT 53.1 Wed 15:00 HSZ/0105

Nonlocal Correlation Effects in the Relaxation Dynamics of the Photo-Excited Hubbard Model — •Gusein Bedirkhanov[1], Nagamalleswararao Dasari[2], Alexander I. Lichtenstein[2], and Evgeny A. Stepanov[1] — [1]CPHT, CNRS, École polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France — [2]Institut für Theoretische Physik, Universität Hamburg, 22607 Hamburg, Germany

Experiments on ultrafast irradiation of correlated materials have revealed a variety of exotic nonequilibrium phenomena. A theoretical investigation of these phenomena requires methods capable of accurately describing a complex interplay between the non-perturbative local correlations and nonlocal collective electronic fluctuations throughout their relaxation pathway. A recently developed real-time nonequilibrium *D-GW* method allows for such a description by incorporating nonlocal charge and spin fluctuations diagrammatically, going beyond the dynamical mean-field theory solution. In this work, we apply *D-GW* to track the relaxation dynamics of a photo-excited Hubbard model across different interaction strengths, including the particularly challenging region near the Mott transition. To simulate the transfer of electronic energy to other degrees of freedom, we introduce controlled cooling by coupling the electronic system to various relaxation baths and compare their efficiency and physical implications. We analyze the emergent steady and metastable states, and investigate how interaction strength and nonlocal correlations shape the relaxation pathway.

TT 53.2 Wed 15:15 HSZ/0105

Optimizing energy conversion with nonthermal resources in steady-state quantum devices — •Elsa Danielsson, Henning Kirchberg, and Janine Splettstoesser — Chalmers University of Technology, Sweden

In quantum transport, particle currents are investigated through quantum devices coupled to multiple contacts, which are defined by their electrochemical potentials and temperatures. However, when reaching the nanoscale, particles might no longer equilibrate with their thermal surroundings. Consequently, in the investigation of energy conversion processes, nonthermal distributions become highly relevant descriptors of the particles' environment. I will present how a nonthermal resource can be exploited to generate power or cool a contact and how to maximize the efficiency or precision for these processes. Utilizing coherent electron scattering, the optimization is made by adjusting the transmission probabilities of electrons at different energies. Importantly, we also address the issue of how to define an efficiency as the energy current cannot be neatly divided into heat and work, due to the presence of a nonthermal resource. Based on this, we show that for a fixed output current the optimal transmission function is a series of band-passes in the energy spectrum, depending on the shape of the nonthermal distribution. When applying this result on example systems with nonthermal resources we find that all performance quantifiers improve compared to thermal counterparts. These findings highlight the importance of designing nanoelectronic devices according to the electron distributions their contacts.

TT 53.3 Wed 15:30 HSZ/0105

Excited State Phases of Matter in the SymTFT Paradigm — •Ludwig Zweng[1,2], Apoorv Tiwari[3], and Sanjay Moudgalya[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences — [2]Munich Center for Quantum Science and Technology (MCQST) — [3]Southern Denmark University, Center for Quantum Mathematics at IMADA

Recent works have developed a unifying framework for classifying ground state phases of matter with a wide range of discrete symmetries—both group-like and non-invertible symmetries—via a holographic correspondence between symmetric operators in d dimensions and topological operators in a d+1 dimensional system often known as the SymTO or SymTFT. Its lattice formulation naturally yields fixed-point commuting Hamiltonians that realize these phases in their ground state. In this work, we extend this framework to non-equilibrium settings by analyzing excited states of these fixed-point models. Characterizing symmetry breaking patterns in the excited states requires new tools and diagnostic methods, which we develop to find that they can differ dramatically from their ground state counterparts, leading to a rich and sometimes surprising phenomenology. We illustrate these phenomena by constructing lattice models for

a variety of invertible and non-invertible symmetries, classifying the distinct excited state phases that arise in each case. Finally, we propose a concrete definition of excited state phases of matter and argue that the SymTFTs that capture ground state phases do not fully capture the intricacies of the excited states.

TT 53.4 Wed 15:45 HSZ/0105

Improving the stability of the hierarchical equations of motion approach for generic bosonic spectral densities — •Salvatore Gatto, Samuel Rudge, and Michael Thoss — University of Freiburg

The hierarchical equations of motion (HEOM) constitute a numerically exact method for investigating the dynamics of open quantum systems across a wide range of environmental conditions [1]. In this contribution, we investigate the stability of HEOM for generic bosonic spectral densities and identify temperature- and coupling-dependent instabilities in the time evolution. We show that, upon increasing the system-bath coupling strength, the conventional HEOM formulation may become unstable, and that simply extending the hierarchy depth does not cure these long-time divergences [2]. Starting from the HEOM structure, we derive a multidimensional phase-space differential equation that generalizes the Quantum Fokker-Planck equation to arbitrary temperature [3]. We further demonstrate that expanding this new equation in an alternative basis removes the numerical instabilities inherent to the standard HEOM representation.

[1] J. Bätge, Y. Ke, C. Kaspar, M. Thoss, PRB 103, 235413 (2021)
[2] I. S. Dunn, R. Tempelaar, D. R. Reichman, J. Chem. Phys. 150, 184109 (2019)
[3] T. Li, Y. Yan, and Q. Shi, J. Chem. Phys. 156, 064107 (2022)

TT 53.5 Wed 16:00 HSZ/0105

Non-Local Correlation effects in DC and optical conductivity of the Hubbard model — Nagamalleswararao Dasari[1], Hugo Strand[2], Martin Eckstein[1], Alexander Lichtenstein[1], and •Evgeny Stepanov[3] — [1]Universität Hamburg, Germany — [2]Örebro University, Sweden — [3]CPHT, CNRS, École polytechnique, France

Many-body effects in correlated materials can be explored through various response functions, with transport measurements being among the simplest and most direct probes. Accurately addressing the unconventional transport properties of materials requires accounting for spatial electronic correlations. These correlations can significantly influence transport characteristics by modifying the electronic spectral function and giving rise to complex multi-electron scattering processes, known as vertex corrections, which can both strongly impact the conductivity. In this talk, I will discuss the impact of non-local correlations on the conductivity of the single-band Hubbard model within the recently developed D-GW method [arXiv:2507.16673]. I will demonstrate that the impact of non-local correlations on the conductivity differs between the correlated metallic and Mott insulating phases. Incorporating nonlocal correlations in both the electronic spectral function and vertex corrections is crucial for accurately describing the optical conductivity at finite frequencies in both these regimes. The crossover between the metallic and Mott insulating phases can be identified by a vanishing contribution of vertex corrections to the DC conductivity.

15 min. break

TT 53.6 Wed 16:30 HSZ/0105

Conditioning Subsystem Magnetization into the Large-Deviation Regime in Quantum Spin Chains — •Kriti Baweja[1], Samuel Garratt[2], David Luitz[1], Ali Zahra[3,4], and Jérôme Dubail[3,5] — [1]Institute of Physics, University of Bonn, Germany — [2]Department of Physics, Princeton University, USA — [3]Laboratoire de Physique et Chimie Théoriques, University of Lorraine, France — [4]Centro de Análise Matemática, Departamento de Matemática, Universidade de Lisboa, Portugal — [5]Centre Européen de Sciences Quantiques and ISIS, University of Strasbourg, France

We investigate the ground-state and finite-temperature properties of free-fermion and XXZ spin systems when a contiguous spatial region of the chain is conditioned to have a fixed value of its total S^z. We analyze how this conditioning operation reshapes the local magnetization profile and longitudinal spin-spin correlations both within the constrained region and in its surrounding environment. To access regimes beyond analytically tractable limits, we extend an existing post-measurement Quantum Monte Carlo (QMC) framework by introducing new update rules that enable efficient sampling of states with arbitrary subsystem magnetization. Using this post-measurement QMC approach, we probe the finite-temperature properties of these conditioned states and characterize how magnetization constraints modify local structure in both interacting and non-interacting spin models. Our results provide a computational tool for exploring measurement-induced constraints and conditioned ensembles in quantum many-body systems.

TT 53.7 Wed 16:45 HSZ/0105

Consistent quantum treatments of nonconvex kinetic energies — Christina Koliofoti, Mohammad Atif Javed, and •Roman-Pascal Riwar — Peter Grünberg Institut (PGI-2), Forschungszentrum Jülich, 52428 Jülich, Germany

The task of finding a consistent relationship between a quantum Hamiltonian and a classical Lagrangian is of utmost importance for basic, but ubiquitous techniques like canonical quantization and path integrals. Nonconvex kinetic energies (which appear, e.g., in nonlinear capacitors or classical time crystals) pose a fundamental problem: the Legendre transformation is ill-defined, and the more general Legendre-Fenchel transformation removes nonconvexity essentially by definition. Arguing that such anomalous theories follow from suitable low-energy approximations of well-defined, harmonic theories, we show that seemingly inconsistent Hamiltonian and Lagrangian descriptions can both be valid, depending on the coupling strength to a dissipative environment. There occurs a dissipative phase transition from a nonconvex Hamiltonian to a convex Lagrangian regime, involving exceptional points in imaginary time. Our approach thus resolves apparent inconsistencies and provides computationally effcient methods to treat anomalous, nonconvex kinetic energies.

TT 53.8 Wed 17:00 HSZ/0105

Lanczos-Pascal approach to correlation functions in chaotic quantum systems — •Merlin Füllgraf, Jiaozi Wang, Robin Steinigeweg, and Jochen Gemmer — University of Osnabrück, Departement of Mathematics/Computer Science/Physics, D-49076 Osnabrück, Germany

We suggest a method to compute approximations to temporal correlation functions of few-body observables in chaotic many-body systems in the thermodynamic limit based on the respective Lanczos coefficients. Given the knowledge of these Lanczos coefficients, the method is very cheap. Usually accuracy increases with more Lanczos coefficients taken into account, however, we numerically find and analytically argue that the convergence is rather quick, if the Lanczos coefficients exhibit a smoothly increasing structure. For pertinent examples we compare with data from dynamical typicality computations for large but finite systems and find good agreement if few Lanczos coefficients are taken into account. From the method it is evident that in these cases the correlation functions are well described by a low number of damped oscillations.

[1] Accepted in Phys. Rev. Lett.

TT 53.9 Wed 17:15 HSZ/0105

Many-body neural network wavefunction for a non-Hermitian Ising chain — •Lavoisier Wah — Max Planck Institute for the Science of Light, 91058 Erlangen, Germany

Non-Hermitian (NH) quantum systems have emerged as a powerful framework for describing open quantum systems, non-equilibrium dynamics, and engineered quantum optical materials. However, solving the ground-state properties of NH systems is challenging due to the exponential scaling of the Hilbert space, and exotic phenomena such as the emergence of exceptional points. Another challenge arises from the limitations of traditional methods like exact diagonalization (ED). For the past decade, neural networks (NN) have shown promise in approximating many-body wavefunctions, yet their application to NH systems remains largely unexplored. In this paper, we explore different NN architectures to investigate the ground-state properties of a parity-time-symmetric, one-dimensional NH, transverse field Ising model with a complex spectrum by employing a recurrent neural network (RNN), a restricted Boltzmann machine (RBM), and a multilayer perceptron (MLP). We construct the NN-based many-body wavefunctions and validate our approach by recovering the ground-state properties of the model for small system sizes, finding excellent agreement with ED. Then, for larger system sizes, we demonstrate that the RNN outperforms both the RBM and MLP. These results highlight the potential of neural network-based approaches - particularly for accurately capturing the low-energy physics of NH quantum systems both in case of weak and strong non-Hermiticity.

TT 54: Graphene: Electronic structure, excitations, etc. (joint session O/TT)

Time: Wednesday 15:00–17:45 Location: HSZ/0204

TT 54.1 Wed 15:00 HSZ/0204

Magneto-photoelectric effect in graphene via tailored potential landscapes — •Friedemann Queisser[1], Joris Josiek[1,2], Stephan Winnerl[1], and Ralf Schützhold[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

We consider the propagation of charge carriers in planar graphene under the combined influence of a constant transversal magnetic field and an in-plane

varying electric potential. By suitably designing the potential landscape, we may effectively steer charge carriers generated by photo-excitation, for example, in order to achieve an efficient charge separation. These finding may pave the way for transport schemes or photoelectric/photovoltaic applications. Funding by the DFG through the SFB 1242 is gratefully acknowledged.

TT 54.2 Wed 15:15 HSZ/0204

Topological obstruction in twisted bilayer graphene — Florie Mesple[1], Pierre Mallet[2], •Guy Trambly de Laissardière[3], Clement Dutreix[4], Gérard Lapertot[5], Jean-Yves Veuillen[2], and Vincent T. Renard[5] — [1]Dept. Physics, Univ. of Washington, Seattle, USA — [2]CNRS, Univ. Grenoble Alpes, Inst. Néel, Grenoble, France — [3]CY Cergy Paris Univ., CNRS, LPTM, Cergy-Pontoise, France — [4]Univ. Bordeaux, CNRS, LOMA, Talence, France — [5]Univ. Grenoble Alpes, CEA, IRIG, PHELIQS, Grenoble, France

The rich physics of magic angle twisted bilayer graphene (TBG) results from the Coulomb interactions of electrons in nearly flat bands of non-trivial topology [1]. Here [2], we perform STM/STS measurements on a moiré pattern generated in a TBG tilted by 4.3°, focusing on a point-like defect. We observe quasiparticle interferences (QPIs) resulting from intravalley backscattering between Dirac cones of graphene layers 1 and 2. Rationalized by tight binding calculations and T-matrix theory, our work shows that the QPIs are strongly impacted by the relative chirality of the Dirac cones of layer 1 and 2 in each valley. It establishes that, within a given moiré valley, the two Dirac cones have the same electronic chirality, as expected in the usual continuum model [3]. This peculiar topology leads to a topological obstruction.

[1] B. A. Bernevig, D. K. Efetov, Physics Today **77**, 38 (2024)
[2] F. Mesple, et al., arXiv:2506.08913 (2025)
[3] R. Bistritzer, A. H. MacDonald, PNAS **108**, 12233 (2011)

TT 54.3 Wed 15:30 HSZ/0204

Quasiparticle Interferences in 30°-twisted graphene quasicrystal — •Jean-Maxime Schlachter[1], Ahmed El Alouani[2], Vincent S Renard[2], Abhishek Karn[1], Ileana Florea[2], Stéphane Vézian[2], Adrien Michon[2], Clemens B Winkelmann[1], and Vincent T Renard[1] — [1]Univ. Grenoble Alpes, CEA, Grenoble INP, IRIG, PHELIQS, 38000 Grenoble, France — [2]CNRS-CRHEA, Université Côte d'Azur, rue B. Grégory, 06560 Valbonne, France

Quasicrystals are materials that have clean diffraction pattern but no translational symmetry. The advent of van der Waals stacking has opened the possibility to engineer quasicrystals. For example, the moiré pattern in 30°-twisted graphene bilayers has 12-fold rotational symmetry which is not compatible with translation symmetry in 2D, hence it is a quasicrystal (1). Studying this system gives insight into the behavior of Dirac fermions in 2D quasicrystals. ARPES experiments (2) demonstrated the existence of multiple Dirac cone replicas, originating from the incommensurate interlayer coupling. The goal of this study is to determine to what extend these Dirac cone replicas influence the electronic properties of the Dirac fermions. Our low temperature scanning tunneling microscope (STM) experiments evidence the replicated Dirac cones by specific patterns in the local density of states patterns associated with scattering between them, contrary to previous STM experiments (3).

(1) P. Moon et al., Phys. Rev. B, **99**, 16, :165430 (2019) ; (2) S. J. Ahn et al., Science, **361**, 6404, :782-786 (2018) ; (3) C. Yan et al., 2D Mater., **6**, 4, :045041 (2019)

TT 54.4 Wed 15:45 HSZ/0204

Machine Learning for Bandstructure-Structure Relationships in Doped Graphene — •Benedict Saunders[1], Lukas Hörmann[1,2], Valdas Vitartas[1], Chen Qian[1], and Reinhard J Maurer[1,2] — [1]University of Warwick, Coventry, United Kingdom — [2]University of Vienna, Vienna, Austria

The introduction of topological defects or dopants to graphene's honeycomb lattice is a common approach to tuning the electronic and transport properties of the material to suit a specific application. Nitrogen is a widely investigated dopant, which can be introduced into the lattice in various configurations, each with a distinct effect on the material's bandstructure. However, due to the combinatorial explosion of possible dopant configurations, conventional first-principles screening of the electronic bandstructure for all possible configurations is not feasible. Here, we address this limitation by employing the recently developed MACE-H machine learning model to predict the electronic Hamiltonian of nitrogen-doped graphene configurations directly for a series of previously generated defect configurations. This allows us to rapidly generate accurate bandstructures and densities-of-states for large numbers of configurations, enabling the identification of structure-property relationships as a function of temperature and composition.

TT 54.5 Wed 16:00 HSZ/0204

Electronic structure of intercalated epitaxial graphene: A first principles study — •Andres Unigarro[1], Florian Günther[2], and Sibylle Gemming[1] — [1]Institute of physics, TU Chemnitz, Chemnitz, Germany — [2]UNESP, Rio Claro, Brazil

Two-dimensional materials such as graphene are particularly intriguing due to their exceptional mechanical and electronic properties. A natural next step involves combining different 2D materials to form heterostructures with enhanced functionalities. In epitaxial graphene on silicon carbide (SiC), intercalation provides an effective means to tune the electronic, optical, and transport properties of graphene while preserving its honeycomb lattice. Moreover, intercalation enables the synthesis of otherwise unstable 2D layers. In particular, the intercalation of heavy elements such as Pb [1] and Bi [2] is especially promising, as these can introduce strong spin-orbit coupling (SOC) effects [3] (e.g. Rashba effect, gap opening) in graphene. In this work, we use first-principles calculations to investigate the electronic properties of heterostructures formed by Pb and Bi intercalation.

[1] Schölzel, Franziska, et al. ,Small Structures (2024), 2400338
[2] Tilgner, N., et al. Nat Commun 16, (2025), 6171.
[3] Unigarro A., et al. J. Phys. Chem. C (2025), 129, 11, 5617-5624

TT 54.6 Wed 16:15 HSZ/0204

Domain-resolved electronic structure of AgTe-intercalated graphene on SiC(0001): From semiconducting Te-rich interlayer bands to metallic AgTe alloy states — •Vibha Reddy[1], Sawani Datta[1], Bharti Matta[1], Philipp Rosenzweig[2], Ulrich Starke[1], and Kathrin Küster[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, — [2]Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart

Intercalation at the graphene/SiC(0001) interface provides a powerful route towards engineering the electronic properties of both the graphene and the intercalant. Here, we present the first realization of a transition-metal chalcogen alloy intercalated into the graphene/SiC(0001) interface via AgTe intercalation. The nominally AgTe-intercalated system segregates into multiple microscale intercalation phases, namely, Te-rich, Ag-rich and AgTe alloyed domains. Spatially-resolved and angle-resolved photemission spectroscopy (ARPES) reveals that each domain exhibits distinct graphene doping levels and interlayer band dispersions, highlighting the strong interplay between local intercalation chemistry investigated by X-ray photoelectron spectroscopy (XPS) and electronic band structure. Given the intrinsic spin-orbit coupling and topologically non-trivial states associated with Te- and Ag-based 2D materials, the AgTe alloy-intercalated graphene represents a promising platform for realizing domain-specific emergent quantum phenomena, underscoring the chemical versatility and tunability of alloy-based heterostructures in interface engineering.

TT 54.7 Wed 16:30 HSZ/0204

Proximity-induced electronic states in epitaxial graphene/SiC (0001) via Sn intercalation — •Huu Thoai Ngo[1], Zamin Mamiyev[1], Niklas Witt[2,3], Tim Wehling[2], and Christoph Tegenkamp[1] — [1]Solid Surface Analysis, Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [2]Institute of Theoretical Physics & Centre for Ultrafast Imaging, University of Hamburg, Hamburg, Germany — [3]Institute for Theoretical Physics and Astrophysics, University of Würzburg, Würzburg, Germany

Intercalation of heavy elements at the buffer layer/SiC interface is an effective route to decouple it from the substrate while tailoring its electronic properties, for example, energy gap opening [1] and Mott insulating states [2]. In this work, we investigate the Sn-intercalated buffer layer using low-temperature STM/STS, supplemented by SPA-LEED, and DFT calculations. By precisely controlling the intercalation process, we obtain two distinct Sn phases beneath graphene: Sn(1x1) that induces Kekulé-O distortion, and honeycomb-Sn structure that gives rise to Moiré patterns. Remarkably, our STS results reveal a gap opening in Kekulé-O graphene due to Sn-induced sublattice symmetry breaking. In contrast, the honeycomb-Sn phase exhibits Mott insulating states. These findings demonstrate how Sn intercalants modify the structural and electronic properties of graphene at both nano- and microscale. [1] Ghosal, Tegenkamp, C. et al. Phys. Rev. Lett. 129, 116802 (2022). [2] Ghosal, Tegenkamp, C. et al. Phys. Rev. B 111, 235426 (2025).

TT 54.8 Wed 16:45 HSZ/0204

Doping monolayer graphene to the Van Hove singularity — •Guangyao Miao[1], Daniel Jansen[1], Bilal Hawashin[2], Julian Kleeschulte[2], Katharina Offermann[1], Christian Krämer[1], Affan Safeer[1], Abdallah Karaka[1], Jeison Fischer[1], Thomas Michely[1], Michael M. Scherer[2], and Wouter Jolie[1] — [1]II. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Cologne, Germany — [2]Theoretische Physik III, Ruhr-Universität Bochum, D-44801 Bochum, Germany

Tuning correlated states in graphene is an intriguing topic, particularly since the experimental realization of superconductivity, correlated insulator states, and magnetic states in twisted-angle bilayer graphene near the magic angle, along with Van Hove singularities (VHSs) tuned to the Fermi level. Such correlated phenomena have also been predicted in monolayer graphene doped to its van Hove singularity. Motivated by this, we study the effect of Cs doping on a graphene monolayer on Ir(111) using MBE. A $\sqrt{3}\times\sqrt{3}$ superstructure is observed due to the Cs intercalations between graphene and Ir(111). Further deposition of Cs on top of graphene leads to the formation of several surface structures with varying Cs concentrations, including adatoms, stripes, and com-

pact islands. Their morphology and electronic structures are revealed by scanning tunneling microscopy and spectroscopy at low temperature. By optimizing the dosage, we successfully tune the VHS to the vicinity of the Fermi level and observe a $2\sqrt{3}\times2\sqrt{3}$ superstructure with respect to the graphene lattice. Possible origins of the superstructure related to many-body interactions will be discussed.

TT 54.9 Wed 17:00 HSZ/0204

Optimizing quantum transport in multi-barrier graphene systems using differential evolution — •Leon Browne and Stephen R. Power — School of Physical Sciences, Dublin City University, Ireland

Potential and mass barriers in graphene introduce electron scattering, modulating transmission probabilities. Complex multi-barrier setups allow electron transmission to be controlled with high precision, but have a huge design space of possible barrier geometries. This work presents a framework to optimize electronic transport in such systems using differential evolution algorithms. First, transfer matrix methods are employed to efficiently compute quantum transport through multi-barrier structures, before optimization is applied to find barrier configurations whose transmission profiles closely match a predefined target profile. To address the trade-off between the accuracy and complexity of resulting barrier configurations, regularization techniques are incorporated into the optimization process. Our approach demonstrates the potential for highly tunable electronic transport in graphene-based systems by exploiting evolution-inspired optimization techniques.

TT 54.10 Wed 17:15 HSZ/0204

Comparative study of plasmons in half-filled graphene via Quantum Monte Carlo and kinetic theory — Maksim Ulybyshev[1], •Adrien Reingruber[1], and Kitinan Pongsangangan[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg — [2]Department of Physics, Faculty of Science, Mahidol University, Bangkok

A quantitative description of hydrodynamic electronic transport in strongly correlated materials requires accurate knowledge of collective excitations such as plasmons, which can notably influence viscosity. In free-standing graphene, where long-range interactions are important, standard Dirac-cone perturbation theory misses important finite Brillouin-zone and strong-coupling effects. We investigate plasmons in half-filled free-standing graphene using unbiased Quantum Monte Carlo simulations. Our results reveal well-defined plasmon peaks near the Gamma-point, map their dispersion, and extract the momentum dependence of their quasiparticle residue. Comparing to perturbative predictions, we find substantial deviations arising from the interaction and lattice effects captured only beyond the Dirac approximation. These results underscore the need to incorporate such corrections in analytical theories of electronic transport in graphene.

TT 54.11 Wed 17:30 HSZ/0204

NanoARPES Facility in Shanghai Synchrotron Radiation Facility and Investigation of the Moiré bands in Graphene Devices — •Zhongkai Liu — Shanghaitech University

Spatially resolved angle-resolved photoemission spectroscopy (NanoARPES) is an indispensable tool for probing the electronic structure of exfoliated sample flakes, fabricated devices, and more. In this presentation, we describe the construction, specifications, capabilities, and operation of BL07U-the NanoARPES endstation at the Shanghai Synchrotron Radiation Facility (SSRF) [1]. We will showcase our research on the electronic structure of emerging graphene devices, with a focus on moiré and flat bands. For example, our ARPES studies on magic-angle twisted trilayer graphene clearly reveal the coexistence of moiré flat bands and Dirac bands [2]. In aligned bilayer graphene/hBN heterostructures, we demonstrate that in-situ back gating enables precise tuning of the moiré electronic structure [3]. We directly observe the characteristic topological electronic structures of rhombohedral multilayer graphene, from a 3D generalization of the 1D Su-Schrieffer-Heeger (SSH) chain in thin layers to a topological Dirac nodal spiral semimetal in bulk rhombohedral graphite [4]. Finally, we present our work on the moiré band in bulk alternating twist graphene, which becomes flat at "magic momenta".

Reference: [1] H. Gao et al., Synchrotron Radiation News 37, 12-17 (2024) [2] Y. W. Li et al., Advanced Materials 202205996 (2022) [3] H. B. Xiao et al., Advanced Science 202412609 (2025) [4] H. B. Xiao et al., Science Bulletin 70, 1030-1033 (2025)

TT 55: Topology and symmetry protected materials & Topological insulators (joint session O/HL/TT)

Time: Wednesday 15:00–17:45 Location: HSZ/0401

TT 55.1 Wed 15:00 HSZ/0401

Majorana or Not? An Insight from Atomic-Scale Shot-Noise — •Abhishek Maiti[1], Genda Gu[2], and Freek Massee[1] — [1]Université Paris-Saclay, CNRS, Laboratoire de Physique des Solides, 91405, Orsay, France — [2]Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, NY, USA

The search for non-abelian states of matter has become a central theme of modern quantum material research. Notably, Majorana zero modes are of special interest, as they can serve as the foundation for topological qubits. A robust zero-bias conductance peak, observed in scanning tunneling spectra, is often regarded as the primary signature of a Majorana zero mode. Yet similar features can also arise from trivial bound states, raising a long-standing challenge of how to distinguish a genuine Majorana from imposters. In my talk, I will address this problem with a new approach, atomic-scale shot-noise spectroscopy, that goes beyond conductance measurements. Through a detailed investigation on multiple defect- and vortex-bound zero-bias states in the widely studied (putative) topological superconductor Fe(Se,Te), I will show that while differential conductance measurements might sometimes fail to detect an imposter Majorana state locally, noise measurements consistently provide a conclusive diagnostic, offering a powerful complementary probe. Looking ahead, this technique can be applied to other reported platforms to verify whether their Majorana-like signature in tunneling conductance can pass the shot-noise test.

TT 55.2 Wed 15:15 HSZ/0401

Intrinsic topological superconductivity revealed by surface-extended Andreev bound states in $PtBi_2$ — •Xiaochun Huang[1], Lingxiao Zhao[2], Sebastian Schimmel[3,4], Julia Besproswanny[3,4], Patrick Härtl[1], Christian Hess[3,4], Bernd Büchner[4,5], and Matthias Bode[1] — [1]Experimentelle Physik 2, Physikalisches Institut, Universität Würzburg, Germany — [2]Quantum Science Center of Guangdong, Shenzhen, China — [3]Fakultät für Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, Germany — [4]Leibniz-Institute for Solid State and Materials Research, Dresden, Germany — [5]Technische Universität Dresden, Germany

Intrinsic topological superconductivity remains a central question in condensed-matter physics. The three-dimensional Weyl semimetal $PtBi_2$ was recently shown by angle-resolved photoemission spectroscopy to host a superconducting gap that opens exclusively on its Fermi-arc surface states with a nodal structure, establishing it as a prime candidate for intrinsic topological superconductivity [1]. Using scanning tunneling microscopy and spectroscopy, we directly visualize surface-extended Andreev bound states (ABSs) across atomically pristine terraces within a sizable superconducting gap ($\Delta > 10$ meV) in $PtBi_2$. Quantitative analysis of the tunneling spectra within an anisotropic chiral pairing framework identifies these ABSs as signatures of an emergent Majorana-cone dispersion. Our findings provide a definitive real-space spectroscopic fingerprint of intrinsic topological superconductivity in $PtBi_2$.

[1] A. Kuibarov *et al.*, Nature **626**, 294 (2024)

TT 55.3 Wed 15:30 HSZ/0401

Probing chiral symmetry with a topological domain wall sensor — •Artem Odobesko[1], Glenn Wagner[2], Titus Neupert[2], Ronny Thomale[1], and Matthias Bode[1] — [1]Physikalisches Institut, Universität Würzburg, Würzburg, Germany — [2]Department of Physics, University of Zurich, Zürich, Switzerland

Chiral symmetry is a fundamental property with profound implications for the properties of elementary particles, that implies a spectral symmetry (i.e. E -> -E) in their dispersion relation. In condensed matter physics, chiral symmetry is frequently associated with superconductors or materials hosting Dirac fermions such as graphene or topological insulators. There, chiral symmetry is an emergent low-energy property, accompanied by an emergent spectral symmetry. While the chiral symmetry can be broken by crystal distortion or external perturbations, the spectral symmetry frequently survives. As the presence of spectral symmetry does not necessarily imply chiral symmetry, the question arises how these two properties can be experimentally differentiated. Here, we demonstrate how a system with preserved spectral symmetry can reveal underlying broken chiral symmetry using topological defects. Our study shows that these defects induce a spectral imbalance in the Landau level spectrum, providing direct evidence of symmetry alteration at topological domain walls. Using high-resolution STM/STS we demonstrate the intricate interplay between chiral and translational symmetry which is broken at step edges in topological crystalline insulator $Pb_{1-x}Sn_xSe$.

[1] G. Wagner et al., Newton **1**, 100009 (2025)

TT 55.4 Wed 15:45 HSZ/0401

Quantifying quasiparticle chirality in a chiral topological semimetal — •Jiaju Wang[1], Amit Kumar[1], Markel Pardo-Almanza[1], Jaime Sanchez-Barriga[2], Jorge Cardenas-Gamboa[3], Maia Vergniory[3], Vladimir Strokov[4], Moritz Hoesch[5], Chandra Shekhar[6], Claudia Felser[6], Stuart Parkin[1], and Niels Schröter[1] — [1]Max Planck Institute of Microstructure Physics, Halle (Saale), Germany — [2]Helmholtz-Zentrum Berlin, Berlin, Germany — [3]Donostia International Physics Center, San Sebastián, Spain — [4]Paul Scherrer Institute, Villigen, Switzerland — [5]Deutsches Elektronen-Synchrotron, Hamburg, Germany — [6]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Recently, electron chirality has been proposed as an order parameter to quantify chirality. In chiral topological semimetals with the B20 structure, electron chirality is linked to parallel spin-momentum locking (SML) and spin deviations from SML, which affects numerous physical properties. However, experimental quantification of spin deviation still remains a big challenge. To achieve this, we have used spin and angle-resolved photoemission spectroscopy to directly probe the spin texture of Weyl cones in RhSi, a chiral topological semimetal with strong spin-orbit coupling (SOC). The spin-resolved spectra at different azimuthal angles are intricately fitted to extract numerical values of spin deviation for Weyl cones, allowing us to calculate the normalized electron chirality density (NECD). It was found that deviations can decrease the NECD from 1 down to 0.8. This observation may help interpret physical phenomena in chiral topological semimetals.

TT 55.5 Wed 16:00 HSZ/0401

Topology and Real-Space Obstruction: The Phase Diagram of the Triangular p-Orbital Lattice — •Jonas Erhardt[1,2], Sven Schemmelmann[3], Fabian Schöttke[3], Jörg Schäfer[1,2], Giorgio Sangiovanni[2,4], Markus Donath[3], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Universität Würzburg — [2]Würzburg-Dresden Cluster of Excellence ctd.qmat — [3]Physikalisches Institut, Universität Münster — [4]Institut für Theoretische Physik und Astrophysik, Universität Würzburg

Triangular p-orbital monolayers (MLs) host a rich topological phase diagram governed by the competition between spin-orbit coupling (SOC) and substrate-induced inversion-symmetry breaking (ISB). The SOC-dominated quantum spin Hall insulator (QSHI) phase arises from a band inversion in the $p_\pm$ manifold and was first realized in indenene, a triangular ML of In atoms on SiC [1]. Real-space interference shifts the associated Wannier centers away from the atoms to interstitial sites A/B, which for the QSHI phase produces an alternating ABAB energy sequence in the charge localization, as demonstrated by scanning tunneling microscopy (STM) [1]. Using the same STM approach, we identify the complementary ISB-dominated regime in a Tl ML on Si(111), where strong adsorption-induced ISB exceeds Tl's SOC. The charge likewise shifts off the atoms but evidences a non-alternating AABB sequence, characterizing Tl/Si(111) as a trivial obstructed atomic insulator. These results complete the experimental validation of the topological phase diagram for triangular p-orbital MLs.

[1] Nat. Commun. **12**, 5396 (2021).

TT 55.6 Wed 16:15 HSZ/0401

Majorana-metal transition in a disordered superconductor: percolation in a landscape of topological domain walls — Vladimir A Zakharov[1], Ion Cosma Fulga[2,3], •Gal Lemut[4], Jakub Tworzydło[5], and Carlo W. J. Beenakker[1] — [1]Instituut-Lorentz, Universiteit Leiden, PO Box 9506, 2300 RA Leiden, The Netherlands — [2]Institute for Theoretical Solid State Physics, IFW Dresden, Germany — [3]Würzburg-Dresden Cluster of Excellence ct.qmat, Dresden, Germany — [4]Dahlem Center for Complex Quantum Systems and Physics Department, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [5]Faculty of Physics, University of Warsaw, ul. Pasteura 5, 02-093 Warszawa, Poland

Most superconductors are thermal insulators. A disordered chiral p-wave superconductor, however, can make a transition to a thermal metal phase. Because heat is then transported by Majorana fermions, this phase is referred to as a Majorana metal. Here we present numerical evidence that the mechanism for the phase transition with increasing electrostatic disorder is the percolation of boundaries separating domains of different Chern number. We construct the network of domain walls using the spectral localizer as a "topological landscape function", and obtain the thermal metal-insulator phase diagram from the percolation transition.

TT 55.7 Wed 16:30 HSZ/0401

fabrication and characterization of the Moiré surface state on a topological insulator — •yi zhang — Shanghai Jiao Tong University, Shanghai, China

A Moire* superlattice on the topological insulator surface is predicted to exhibit many novel properties but has not been experimentally realized. Here, we developed a two-step growth method to successfully fabricate a topological insulator Sb2Te3 thin film with a Moire* superlattice, which is generated by a twist of the topmost layer via molecular beam epitaxy. The established Moire* topological surface state is characterized by scanning tunneling microscopy and spectroscopy. By application of a magnetic field, new features in Landau levels arise on the Moire* region compared to the pristine surface of Sb2Te3, which makes the system a promising platform for pursuing next-generation electronics. Notably, the growth method, which circumvents contamination and the induced interface defects in the manual fabrication method, can be widely applied to other van der Waals materials for fabricating Moire* superlattices.

TT 55.8 Wed 16:45 HSZ/0401

Backscattering in topological edge states despite time-reversal symmetry — Jonas Erhardt[1,2], •Mattia Iannetti[3,4], Fernando Dominguez[2,5], Ewelina M. Hankiewicz[2,5], Björn Trauzettel[2,5], Gianni Profeta[3,4], Domenico Di Sante[6], Giorgio Sangiovanni[2,5], Simon Moser[1,2], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Universität Würzburg — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg — [3]Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell'Aquila — [4]CNR-SPIN C/o Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell'Aquila — [5]Institut für Theoretische Physik und Astrophysik, Universität Würzburg — [6]Department of Physics and Astronomy, University of Bologna

Quantum Spin Hall Insulators (QSHI) are promising materials for many applications based on Dirac fermions and topologically-protected edge states. Indium adatoms on a silicon carbide surface, the so-called Indenene, was the first material in which a topological classification solely based on an inspection of the bulk wave functions has been demonstrated. In this work, we present a combined experimental and theoretical study of finite-sized Indenene systems, using STM/STS measurements and a quantitative tight-binding model revealing the rich physics of edge states. We find that a strongly non-linear edge dispersion leads to inter-Kramers pair backscattering, thereby extending the conventional understanding of backscattering protection in topological edge states.

TT 55.9 Wed 17:00 HSZ/0401

Quantized Subband Tunneling from Topological Insulator Nanowire Scanning Probe Tips — •Abhisek Kole[1,2], Felix Münning[3,4], Xiaosheng Yang[1,5], Jia G. Lu[6], Oliver Breunig[4], F. Stefan Tautz[1,2], Yoichi Ando[4], and Felix Lüpke[1,4] — [1]Peter Grünberg Institute (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institute for Experimental Physics IV A, RWTH Aachen University, Otto-Blumenthal-Straße, 52074 Aachen, Germany — [3]Institute of Physics I, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [4]Institute of Physics II, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [5]School of Optical and Electronic Information, Huazhong University of Science and Technology, Wuhan 430074, China — [6]Department of Physics/Electrophysics, University of Southern California, Los Angeles, CA 90089, USA

In topological insulator nanowires, the interplay between size quantization and the surface states wrapping the nanowire circumference gives rise to a magnetic-flux-tunable band structure. We demonstrate the controlled fabrication of (Bi_(1-x) Sb_x)_2 Te_3 (BST) topological insulator nanowires into scanning tunneling microscopy tips. Tunneling spectroscopy reveals a series of distinct peak-like features that exhibit a characteristic 1D DOS, indicating tunneling into the quantized 1D subbands of the BST nanowire tips. Furthermore, a magnetic-field-induced gap-closing and reopening transition is observed, consistent with the Dirac-like gap-closing transition expected for such wires. Moreover, we find indications of spin-selective helical tunneling between the nanowire tip and the Rashba surface states of Au(111).

TT 55.10 Wed 17:15 HSZ/0401

Simultaneous Characterization of Dispersion and Orbital Character of the Topological Surface State on the Topological Insulator Bi_2Te_3 — •Christoph Stephen Setescak, Adrian Weindl, and Franz Josef Giessibl — Universität Regensburg, D-93053 Regensburg

Scanning probe microscopy (STM and AFM) allows one to locally probe properties of topological insulators (TIs). On the compound Bi_2Te_3, atomic-scale electronic standing waves can be observed at crystalline step edges, which are associated with the hexagonal warping of the Dirac cone. These real-space oscillations provide a direct means to study the dispersion relation of the topological boundary mode. The interpretation relies on comparing the experimental data to calculations including not only the properties of the TI but also of the tip. In this framework, the tunneling current and differential conductance is modelled using Chen's derivative rule. Bending of the CO molecule at the tip apex due to lateral tip-sample forces is also included in the model. The relevant Bloch functions of the sample are obtained from Wannier-interpolated tight-binding Hamiltonians using maximally localized Wannier functions derived from first-principles DFT + GW computations. In combination with the high spatial resolution obtained with CO-terminated tips, not only the dispersion, but also the orbital character of the band structure can be probed.

TT 55.11 Wed 17:30 HSZ/0401

Defect-induced displacement of topological surface state in magnetic topological insulator $MnBi_2Te_4$ — •Felix Lüpke[1,2], Marek Kolmer[3,4], Hengxin Tan[5], Adam Kaminski[3,4], and Binghai Yan[5,6] — [1]Peter Grünberg Institute (PGI-3) and JARA-FIT, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany — [3]Ames National Laboratory, Ames, Iowa 50011, USA — [4]Iowa State University, Ames, Iowa 50011, USA — [5]Weizmann Institute of Science, Rehovot 7610001, Israel — [6]The Pennsylvania State University, University Park, Pennsylvania 16802, USA

The gapped topological surface states of $MnBi_2Te_4$ (MBT) are an attractive platform for the realization of quantum anomalous Hall and Axion insulator states. However, experimentally observed surface state gaps fail to meet theoretical predictions, with the exact mechanism behind the gap suppression still being debated. We report on the effect of intrinsic anti-site defects on the MBT surface states, which we study using scanning tunneling microscopy (STM), angle-resolved photoemission (ARPES), and density functional theory (DFT). Our results show that high defect concentrations lead to a displacement of the surface states into the interior of the MBT crystal, consistent with theoretical predicitons [PRL 130, 126702 (2023)].

TT 56: Superconductivity: Theory I

Time: Wednesday 15:00–18:30 Location: CHE/0089

TT 56.1 Wed 15:00 CHE/0089

Non-thermal pairing glue of electrons in the steady state — •Michele Pini[1,2], Christian H. Johansen[3,2], and Francesco Piazza[1,2] — [1]University of Augsburg, Augsburg, Germany — [2]MPI-PKS, Dresden, Germany — [3]Pitaevskii BEC Center, CNR-INO and Department of Physics, Trento, Italy

The study of mechanisms for enhancing superconductivity has been a central topic in condensed matter physics due to the combination of fundamental and technological interests. One promising route is to exploit non-equilibrium effects in the steady state. Efforts in this direction have so far focused on enhancing the pairing mechanism known from thermal equilibrium through modified distributions for the electrons or the bosons mediating the electron-electron interaction. In this work, we identify an additional pairing mechanism that is active only outside thermal equilibrium. By generalizing Eliashberg theory to non-equilibrium steady states using the Keldysh formalism, we derive a set of Eliashberg equations that capture the effect of this genuinely non-thermal pairing glue even in the weak-coupling regime. We discuss two examples where this mechanism has a major impact. First, in a temperature-bias setup, we find that superconductivity is enhanced when the boson mediator is colder than the electrons. Second, we find that an incoherent drive of the boson mediator at energies much greater than the temperature pushes the system far from thermal equilibrium but leaves the critical coupling essentially unchanged, owing to a competition between electron heating and the enhancement of pairing by the non-thermal glue.

TT 56.2 Wed 15:15 CHE/0089

Critical behavior of the Superconducting Phase Transition in a Lattice Gauge Theory Approach — •Greta S. Reese[1,2] and Ludwig Mathey[1,2] — [1]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany — [2]Center for Optical Quantum Technologies, University of Hamburg, 22761 Hamburg, Germany

We present a U(1) lattice gauge model to describe the superconducting phase transition of a type-II superconductor. Using the Landau Ginzburg free energy, we perform Monte Carlo simulations to investigate how the presence of a gauge field influences the nature of the phase transition. In particular, we study the effects of the gauge field on the Cooper pair density and the heat capacity.

TT 56.3 Wed 15:30 CHE/0089

Enhancing superconductivity using thermal bosons — •Ekaterina Vlasiuk[1], Eugene Demler[2], and Richard Schmidt[1] — [1]Institute for Theoretical Physics, Heidelberg University, Philosophenweg 16, 69120 Heidelberg, Germany — [2]Institute for Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland

We investigate how the strong coupling of a superconductor to thermal bosons can enhance its superconducting critical temperature. To tackle this problem, we use a functional Renormalization Group (FRG) approach that allows us to describe the competition between the build-up of boson-induced attraction between fermions and diametral density fluctuations in the scattering channel between bosons and fermions. Thus self-consistently treating the mutual influence of bosonic and fermionic sectors allows us to uncover an increase of the critical temperature which is pronounced in the BCS limit but self-regulated as unitary fermion interactions are approached. Also, we find that the mutual influence leads to a nontrivial dependence of the critical temperature on the mass ratio between particles. We identify the regimes where our theory is applicable by investigating the phase diagram of enhanced/induced superconductivity for bosons being in either a condensed or thermal state. Moreover, we outline possible experimental realizations in cold atomic systems as well as discuss the implementation in an alternative solid-state platform - bilayer TMD materials - where excitons play the role of bosons.

TT 56.4 Wed 15:45 CHE/0089

Generalized condition for odd-frequency pairing in multiband materials — •Florian Kayatz[1,2], Annica M. Black-Schaffer[1], and Jorge Cayao[1] — [1]Department of Physics and Astronomy, Uppsala University, Box 516, SE-752 37 Uppsala, Sweden — [2]WISE - allenberg Initiative Materials Science for Sustainability, Department of Physics and Astronomy, Uppsala University, Sweden

Odd-frequency superconductivity has been predicted to arise in various physical systems, including multiband materials, and is known to lead to phenomena such as the unusual Meissner response and long-range proximity effect [1]. The emergence of odd-frequency superconductivity is often explained in terms of a condition derived up to first order in the superconducting order parameter [2], leaving higher order corrections unaccounted. Here, we extend this analysis and derive the odd-frequency condition involving higher-order contributions of the order parameter, as well as a generalized expression valid to all orders. In addition, we explore the conditions for the emergence of odd-frequency correlations between individual bands. This allows us to identify cases where the structure of the Hamiltonian inherently forbids odd-frequency pairing. As an example, we apply our condition to a weakly coupled system consisting of a transition metal dichalcogenide monolayer proximitzed by a conventional spin-singlet s-wave superconductor.

[1] J. Linder and A. V. Balatsky, *Rev. Mod. Phys.* **91**, 045005 (2019)
[2] C.Triola,J.Cayao,A.M.Black-Schaffer*Ann.Phys.***532**,1900298(2020)

TT 56.5 Wed 16:00 CHE/0089

Enhanced Superconductivity in Proximity to Peaks in Densities of States — •Joshua Althüser[1], Ilya Eremin[2], and Götz S. Uhrig[1] — [1]TU Dortmund, Otto-Hahn-Straße 4, 44227 Dortmund, Germany — [2]Institut für Theoretische Physik III, Ruhr-Universität Bochum, 44801 Bochum, Germany

For the BCS theory of superconductivity, the electron-phonon interaction is transformed to an attractive electron-electron interaction in the vicinity of the Fermi energy only. An optimized transformation, however, reveals that the electrons attract one another whenever their energies do not differ more than the phonon energy ω_D. Consequently, the order parameter becomes finite even away from the Fermi energy. Intriguingly, an accumulation of density-of-states at an energy $\varepsilon_{\text{Peak}}$ in proximity to the Fermi energy induces a significant order parameter around $\varepsilon_{\text{Peak}}$, which easily exceeds the one at E_F for moderate coupling strengths. We predict measurable signatures in the thermodynamic and spectroscopic response of this unexpected phenomenon, guiding future experimental searches for it.

TT 56.6 Wed 16:15 CHE/0089

Fluctuation conductivity in multicomponent superconductors — •Sondre Duna Lundemo and Asle Sudbø — Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway

Multicomponent superconductors exhibit many properties that have no counterpart in single-component superconductors, ranging from Leggett modes to novel topological phase transitions. These features derive from the multiorbital character of the parent metallic state, and sometimes leave universal signatures in physical observables. In this talk, we scrutinize the electrodynamic response of such a metal as it approaches the superconducting critical point. In particular, we will elucidate whether the multicomponent character of the incipient superconducting order affects the electrical conductivity and highlight the importance of using a gauge-invariant approximation scheme for calculating it.

TT 56.7 Wed 16:30 CHE/0089

Constraints on the theoretical modeling of hole-doped La_2CuO_4 — •qiwei li[1], hanif hadipour[2], xue-jing zhang[1], and eva pavarini[1] — [1]Peter Grünberg Institute, Forschungszentrum Jülich, 52428 Jülich, Germany — [2]Department of Physics, University of Guilan, Rasht 41335-1914, Iran

The low-energy electronic properties of hole-doped La_2CuO_4 are believed to be well captured by the single-band Hubbard model describing x^2-y^2 electrons.

This finds support, e.g., on Fermi surface and angle resolved photoemission experiments. Here we show [1] that this imposes constraints on the microscopic description of the system. Results are obtained via the LDA+DMFT method using a continuous time hybridization expansion Quantum Monte Carlo impurity solver, as implemented in [2].

[1] Q. Li, H. Hadipour, X-J Zhang, E. Pavarini, in preparation
[2] A.Flesch, G.Zhang, E.Koch, E.Pavarini, PRB **85**, 035124 (2012)

15 min. break

TT 56.8 Wed 17:00 CHE/0089

Superlinear Hall angle, magnetotransport, and superconductivity in solvable models for strange metals — •Davide Valentinis[1,2], Aavishkar A. Patel[3,4], Subir Sachdev[5], and Joerg Schmalian[2,1] — [1]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, Karlsruhe (DE) — [2]Institute for Theoretical Condensed Matter physics, Karlsruhe (DE), Karlsruhe Institute of Technology — [3]Center for Computational Quantum Physics, Flatiron Institute, New York (USA) — [4]International Centre for Theoretical Sciences, Tata Institute of Fundamental Research, Bengaluru (IN) — [5]Harvard University, Cambridge, MA (USA)

We provide exact numerical solutions from the Kubo formula for the DC magnetoconductivity tensor of the two-dimensional (2D) spatially disordered Yukawa-Sachdev-Ye-Kitaev (2D-YSYK) model on a square lattice, at first order in applied perpendicular magnetic field. This system describes fermions endowed with a Fermi surface and coupled to a bosonic scalar field through spatially random Yukawa interactions, which admit mean-field exact numerical solutions. From the interplay between YSYK interactions and square-lattice embedding, and the non-Boltzmann frequency dependent self energies, we find a superlinear evolution of the Hall-angle cotangent and the inverse carrier mobility with temperature, concomitant with linear-in-temperature resistivity, in an extended crossover regime above the low-temperature Marginal Fermi Liquid (MFL) ground state. In addition, a superconducting state with finite phase stiffness, mediated by the same YSYK interactions, emerges out of the MFL.

TT 56.9 Wed 17:15 CHE/0089

Achieving analogue states of high-T_c superconductivity with current quantum simulators — •Thomas Köhler and Adrian Kantian — SUPA, Institute of Photonics and Quantum Sciences, Heriot-Watt University, EH14 4AS Edinburgh, Scotland, United Kingdom

Employing the recently introduced matrix-product states plus mean-field method (MPS+MF) [Bollmark et al. 2020; 2023; 2025, Marten et al. 2023], we show how to realize the analogue of a high-T_c superconducting state in a t-J bi-plane lattice model with strongly enhanced inter-plane spin-spin coupling. Implementation of such systems using ultra cold atomic lattice gases has been demonstrated using metastable tilted Fermi-Hubbard systems [Hirthe et al. 2023]. We show that t-J bi-planes constructed in this way can achieve a critical temperature T_c for the onset of a correlated state analogous to high-T_c superconductivity that would be accessible within currently reachable entropy-per-particle. We further identify the optimal parameter regimes for such states to be realized, rule out the existence of any competing charge density wave-instabilities, and show how to unambiguously detect the onset of superconducting order.

TT 56.10 Wed 17:30 CHE/0089

Understanding and enhancing superconductivity in cuprates with low-energy Hamiltonians and explicit machine learning — •Jean-Baptiste Morée[1] and Ryotaro Arita[1,2] — [1]RIKEN Center for Emergent Matter Science, Wako, Saitama 351-0198, Japan — [2]Department of Physics, University of Tokyo, Bunkyo-ku, Tokyo 113-0033, Japan

Cuprate superconductors exhibit a wide range of transition temperatures $T_c \approx$ 6–166 K despite sharing a common electronic structure dominated by a Cu $3d_{x^2-y^2}$–O $2p_\sigma$ antibonding orbital. Ab initio low-energy Hamiltonians combined with many-variable variational Monte Carlo have shown that T_c is primarily controlled by the nearest-neighbor hopping $|t_1|$ and the ratio $u = U/|t_1|$ (with U the onsite effective Coulomb repulsion), with only minor influence from longer-range terms. Applied pressure enhances T_c mainly by increasing $|t_1|$.

In this talk, I present recent progress [1] on the material dependence of these parameters using a new explicit, interpretable machine-learning approach. By analyzing structural and chemical descriptors across 36 cuprates, the algorithm reveals that $|t_1|$ increases when ionic radii in the block layer are reduced, while u can be tuned through the ionic charges. These results provide simple, physically transparent guidelines for designing cuprates with enhanced superconducting properties.

[1] J.-B. Morée and R. Arita, Phys. Rev. B **110**, 014502 (2024).

TT 56.11 Wed 17:45 CHE/0089

Strong-coupling superconductivity near Gross-Neveu quantum criticality in Dirac systems — •Veronika Stangier[1], Daniel Sheehy[2], and Jörg Schmalian[1] — [1]Karlsruhe Institute for Technology, Karlsruhe, Germany — [2]Louisiana State University, Baton Rouge, USA

We investigate superconductivity in two-dimensional massless Dirac fermions at charge neutrality, coupled to bosonic collective modes via a Yukawa interaction. Despite the absence of carriers at zero temperature, we uncover the surprising possibility that such systems can become superconducting near a Gross-Neveu quantum critical point. Remarkably, superconductivity emerges precisely when the fermionic excitations lose coherence - once their anomalous dimension in the normal state becomes sufficiently large. In other words, well-defined quasiparticles fail to superconduct, whereas strongly incoherent ones can. To capture this behavior, we develop a general framework for four-component Dirac systems and derive explicit algebraic criteria for the onset of pairing. Within this description, different bosonic modes - classified by their transformation under time-reversal and internal symmetries - select distinct superconducting channels. We then apply this approach to Dirac models of spin-orbit-coupled systems with orbitals of opposite parity and extend it to analyze superconductivity in moiré Dirac materials such as double-bilayer WSe_2 and twisted bilayer graphene.

TT 56.12 Wed 18:00 CHE/0089

Chiral superconductivity in time-reversal symmetry broken honeycomb systems — •Lucca Marchetti[1], Matthew Bunney[1,2], and Stephan Rachel[1] — [1]School of Physics, University of Melbourne, Melbourne, Australia — [2]Institute for Theoretical Solid State Physics, RWTH Aachen University, Aachen, Germany

Rhombohedral graphene — stacked graphene layers in the ABC configuration — has emerged as an exciting playground for strongly correlated physics and superconductivity. Recent experiments on N-layer rhombohedral graphene reveal signatures of spin-valley polarised Fermi surfaces. Probes at low temperature exhibit several regions of superconductivity, with signs of chiral triplet pairing states.

To better discern how broken symmetries in the normal state affect underlying many-body states we focus on 2D single-layer honeycomb systems in the presence of various symmetry breaking terms. We employ the truncated-unity functional renormalization group technique to analyse the leading instabilities of the associated Hubbard model. We discuss how the different broken symmetries affect the resulting superconductivity, and the implications this has for chiral and/or triplet pairing states. We further characterise the superconducting states in a topological context through calculation of Chern number landscapes, where we find regions of topological superconductivity.

TT 56.13 Wed 18:15 CHE/0089

A universal route to chiral Ising superconductivity in monolayer TaS_2 and $NbSe_2$ — •Lucia Gibelli[1], Simon Höcherl[1], Julian Siegl[1], Viliam Vano[2], Somesh C.Ganguli[2], Magdalena Marganska[3], and Milena Grifoni[1] — [1]University of Regensburg, Germany — [2]University of Aalto, Finland — [3]University of Science and Technology, Wroclaw

Ising superconductivity in two archetypal intrinsic superconductors, monolayer 1H-TaS_2 and 1H-$NbSe_2$, is investigated in a bottom-up approach [1]. Using ab initio-based tight-binding parameterizations for the relevant low-energy d-bands, the screened interaction is evaluated microscopically, in a scheme including Bloch overlaps. In direct space, the screened potential displays for both systems long-range Friedel oscillations alternating in sign. Upon scaling, the oscillation pattern becomes universal, with the location of minima and maxima locked to the lattice. Solving the momentum-resolved gap equations, a chiral ground state with p-like symmetry is generically found. Due to the larger Ising spin-orbit coupling, the chiral gap is more anisotropic in TaS_2 than in $NbSe_2$. This is reflected in tunneling spectra displaying V-shaped features for the former, in quantitative agreement with low-temperature scanning tunneling experiments on TaS_2. At the same time, our results reconcile the apparent discordance with hard gap tunneling spectra reported for the sibling $NbSe_2$ [2]. They also agree with recent top-down calculations on the same material.

[1] L. Gibelli et al., arXiv:2509.05784 (2025)
[2] J. Siegl et al., Nature Communications, 16(1):8228 (2025)

TT 57: Correlated Magnetism – Kagome Systems

Time: Wednesday 15:00–18:15 Location: CHE/0091

TT 57.1 Wed 15:00 CHE/0091

Probing Spin Dynamics and Hyperfine Coupling in the Frustrated Quantum Magnet Clinoatacamite: An NMR Study — •Roni Bose[1], Hans-Joachim Grafe[1], Bernd Büchner[1], Anja U. B. Wolter[1], Leonie Stödter[3], Caroline Kastner[2], and Stefan Süllow[2] — [1]IFW Dresden, Helmholtzstraße 20, 01069, Germany — [2]IPKM, TU Braunschweig, Braunschweig, Germany — [3]FZ Jülich, JCNS at MLZ, Garching, Germany

Recent work on Atacamite reveals a quantum critical point above 21.9 T with a dimensional reduction from 3 D AFM ordering to 1 D quantum spin liquid behavior. Clinoatacamite has same chemical formula as Atacamite, but displays distinct magnetic behaviour due to different crystal structure. Previous μSR studies on polycrystals reveal coexistence of long range magnetic ordering and fluctuations below 18 K, which transforms into a metastable state below 6.5 K, while neutron-diffraction observes magnetic reflections only below 6.5 K, but not below 18 K.

To address the discrepancy in reported ordering temperatures and to investigate the magnetic behaviour below 18 K, we performed ^{1}H-NMR measurements with magnetic field orientations $B \parallel [201]$ (perpendicular to the Kagome plane) and $B \parallel [010]$. For both field directions, the NMR spectra show splittings near 18 K and again near 6 K, indicating magnetic transitions. Furthermore, the temperature dependence of the spin-lattice relaxation rate at different proton sites reveals a coexistence of partial spin freezing and strong fluctuations below 18 K, followed by a fully ordered state below 6 K.

TT 57.2 Wed 15:15 CHE/0091

Competing ordering modes in the distorted quantum Kagome material clinoatacamite $Cu_2Cl(OH)_3$ — •Leonie Stödter[1,2], Carolin Kastner[1], Harald O. Jeschke[3], Manfred Reehuis[4], Ketty Beauvois[5], Bachir Ouladdiaf[5], Edmond Chan[5], Fabiano Yokaichiya[4], Fabrice Bert[6], Thomas J. Hicken[7], Jonas A. Krieger[7], Hubertus Luetkens[7], Jackson L. Allen[8], Ralf Feyerherm[4], Michael Tovar[4], Dirk Menzel[1], Anja U. B. Wolter[9], Kirrily C. Rule[10], F. Jochen Litterst[1], Ulrich K. Rössler[9], and Stefan Süllow[1] — [1]IPKM, TU Braunschweig, Braunschweig, Germany — [2]FZ Jülich, JCNS at MLZ, Garching, Germany — [3]RIIS, Okayama University, Okayama, Japan — [4]HZB, Berlin, Germany — [5]ILL, Grenoble, France — [6]SQM, Université Paris-Saclay, Orsay, France — [7]PSI, Villigen, Switzerland — [8]ISEM, University of Wollongong, Australia — [9]Leibniz IFW Dresden, Dresden, Germany — [10]ANSTO, Lucas Heights, Australia

Structurally, the mineral clinoatacamite $Cu_2Cl(OH)_3$ is closely related to the Kagome material herbertsmithite $ZnCu_3Cl_2(OH)_6$, however, its Kagome motif of Cu sites is embedded into a low-symmetry crystal structure. The magnetic ground states of clinoatacamite below an ordering temperature of 18.1 K have remained inconclusive to date. Here, we revisit the magnetic properties using single-crystalline material. We have characterized clinoatacamite by means of thermodynamic measurement techniques, μSR as well as neutron diffraction. We reveal a complex zero-field sequence of phases and discuss our data within a scenario of competing antiferromagnetic ordering modes.

TT 57.3 Wed 15:30 CHE/0091

High-field μSR on the frustrated quantum magnet clinoatacamite $Cu_2Cl(OH)_3$ — •Carolin Kastner[1], Fabrice Bert[2], Andrin Doll[3], Thomas J. Hicken[3], Jonas A. Krieger[3], Hubertus Luetkens[3], Dirk Menzel[1], F. Jochen Litterst[1], Leonie Stödter[4], Kirrily C. Rule[5], Anja U. B. Wolter[6], and Stefan Süllow[1] — [1]IPKM, TU Braunschweig, Braunschweig, Germany — [2]SQM, Université Paris-Saclay, Orsay, France — [3]PSI, Villigen, Switzerland — [4]FZ Jülich, JCNS at MLZ, Garching, Germany — [5]ANSTO, Lucas Heights, Australia — [6]Leibniz IFW Dresden, Dresden, Germany

The natural mineral clinoatacamite $Cu_2Cl(OH)_3$ is a distorted Kagome system with antiferromagnetic in-plane couplings of the order of a few hundred K and ferromagnetic interplane couplings of the order of a few tens of K. This dominance of the antiferromagnetic couplings within the Kagome planes establishes clinoatacamite as a frustrated quantum magnet in its own right. In recent years, we have extensively characterized the complex magnetic phase diagram of clinoatacamite which contains a sequence of magnetic transitions of unknown symmetry. In particular, we have performed a detailed μSR study in zero magnetic field, thus characterizing the different magnetic regions below T_N = 18.1 K using this experimental technique.

To provide further insight into the microscopic details of the different magnetic regions we now have performed a μSR study on single-crystalline clinoatacamite in high magnetic fields up to 6.5 T and will discuss the results in this presentation.

TT 57.4 Wed 15:45 CHE/0091

Pathway to the ground state in Kagome spin ice HoAgGe — •Philipp Gegenwart — Lehrstuhl für Experimentalphysik VI, Universität Augsburg

HoAgGe represents the first crystalline realization of Kagome spin ice and displays striking fractionalized plateau states in magnetic and transport experiments [1,2]. We report single crystal neutron diffuse scattering to map the pathway from paramagnetism via partial order to the Kagome spin ice ground state [3]. The symmetry-broken nature of the latter is evidenced by the nonlinear magnetic susceptibility.

[1] K. Zhao, H. Deng, H. Chen, K.A. Ross, V. Petricek, G. Günther, M. Russina, V. Hutanu, P. Gegenwart, Science 367, 1218 (2020)
[2] K.Zhao, Y.Tokiwa, H.Chen, P.Gegenwart, Nat.Phys. 20,442 (2024)
[3] K.Zhao, H.Deng, H.Chen, N.Ma, N.Oefele, J.Guo, X.Cui, Ch.Tang, M. J. Gutmann, T. Mueller, Y. Su, V. Hutanu, Ch. Jin, P. Gegenwart, arXiv:2505.22544

TT 57.5 Wed 16:00 CHE/0091

Pressure-tuned Kagome spin liquid in Herbertsmithite $ZnCu_3(OH)_6Cl_2$ — •Victoria Ginga[1], Rodolfo A. Rangel Hernandez[1], Bin Shen[2], Louis Stein[3], Ece Uykur[3], Philipp Gegenwart[2], and Alexander A. Tsirlin[1] — [1]Felix Bloch Institute, University of Leipzig, Germany — [2]EP VI, EKM, University of Augsburg, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, Germany

Herbertsmithite is a benchmark S = 1/2 Kagome quantum spin-liquid candidate. At ambient pressure, our magnetization data confirm the absence of long-range order down to 2 K while revealing a low-field spin-freezing that is suppressed by moderate fields. High-pressure single-crystal diffraction shows that the trigonal structure remains stable up to 22 GPa, beyond which the material becomes amorphous. Whereas an earlier study [1] reported non-monotonic changes in Cu-O distances and Cu-O-Cu angles near 2.5 GPa concomitant with pressure-induced T_N around 6 K, our high-pressure structural data show no such behavior. Our pressure-dependent magnetization up to 4.2 GPa shows no transition, while spin freezing persists with an almost constant freezing temperature of 7 K. Using experimentally determined high-pressure structures, we quantify exchange couplings via DFT and map how the dominant interactions evolve with bond geometry. Our findings show that, to at least 4.2 GPa, Herbertsmithite preserves its quantum-disordered ground state and provides a reference framework for pressure tuning in Kagome spin-liquid candidates.

[1] Phys. Rev. Lett. 108, 187207

TT 57.6 Wed 16:15 CHE/0091

Anisotropic Transient Reflectivity Observed in Fe-Sn Kagome Binary Compounds — •Marcos Vinicius Goncalves Faria[1,2], Alexej Pashkin[1], Stephan Winnerl[1], Manfred Helm[1,2], Hechang Lei[3], Qi Wang[3], Jure Demsar[4], Chandra Kotyada[4], Lilian Prodan[5], István Kézsmárki[5], and Ece Uykur[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf — [2]Technische Universität Dresden — [3]Renmin University of China — [4]Johanes Gutenberg University Mainz — [5]Universität Augsburg

In this work, we investigate the interlayer coupling in Fe-Sn Kagome binaries using ultrafast transient reflectivity. Previous pump-probe studies have revealed that many Kagome metals exhibit similar relaxation features when probing the Kagome plane. However, the ultrafast response changes significantly by moving the probe direction from in-plane to out-of-plane, which we ascribe to the confinement of localized carriers in the Kagome layers. Such anisotropic behavior is consistent with what has also been observed with resistivity and broadband optics. The strong coupling between the Kagome layers shows that the single-Kagome layer approximation is not sufficient to describe the physics in this material family.

Beyond electronic anisotropy, the presence of magnetism, CDW and other lattice instabilities can strongly influence the nonequilibrium response of Kagome metals. Fe_3Sn and Fe_3Sn_2 are systems where there is an in-plane breathing mode and a coherent optical phonon can be excited. However, for FeSn, which has a pristine Kagome lattice, no coherent phonon could be observed.

15 min. break

TT 57.7 Wed 16:45 CHE/0091

Many-body interference in Kagome crystals — •Chunyu Guo[1], Kaize Wang[1], Ling Zhang[1], Carsten Putzke[1], Dong Chen[2], Takashi Oka[3], Roderich Moessner[4], Mark Fischer[5], Titus Neupert[5], Claudia Felser[2], and Philip Moll[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]The Institute for Solid State Physics, The University of Tokyo, Kashiwa, Japan — [4]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [5]Department of Physics, University of Zurich, Zurich, Switzerland

When electrons in metals act collectively, they create emergent phenomena that exceed the behavior of individual particles. We present experimental evidence of coherent charge transport in the normal state of the Kagome metal CsV_3Sb_5.

This is evidenced by magnetoresistance oscillations in mesoscopic crystalline pillars under in-plane magnetic fields, with periodicity determined by magnetic flux quanta, h/e, between adjacent Kagome layers, resembling an interlayer Aharonov-Bohm interferometer. The oscillation amplitude also correlates directly with other unusual electronic responses in CsV_3Sb_5, suggesting an intrinsic coherence mechanism. These findings shed light on the debated nature of correlated order in Kagome metals, positioning CsV_3Sb_5 as a unique platform for long-range coherent charge transport outside of superconductivity, and opening new avenues for understanding coherence in correlated electron systems.

TT 57.8 Wed 17:00 CHE/0091

Correlation effects in extended Kagome Hubbard models — •Alon Strugatsky and Roser Valenti — Goethe-Universität Frankfurt, Frankfurt am Main, Germany

Kagome materials display a rich interplay of topology, strong electronic correlations, and lattice dynamics. Recently, attention has focused on a class of Kagome metals whose nearly flat bands sit close to the Fermi level. Examples include FeGe, CsV_3Sb_5, $YbCr_6Ge_6$. Such systems are natural hosts for flat-band phenomena (for instance, flat-band ferromagnetism and unconventional superconsuctivity), but their large density of states makes perturbative diagrammatic approaches challenging. Here, we present a systematic study using dynamical mean-field theory (DMFT) and cluster DMFT on an extended Kagome Hubbard model, and map the phase diagram at various fillings.

TT 57.9 Wed 17:15 CHE/0091

Emergent Network of Josephson Junctions in a Kagome Superconductor — •Tycho Blom[1], Matthijs Rog[1], Marieke Altena[2], Andrea Capa Salinas[3], Stephen Wilson[3], Milan Allan[1,4], Chuan Li[2], and Kaveh Lahabi[1] — [1]Huygens-Kamerlingh Onnes Laboratory, Leiden University, 2300 RA Leiden, The Netherlands — [2]MESA+ Institute for Nanotechnology, University of Twente, 7500 AE, Enschede, The Netherlands — [3]Materials Department, University of California Santa Barbara, Santa Barbara, California 93106, USA — [4]Munich Center for Quantum Science and Technology (MCQST), Ludwig-Maximilians- University Munich, Munich 80799, Germany

Materials with a Kagome lattice are intensely studied because they host exotic states that combine strong correlations and topology. In this talk, I will describe several unique phenomena that are observed in the Kagome superconductor $CsV_3Sb_{5-x}Sn_x$ (x = 0.03-0.04), and show that a network of Josephson junctions spontaneously emerges below the transition temperature in thin, homogeneous flakes. Using magnetotransport experiments under both DC and radio frequency current bias, I will demonstrate that the junctions are localized and stable, and that supercurrent must flow in filaments. These results pave the way for determining the exact nature of superconductivity in the AV_3Sb_5 family.

TT 57.10 Wed 17:30 CHE/0091

Unconventional gap structure in Kagome superconductor coupled to hybrid microwave resonators — •Yejin Lee, Haolin Jin, Berit Goodge, Edouard Lesne, Sushmita Chandra, and Uri Vool — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Kagome superconductors have been recently discovered, offering a rich platform to study strongly correlated systems, including superconductivity, charge density wave, and time reversal symmetry broken states, and their electronic properties, featuring flat bands and van Hove singularities. Finding a pairing symmetry is crucial to understand the quantum phases interplay. Despite numerous experimental efforts focused on bulk crystals, there is no consensus for microscopic origin so far. Additionally, van der Waals flakes show distinct phases that are hard to probe with conventional methods. Superconducting microwave resonator is highly sensitive to detect the kinetic inductance and allows for studying the microwave response when hybridized with vdW layered flakes. Using this technique we investigate the pairing symmetry of the Kagome superconductor. We fabricate the CVS flake-coupled circuits with cryogenic transfer method, which preserves the pristine property and atomically sharp interface. We find any disorder in the flake disrupts coupling in the circuits that hinders the investigation of the low temperature properties. The temperature dependent resonance frequency shows a linear behavior, which deviate from a conventional fully gapped structure. The linear dependence is a signature for a nodal structure, as a hallmark of unconventional superconductivity.

TT 57.11 Wed 17:45 CHE/0091

Superconductivity in Kagome metals due to soft loop-current fluctuations — •Daniel Schultz[1], Grgur Palle[2], Asimpunya Mitra[3], Yong-Baek Kim[3], Rafael Fernandes[2], and Jörg Schmalian[1] — [1]Institute for Theoretical Condensed Matter Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Department of Physics, The Grainger College of Engineering, University of Illinois Urbana-Champaign, Urbana, Illinois 61801, USA — [3]Department of Physics, University of Toronto, Toronto, Ontario M5S 1A7, Canada

We demonstrate that soft fluctuations of translation symmetry-breaking loop currents provide a mechanism for unconventional superconductivity in Kagome metals that naturally addresses the multiple superconducting phases observed under pressure. Focusing on the rich multi-orbital character of these systems, we show that loop currents involving both vanadium and antimony orbitals generate low-energy collective modes that couple efficiently to electrons near the Fermi surface and mediate attractive interactions in two distinct unconventional pairing channels. While loop-current fluctuations confined to vanadium orbitals favor chiral d+id superconductivity, which spontaneously breaks time-reversal symmetry, the inclusion of antimony orbitals stabilizes an $s^{\pm}$ state that is robust against disorder. We argue that these two states are realized experimentally as pressure increases and the antimony-dominated Fermi surface sheet undergoes a Lifshitz transition.

TT 57.12 Wed 18:00 CHE/0091

Strain Tuning of the Kagome Metal GdV_6Sn_6 — •Francisco Lieberich[1,2], Ganesh Pokharel[3], Stephen Wilson[4], and Elena Gati[1,2,5] — [1]MPI−CPfS, Dresden, Germany — [2]TUD, Dresden, Germany — [3]UWG, Georgia, USA — [4]UCSB, Santa Barbara, USA — [5]Goethe Universität, Frankfurt, Germany

Kagome metals are a fertile ground for exotic states of matter, driven by the interplay of nontrivial band topology and strong correlation effects [1]. In the RV_6Sn_6 series, alternating rare-earth (R) triangular-lattice and V Kagome layers generate a unique environment for exploring the interaction of correlated topological behavior with magnetic frustration. GdV_6Sn_6, in particular, exhibits strong coupling between Gd local magnetic moments and Kagome-plane itinerant electrons [2], giving rise to a fascinating interplay of commensurate and incommensurate spin modulations under applied magnetic field [3]. In this talk, we discuss the effects of uniaxial pressure, which lifts the inherent lattice frustration, on the thermodynamic properties of GdV_6Sn_6. Using high-resolution elastocaloric effect [4] measurements we establish a rich phase diagram and show that the balance of commensurate and incommensurate spin modulations is highly tunable by uniaxial pressure. These findings highlight the exceptional sensitivity of magnetic Kagome metals to lattice tuning by uniaxial pressure.

[1] Sante *et al*, arXiv:2511.12731 (2025)
[2] Ishikawa *et al*, JPSC 90, 124704 (2021)
[3] Porter *et al*, PRB 108, 035134 (2023)
[4] Ikeda *et al*, RSI 90, 083902 (2019)

TT 58: Quantum Transport and Quantum Hall effects (joint session HL/TT)

Time: Wednesday 15:00–16:15 Location: POT/0006

TT 58.1 Wed 15:00 POT/0006

High Harmonic Hall Currents Driven by Curved Conducting Nanoarchitecture — •Ching-Hao Chang[1,2], Botsz Huang[1,2], Wei-Xiang Yin[1,2], and Xiao Zhang[3] — [1]Department of Physics, National Cheng Kung University Tainan, Taiwan — [2]Center for Quantum Frontiers of Research and Technology (QFort), National Cheng Kung University Tainan 70101, Taiwan — [3]Institute for Theoretical Solid State Physics Leibniz Institute for Solid State and Materials Research Dresden Helmholtzstr. 20, D-01069 Dresden, Germany

We theoretically establish a realizable non-perturbative mechanism for generating high harmon- ics (up to 6th order) in Hall currents within curved two-dimensional nanoarchitectures. Unlike previously explored perturbative mechanisms based on inversion symmetry breaking or Berry curvature, the high-harmonic generation demonstrated here is driven by magnetic-field dipoles induced purely by nanoscale curvature under an applied uniform magnetic field. We develop a theory showing that these harmonics originate from unique snake orbits induced by the interplay between an alternating electric field and curvature-induced magnetic-field dipole. Moreover, we establish quantitative control over harmonic suppression and enhancement by tuning the amplitude and orientation of the magnetic field, uncovering distinct symmetry-based even/odd harmonic selection rules. These findings provide a tunable platform for engineering nonlinear currents in curved electronics, with potential applications in developing high-frequency Hall sensors and THz devices.

TT 58.2 Wed 15:15 POT/0006

Gate-tunable isospin switching in graphene Mach-Zehnder electronic interferometers — •Antonio Lacerda-Santos, Lilian Seyve, Yassine Setti, Bikash Barik, Leo Pugliese, Preden Roulleau, and Cosimo Gorini — SPEC, CEA, CNRS, Université Paris-Saclay, 91191 Gif-sur-Yvette, France

Graphene has become an exciting platform for electron (quantum) optics experiments [1]. Compact electronic interferometers can be realised via p-n interfaces,

which in quantizing magnetic fields host counter-propagating chiral edge states. In a paradigmatic architecture with a single junction, such quantum Hall states form a Mach-Zehnder interferometer [2, 3]. The precise position of such edge states is set by the electrostatics of a given device [4], which can be determined to great accuracy with the self-consistent Schrödinger-Poisson solver Pescado [5].

We perform electrostatic and quantum transport simulations accompanying conductance measurements in a graphene Mach-Zehnder interferometer, and show that remote gates can be used to control the position of the p-n junction on sub-nanometer scales. Such a fine control does not meaningfully affect the edge state positions and lengths, but induces valley-isospin oscillations. The interferometer thus behaves as a tunable valley-isospin transistor.

[1] H. Chakraborti et al., J.Phys.:Condens.Matter 36 (2024) 393001 [2] D.S.Wei et al, Science Advances 3, e1700600 (2017) [3] M. Jo et al, PRL 126, 146803 (2021) [4] I.M. Flor et al, PRB 105, L241409 (2022) [5] A. Lacerda-Santos, arXiv:2507.03131v1

TT 58.3 Wed 15:30 POT/0006

Phase-coherent autonomous nonequilibrium demon — •José Balduque[1,2] and Rafael Sánchez[1,2,3] — [1]Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Madrid, Spain. — [2]Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, Spain — [3]Instituto Nicolás Cabrera (INC), Universidad Autónoma de Madrid, Madrid, Spain.

Mesoscopic conductors enable the efficient management and useful conversion of not only thermal resources but also nonequilibrium electron distributions. The latter scenario makes it possible to define demonic modes of operation, in which the entropy of a subsystem is autonomously reduced without extracting net particles or energy from the subsystem that provides the nonequilibrium resource [1]. We propose an implementation of such a nonequilibrium demon, or N-demon, in a multiterminal system that exploits carrier coherence. This is achieved by directly coupling the demonic subsystem to an isothermal two-terminal conductor via a scanning tip, enabling the local injection of electrons in a nonthermal distribution that participates in the phase-coherent interference processes governing the system's transport response [2]. In this way, we uncover an extrinsic, nonlocal, and phase-tunable transport response induced by the demon [3].

[1] R. Sánchez, et al., Phys. Rev. Lett. 123, 216801 (2019).
[2] R. Sánchez, et al., Phys. Rev. B, 105, 239903 (2022).
[3] J. Balduque and R. Sánchez, in preparation.

TT 58.4 Wed 15:45 POT/0006

Exploring the Influence of Electron Density on the Giant Negative Magnetoresistance — •Lina Bockhorn[1], Christian Reichl[2], Werner Wegscheider[2], and Rolf J. Haug[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Germany — [2]Laboratorium für Festkörperphysik, ETH Zürich, Switzerland

Ultra-high mobility two-dimensional electron gases exhibit a robust negative magnetoresistance at zero magnetic fields, characterized by a temperature-independent peak around $B = 0$ T and a temperature-dependent giant negative magnetoresistance (GNMR) at higher fields [1-4]. By varying the electron density in situ, we gain valuable insights into the nature of GNMR. Our study shows a significant dependence of GNMR on electron density, suggesting that scattering potential variations [5] may not be fully addressed in current theoretical models. By examining these dependencies for different temperatures, we enhance the understanding of unresolved aspects of GNMR theory, potentially bridging the gap between experimental observations and theoretical predictions.

[1] L. Bockhorn et al., Phys. Rev. B 83, 113301 (2011).
[2] L. Bockhorn et al., Phys. Rev. B 90, 165434 (2014).
[3] L. Bockhorn et al., Appl. Phys. Lett. 108, 092103 (2016).
[4] L. Bockhorn et al., Phys. Rev. B 109, 205416 (2024).
[5] Y. Huang et al., Phys. Rev. Materials 6, L061001 (2022).

TT 58.5 Wed 16:00 POT/0006

A topological field-effect memristor — •Fabian Hartmann[1], Manuel Meyer[1], Selena Barragan[1], Sergey Krishtopenko[1,2], Jean-Baptiste Rodriguez[3], Eric Tournie[3], Benoit Jouault[2], Gerald Bastard[1], Frederic Teppe[2], Lukas Worschech[1], Victor Lopez-Richard[4], and Sven Höfling[1] — [1]Lehrstuhl für Technische Physik, Julius-Maximilians-Universität Würzburg — [2]L2C, CNRS-Université de Montpellier, France — [3]IES, Université de Montpellier, France — [4]Departamento de Fisica, Universidade Federal de Sao Carlos, Brazil

Quantum and neuromorphic computing rely on unconventional materials and device functionalities, yet achieving resilience to imperfections and reliable operation remains a major challenge. This has motivated growing interest in topological materials that provide robust and low-power operation while preserving coherence. However, integrating topological transport with memory functionality into a reconfigurable device has remained elusive. Here, we realize a topological field-effect memristor in which topological protection preserves edge state coherence, enabling the coexistence of coherent transport and non-volatile memory functionality. Utilizing inverted InAs/GaInSb/InAs trilayer quantum wells, we realize a quantum spin Hall insulator that exploits its intrinsic floating-gate behavior. This feature allows one to reconfigure the conventional field-effect transistor operation into memristive functionality with broad electric-field tunability. One resistance state is entirely governed by dissipationless, coherent transport.

TT 59: 2D Materials V – Magnetic, spintronic, and topological properties (joint session HL/TT)

Time: Wednesday 15:00–17:15 Location: POT/0081

Invited Talk TT 59.1 Wed 15:00 POT/0081

Dual proximity engineering of spin-orbit and magnetic effects in graphene heterostructures — •Christoph Kastl — Walter Schottky Institute, School of Natural Sciences, Technical University of Munich — Munich Center for Quantum and Technology (MCQST)

The coexistence of induced spin-orbit coupling (SOC) and magnetic exchange fields is predicted to drive graphene into topological phases, such as the quantum anomalous Hall state. Here, I will discuss the prospect of using monolayer graphene proximitized by WSe_2 (SOC) and $Cr_2Ge_2Te_6$ (magnetic exchange) for such dual proximity control. To determine the type and strength of the induced SOC, I will compare Landau fan analysis, where level anticrossings can serve as direct signatures of spin-orbit splittings, to optoelectronic measurements on graphene/WSe_2 heterostructures, where the photogalvanic effect can provide an indirect fingerprint of SOC. Low-temperature magnetotransport measurements of the heterostructures with combined magnetic and SOC proximity reveal a large and gate-tunable anomalous Hall effect persisting at zero magnetic field, signaling an intrinsic Berry curvature arising from the interplay of SOC and magnetism. These results highlight the coexistence of spin-orbit and magnetic proximity effects in graphene-based van der Waals heterostructures and establish a route toward topological graphene phases.

TT 59.2 Wed 15:30 POT/0081

Twist angle and pressure tuning of proximity-induced spin-orbit coupling in graphene/WSe_2 heterostructures — Tobias Rockinger[1], Bálint Szentpéteri[2], Szabolcs Csonka[2], Marina Marocko[1], Julia Amann[1], Ziyang Gan[3], Antony George[3], Andrey Turchanin[3], Kenji Watanabe[4], Takashi Taniguchi[4], Dieter Weiss[1], Péter Makk[2], and •Jonathan Eroms[1] — [1]Department of Physics, University of Regensburg, Regensburg, Germany — [2]Department of Physics, Budapest University of Technology and Economics, Budapest, Hungary — [3]Institute of Physical Chemistry, Friedrich Schiller University Jena, Jena, Germany — [4]National Institute for Materials Science, Tsukuba, Japan

Proximity-induced spin-orbit interaction in heterostructures of graphene and transition metal dichalcogenides has been studied intensely in the past few years. However, present experiments still suffer from poor reproducibility, as one key parameter, the twist angle between the crystal axes of both materials, has not been systematically controlled during fabrication. Band structure calculations, on the other hand, have predicted a decisive influence of this parameter. In our experiments, we control the twist angle during fabrication by aligning fractured or CVD grown edges and resolving the ambiguity of zigzag and armchair directions using a crystallographic etching process. We employ weak antilocalization to extract the spin-orbit coupling parameters quantitatively, and report excellent reproducibility and a good match to theoretical predictions. We also confirm the influence of high pressure on the proximity effect.

TT 59.3 Wed 15:45 POT/0081

Nonlinear optical probing of local quantum geometry — •Nele Tornow[1], Paul Herrmann[1], Clemens Schneider[2], Jan Wilhelm[2], and Giancarlo Soavi[1,3] — [1]Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany — [2]Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy, Regensburg, Germany — [3]Abbe Center of Photonics, Friedrich Schiller University Jena, Jena, Germany

With its direct relation to many phenomena in solid matter, quantum geometry has become a concept of increasing interest in solid state physics. However, measurements of the local quantum geometry, *e.g.,* Berry curvature, has been possible to date only *via* angle-resolved photoemission spectroscopy [1]. On the other hand, in one of our recent theoretical works [2] we have shown that there is a link between linear circular dichroism and derivatives of Berry curvature in 3D crystals with preserved time-reversal symmetry (TRS).

In this presentation I will further demonstrate both, experimentally and with analytical solutions of semiconductor Bloch equations, that in a 2D semiconductor with broken TRS, the emerging second-harmonic circular dichroism can be used as a direct probe of the Berry curvature at the opposite ± K valleys, providing a new all-optical approach to access the local quantum geometry in 2D materials.

[1] Schüler, M. et al., Sci. Adv. 6, eaay2730 (2020)
[2] Soavi, G. and Wilhelm, J., arXiv:2501.03684 (2025)

15 min. break

TT 59.4 Wed 16:15 POT/0081

Proposal for Resolving Quantized Landau Orbits via Elastic XUV Scattering — •Sabrina Meyer[1], Andreas Knorr[1], Stephen Hughes[2], and Lara Greten[1,2] — [1]Institut für Physik und Astronomie, Technische Universität Berlin, Germany — [2]Department of Physics, Queen's University, Kingston, Canada

In a strong perpendicular magnetic field, a two-dimensional electron gas is quantized into discrete Landau levels. We propose a method to extract the spatial structure of Landau orbits via scattering with extreme ultraviolet radiation, whose wavelength naturally matches the Larmor radius. In a microscopic theory, we derive the far-field spectrum emitted by the optically induced current density. Contributions from Landau orbits within this spectrum are suppressed due to scattering effects imposed by the sample geometry. By normalizing against the zero-magnetic-field reference, however, we define a Landau level scattering spectrum that isolates Landau orbit information. This gives access to the probability density distributions of individual Landau level wave functions featuring radial maxima at the quantized Larmor radii.

TT 59.5 Wed 16:30 POT/0081

Berry Phase Shift in Folded Bilayer Graphene — •Hannes Kakuschke, Lina Bockhorn, and Rolf J. Haug — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

Mono- and bilayer systems of graphene have been extensively researched due to their unique magnetic und electronic transport properties. In more recent works, folded graphene [1-5] has gained interest as a platform for topological phenomena, such as zero-line modes [4]. However, these systems rely on self-assembled folded graphene, found by chance during exfoliation or induced by tearing [1-5]. Our dry-transfer approach allows us to fold graphene around hBN in a controllable manner, decoupling the overlapping graphene regions. In these samples, we observe a Berry phase shift from 2π to π near the edge of folded bilayer graphene, attributed to local strain fields and stacking shifts.

[1] J. C. Rode et al., Ann. Phys. 529, 1700025 (2017).
[2] J. C. Rode et al., 2D Mater. 6, 015021 (2018).
[3] L. Bockhorn et al., Appl. Phys. Lett. 118, 173101 (2021).
[4] S. J. Hong et al., 2D Materials 8, 045009 (2021).
[5] S. J. Hong et al., Phys. Rev. B 105, 205404 (2022).

TT 59.6 Wed 16:45 POT/0081

Probing spin-orbit coupling in graphene/WSe_2 heterostructures by the circular photogalvanic effect — Ernst Knöckl, •Matthias Klein, Alexander Holleitner, and Christoph Kastl — Walter Schottky Institute, School of Natural Sciences, Technical University of Munich

We investigate proximity-induced spin–orbit coupling (SOC) in graphene/WSe_2 heterostructures using the circular photogalvanic effect (CPGE) as a symmetry-selective and experimentally accessible probe of spin–valley-locked band textures [1]. By measuring helicity-dependent photocurrents as a function of gate voltage, excitation energy, and device geometry, we aim to disentangle Rashba and valley-Zeeman SOC contributions and to extract their magnitude and sign as a function of the graphene–WSe_2 twist angle. The observed trends in CPGE sign reversals and scaling behavior provide quantitative indications of interfacial symmetry breaking and moiré-enhanced spin–valley coupling, supported by comparison to microscopic transport models. These results are expected to establish CPGE as a promising metrological probe of proximity SOC in 2D heterostructures and to complement ongoing efforts in twist-angle-dependent spin–orbit engineering in graphene/TMD systems [2,3].

[1] Kiemle, J., et al. ACS nano 16.8, 12338-12344 (2022)
[2] Yang, H., et al. Nat. Mater. 23, 1502-1508 (2024)
[3] Zhang, Y., et al. Natur 641, 625-631 (2025)

TT 59.7 Wed 17:00 POT/0081

Study of the non-trivial spin texture in Tellurium and the consequences in charge-spin interconversion — •Andrés Martínez-García[1], Daniel Gosálvez-Martínez[1], Carlos Sabater[1], and Juan José Palacios[2] — [1]Departamento de Física and Instituto Universitario de Materiales de Alicante (IUMA), Universidad de Alicante, Alicante, Spain. — [2]Departamento de Física de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, Spain.

Tellurium is a chiral semiconducting material with a narrow band gap that can be synthesized with well-defined handedness in nanowires and flakes, making it an excellent platform for studying chirality-related charge-spin interconversion in nanodevices. The coupling between charge and spin degrees of freedom is closely connected to the spin texture in momentum space. In this work, we demonstrate that tellurium exhibits a nontrivial radial spin texture at the top of the valence band, where the spin polarization aligns parallel to the HK direction of the Brillouin zone, while spins in the perpendicular ZHL plane display a nontrivial winding. We investigate the electronic transport and resulting spin polarization within the Landauer transport formalism using first-principles calculations. This approach allows us to map the transport properties along each crystallographic direction and to identify correlations between the spin polarization of the induced current and the underlying momentum-space spin texture. Our results provide microscopic insight into chirality-driven spin responses in tellurium and highlight its potential for spintronic applications.

TT 60: Spintronics (other effects) (joint session MA/TT)

Time: Wednesday 15:00–18:00 Location: POT/0112

Invited Talk TT 60.1 Wed 15:00 POT/0112

Magneto-optic Kerr effects of higher order in magnetization in thin films of different crystal orientations — •Timo Kuschel — Johannes Gutenberg University Mainz, Germany

The magneto-optic Kerr effect (MOKE) is an important tool to study magnetic properties of thin films. While the MOKE contribution linear in magnetization (LinMOKE) is mainly used for Kerr imaging, Kerr spectroscopy, time-resolved MOKE, and vectorial magnetometry of ferromagnetic thin films [1], the MOKE contributions quadratic in magnetization (QMOKE) [2] have been used for investigations of antiferromagnetic materials, spin-orbit torques, and structural order of Heusler compounds [3]. Recently, we have identified MOKE contributions of third order in magnetization (cubic MOKE, CMOKE) [4] and studied its dependence on the structural domain twinning of Ni(111) thin films.

In this talk, I will introduce these MOKE effects of higher order and describe their angular dependencies with respect to the crystal orientations of the thin films. While it is quite simple to find CMOKE in (111)-oriented films, it is not straightforward to identify it in (001)-oriented samples. I will discuss the reasons. Furthermore, I will report on the material systems that have shown CMOKE so far and mention potential applications.

[1] T. Kuschel et al., J. Phys. D: Appl. Phys. 44, 265003 (2011)
[2] R. Silber, TK et al., Phys. Rev. B 100, 064403 (2019)
[3] R. Silber, TK et al., Appl. Phys. Lett. 116, 262401 (2020)
[4] M. Gaerner, TK et al., Phys. Rev. Applied 22, 024066 (2024)

TT 60.2 Wed 15:30 POT/0112

Ignition of spin-triplet supercurrent in a ballistic S/F/S Josephson junction with precessing magnetization — •Elizaveta Andriyakhina, Miad Mansouri, Maxim Breitkreiz, and Piet Brouwer — Freie Universität Berlin, Germany

We develop a theory for a ballistic Josephson junction with a ferromagnetic (including half-metallic) interlayer whose uniformly precessing magnetization generates a controllable equal-spin (triplet) supercurrent. In a co-rotating frame, the driven junction maps to an effective static problem that can be treated with a scattering-matrix approach to obtain Andreev bound states and the dc Josephson current.

A key result is that steady precession produces a spin-dependent non-equilibrium occupation in the rotating frame, yielding a finite dc supercurrent. In the half-metal limit the junction is "off" without precession, but becomes "on" when a finite precession angle induces phase-sensitive Andreev levels and a triplet current.

For small precession angles, the induced current is approximately sinusoidal in phase and the critical current scales quadratically with the precession angle (and with drive parameters), enabling microwave-controlled switching via ferromagnetic resonance.

TT 60.3 Wed 15:45 POT/0112

Magnetic Domain Wall Motion under Microwave Excitation — •Lukas Fischer[1], Rouven Dreyer[2], Jae-Chun Jeon[1], Georg Woltersdorf[2], and Stuart Parkin[1] — [1]Max-Planck Institute of Microstructure Physics, Halle (Saale), Germany — [2]Martin-Luther-University Halle-Wittenberg, Halle (Saale), Germany

Chiral domain walls (DWs) and their synchronous motion via current pulses in magnetic conduits (so-called magnetic racetracks) are of enormous interest due to their fast speed, non-volatility, and capability of creating high bit-density for advanced memory and logic technologies. Most experimental and numerical studies have focused on the motion of the DWs by spin-orbit torque using nanosecond-long current pulses which are not efficient in coupling to magnetization precessions of the magnetic material, typically occurring in the GHz regime.

Here we present that the microwave excitation of chiral Néel DWs in a magnetic microwire with perpendicular magnetic anisotropy significantly impacts the DW motion. We use either magnetic fields or electrical currents at RF-frequencies to explore the pronounced impact on the DW motion. Firstly, we directly visualize the high-frequency response of the DW by using the Super-Nyquist sampling magneto-optical Kerr effect. We then determine the effect of this excitation on the DW motion. When the DW is excited in the presence of a static, transverse magnetic field, it exhibits unidirectional self-propulsion. Moreover, the resonant excitation in a static, longitudinal field leads to a current-triggered, sustained DW motion over micrometer distances, which dramatically increases the effective DW displacement.

TT 60.4 Wed 16:00 POT/0112

Assembly of Magnetic Heterostructures with Chiral Nanographenes — •Chi Fang, Wenhui Niu, Jitul Deka, and Stuart Parkin — Max Planck Institute of Microstructure Physics, Halle(Saale) 06120, Germany

Chirality-induced spin selectivity (CISS) is an emergent phenomenon whereby chiral molecules act as efficient spin filters, selectively transmitting electrons of a particular spin orientation. A central challenge in advancing CISS-based spintronics lies in experimentally verifying spin filtering in structurally defined, laterally extended molecular systems, using standard solid-state device techniques that yield reproducible and robust spin-dependent transport signals. Here, we present direct experimental evidence of the CISS effect in helical nanographenes (NGs), using magnetoresistance (MR) measurements in magnetic heterostructures. The device architecture included a bottom electrode ferromagnetic contact, orthogonally patterned and electrically isolated by an AlOx layer to confine current to the junctions. NG, a synthetically tailored chiral molecule, was spin-coated to form a thin, uniform layer serving as a spin-filter interface. Different from previous works, the ferromagnet layer grown directly on the substrate offers a better performance of the magnetic properties. Both enantiomeric devices showed MR values around 1 % at room temperature, with minimal variation over the 10*400 K temperature range, indicating robust and reproducible spin selectivity. [1] B. Bloom et al. Chem. Rev. 124(4), 2014;[2] S. Ham et al. Micromachines 15(4), 528, 2024;[3] S. Yang et al., Nat. Rev. Phys. 3, 328, 2021.

TT 60.5 Wed 16:15 POT/0112

Alloying-Driven Modifications of the Magnetic Properties in Transition-Metal Iodides — •Paulina Jureczko[1,2] and Martin Gmitra[1,3] — [1]Institute of Experimental Physics, Slovak Academy of Sciences, 04001 Košice, Slovakia — [2]Institute of Physics, University of Silesia in Katowice, 41-500 Chorzów, Poland — [3]Institute of Physics, Pavol Jozef Šafárik University in Košice, 04001 Košice, Slovakia

Single-layer transition-metal dihalides have recently emerged as a platform for exploring two-dimensional magnetism and topology. Using density-functional theory, we investigate the electronic and magnetic properties of MI_2 monolayers and alloyed $M_{1-x}N_xI_2$ systems, where M and N represent Mn, Fe, Co, Ni. We analyze how chemical substitution modifies exchange interactions and spin-orbit-driven topological features by computing the Berry curvature and Chern numbers. The results reveal that alloying provides an efficient route for tuning magnetic anisotropy and topological phases in transition-metal iodides, underscoring their potential relevance for 2D spintronics.

This work has been funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I05-03-V02-00071.

15 min break

TT 60.6 Wed 16:45 POT/0112

Spintronic THz Frequency Conversion Mediated by Ferromagnetic/Oxide Interfaces — •Kang Jin[1], Ruslan Salikhov[1], Stefan Kober[2], Igor Ilyakov[1], Jan-Christoph Deinert[1], Aleksandra Lindner[1], Jürgen Fassbender[1,3], Sebastian F. Maehrlein[1,3], Zhe Wang[2], and Jürgen Lindner[1] — [1]HZDR — [2]TU Dortmund — [3]TU Dresden

Frequency conversion is a key nonlinear phenomenon for communication and data processing technologies. Exploring this phenomenon at terahertz (THz) frequencies is of particular interest, as the high carrier frequency enables faster data transfer and higher operational speeds. Previous experiments have revealed that THz frequency conversion could serve as a distinctive probe for THz-light-induced ultrafast spin-transfer currents (STCs) at Ferromagnetic (FM)/Non-Magnetic (NM) interfaces. Building on these findings, we report THz frequency conversion using cost-effective NM materials (such as SiO2 and Al2O3 films) and demonstrate their origin from the interfacial inverse Rashba-Edelstein effect. We compare conversion efficiencies and characteristics of different samples, revealing that FM interfaces, featuring off-stoichiometric SixOy and AlxOy, achieve conversion efficiencies comparable to heavy metal capping layers (i.e. Ta). The deposition sequence and the oxidation level of the samples were found to critically influence the sign of the spin-charge conversion. The observed THz second harmonic generation represents a spintronic foundation for developing THz frequency mixers and rectifying components.

TT 60.7 Wed 17:00 POT/0112

Magnetic hyperfine fields in solids without inversion symmetry induced by an external electric field — •Alberto Marmodoro[1,2,3,4], Hubert Ebert[1], Sergiy Mankovsky[1], and Jan Minar[3] — [1]LMU Munich, Munich, DE — [2]Inst. of Physics of the Czech Acad. of Sci., Prague, CZ — [3]University of West Bohemia, Pilsen, CZ — [4]Czech Technical University., Prague, CZ

An electric field induces in a solid without inversion symmetry spin and orbital magnetization - a phenomenon called Edelstein effect. This induced magnetization has to have its counterpart in an induced magnetic hyperfine field seen by nuclear magnetic moments. Corresponding NMR experiments have been performed recently on Te with success [1]. Using Kubo's linear response formalism implemented on the basis of the relativistic Korringa-Kohn-Rostoker Green function technique a description for the field induced hyperfine field (EFI-HFF) has been developed in analogy to that for the spin and orbital Edelstein effect [2]. The EFI-HFF drastically differs from that induced by an external magnetic field as the later one does not need missing inversion symmetry. Making use of a Gordon decomposition of the electronic current a splitting of the EFI-HFF into its spin and orbital parts is achieved [3]. This allows to discuss them in relation to their counterparts concerning the magnetization as well as the role of the spin-orbit coupling for them. Corresponding numerical results are presented for Te.

[1] T. Furukawa et al., Phys. Rev. Res., **3**, 023111 (2021). [2] S. Wimmer et al. Phys. Rev B, **103**, 024437 (2021). [3] M. Battoclletti and H. Ebert, Phys. Rev. B, **64**, 094417 (2001).

TT 60.8 Wed 17:15 POT/0112

Theoretical description of the optical activity and directional dichroism of chiral solids — •Hubert Ebert and Sergiy Mankovsky — Ludwig Maximilian University of Munich, Munich, DE

A scheme to deal with the optical activity and directional dichroism of solids on the basis of Kubo's linear response formalism is presented. Accounting for the $\vec{q}$-dependence of the radiation field implies that the corresponding optical transitions described in $\vec{k}$-space are no more vertical. More important, one is led to corrections to the electric dipole matrix element due to the electric quadrupole and magnetic dipole interaction. The scheme is implemented making use of the relativistic Korringa-Kohn-Rostoker Green function (KKR-GF) formalism. Corresponding applications to chiral Te that has time reversal ($\mathscr{T}$) but no inversion ($\mathscr{I}$) symmetry led to a $\vec{q}$-dependent optical conductivity tensor with off-diagonal elements caused by the interference of the electric dipole and its correction terms giving rise to optical activity. In the case of anti-ferromagnetic Cr_2O_3 without $\mathscr{T}$-symmetry the correction terms lead to directional dichroism that strongly depends on whether a magnetic configuration with or without $\mathscr{I}$-but with combined $\mathscr{I}\mathscr{T}$-symmtetry is considered.

TT 60.9 Wed 17:30 POT/0112

Intrinsic and Proximity-Enhanced Spin-Orbit Torques in $Fe_3(Ge,Ga)Te_2$ and WTe_2 Heterostructures — •Gusthavo Brizolla[1], Stepan Tsirkin[2], Yaroslav Zhumagulov[2], and Jaroslav Fabian[1] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]EPFL, Lausanne, Switzerland

Spin-orbit torques (SOTs) in 2D magnets and their heterostructures offer a route to ultra-thin, energy-efficient memories where currents can switch magnetization without external magnetic fields. Materials such as Fe_3GeTe_2 (FGT) and Fe_3GaTe_2 (FGaT), and their interfaces with low-symmetry WTe_2, are especially promising, but the angular dependence and microscopic origin of their SOTs are still not fully understood. Here we compute SOTs in FGT, FGaT

and WTe_2-proximitized heterostructures using first-principles (DFT) calculations and compare two protocols for mapping the angular dependence: self-consistent magnetization rotation and rigid rotation of a fixed exchange field. They agree when spin-orbit mixing is weak, but differ strongly near in-plane alignment, where interband hot spots and evolving spin-orbit hybridization amplify the torkances. In WTe_2 heterostructures, broken symmetry and Te-Te interfacial hybridization further boost torques with out-of-plane spin polarization. These results provide design rules for field-free current control in 2D magnets and show that the angle dependence of spin-orbit coupling must be treated explicitly to obtain reliable SOT angular maps.

TT 60.10 Wed 17:45 POT/0112

Spin vacuum switching — •Eddie Harris-Lee[1,2], John Kay Dewhurst[2], Samuel Shallcross[1], and Sangeeta Sharma[1,3] — [1]Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Berlin, Germany. — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany. — [3]Institut für Theoretische Physik, Freie Universität Berlin, Berlin, Germany.

While physical mechanisms underpinning spin switching are established for nano- to pico-second time scales, here we present a physical route to magnetization toggle control at < 100 femtoseconds. A minority spin current injected into a ferromagnet is shown to create a minority “spin vacuum" that then drives rapid charge redistribution from the majority channel and spin switching. We demonstrate this mechanism reproduces many of the features of recent sub-picosecond switching of ferromagnetic Co/Pt multilayers, and provide simple practical rules for the design of materials to optimize “spin vacuum" control over magnetic order.

Harris-Lee *et al.*, Sci. Adv. **10**, eado6390 (2024). DOI:10.1126/sciadv.ado6390

TT 61: Topology – Poster

Time: Wednesday 15:00–17:00 Location: P4

TT 61.1 Wed 15:00 P4

Topological Surface States for the Implementation of a Landau Level Laser — •Olivier Fayet[1], Jean-Noël Fuchs[2], and Piéchon Frédéric[1] — [1]Laboratoire de physique des solides, université Paris-Saclay et CNRS, Orsay, France — [2]Laboratoire de physique théorique de la matière condensée, Sorbonne Université et CNRS, Paris

Landau levels have since long been proposed for the implementation of a tunable laser in the THz regime. However, rapid non-radiative relaxation processes (Auger processes, disorder) are preventing population inversion. The former may to some extent be circumvented by the choice of a material with a non-equidistant Landau levels spectrum, e.g. in bilayer graphene or in the surface states of a topological heterojunction, called Volkov-Pankratov states. Under a strong magnetic field, the latter are quantised into Landau levels, recently observed in transport and spectroscopic measurements at the LPENS (Paris), based on predictions from the LPS theory group. To study the possibility of obtaining laser emission with these states, a detailed study of the different life times fo electrons in the associated Landau level is required.

TT 61.2 Wed 15:00 P4

Investigating Electrical and Thermal Hall Effect in Topological Insulators — •Karan Singh, Rohit Sharma, Yongjan Wang, Yoichi Ando, Achim Rosch, and Thomas Lorenz — II. Physikalisches Institut, Universität zu Köln, Zülpicher Strasse 77, D-50937 Köln, Germany

3D topological insulators are characterized by a bulk band gap and topologically protected gapless surface states formed by massless Dirac fermions. However, chemical disorder produces spatially fluctuating electric potentials, forming "charge puddles" that allow current to flow through the bulk [1]. With decreasing temperature, charge puddles localize, turning the sample electrically insulating. But these charge puddles remain thermally coupled via phonons and can be probed by the thermal Hall transport measurements [2]. In this work, we grew single crystals of $TlBi_{0.3}Sb_{0.7}Te_2$ and performed electrical and thermal transport measurements. The material shows a metal-semiconductor transition near 100 K and electron-like carriers at all temperatures. Notably, the thermal Hall conductivity (k_{xy}) measured on the same sample deviates from the Wiedemann-Franz law. After subtracting the electronic thermal contribution, the residual thermal Hall signal indicates that heat transport in this system involves contributions beyond conventional electronic carriers.

Work supported by the German Research Foundation via Project No. 277146847-CRC1238 (Subprojects A02 and B01).

[1] O. Breunig et al., Nat. Comm. 8, 15545 (2017).
[2] R. Sharma et al., Phys. Rev. B 109, 104304 (2024).

TT 61.3 Wed 15:00 P4

Synthesis and characterisation of Yb-doped $TlBiSe_2$ delafossite — •Manuel Schulze[1], Isadora Neme[2], Jörg Sichelschmidt[2], Helge Rosner[2], Michael Baenitz[2], and Thomas Doert[1] — [1]Faculty of Chemistry and Food Chemistry, TUD Dresden University of Technology, 01062 Dresden — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden

$TlBiSe_2$ is a three-dimensional (3D) topological insulator with a unique single Dirac cone at the Brillouin-zone centre [1]. $TlYbSe_2$ represents a prototype 2D triangular-lattice quantum spin liquid candidate [2]. Combining the two materials through partial substitution of Bi and Yb provides an interesting platform to investigate the interplay between unconventional electronic and magnetic properties. Polycrystalline samples of the solid-solution series $Tl(Bi,Yb)Se_2$ were synthesised by melting the elements in a rotary setup to enhance homogenisation. Powder X-ray diffraction and Rietveld refinement reveal systematic shifts in the lattice parameters, confirming continuous substitution. First Electron Spin Resonance (ESR) measurements on $Tl(Bi_{0.95}Yb_{0.05})Se_2$ show metallic Yb^{3+} lines with hyperfine structure as expected for a magnetically diluted system. Future work will additionally focus on NMR spectroscopy together with magnetisation and specific-heat studies to analyze the evolution of magnetic and electronic correlations across the series.

[1] K. Kuroda et al., Phys. Rev. Lett. 105, 146801 (2010).
[2] T. Fujii et al., Phys. Rev. B 112, 024426 (2025).

TT 61.4 Wed 15:00 P4

Berry curvature induced giant anomalous and spin texture driven Hall responses in the layered Kagome antiferromagnet $GdTi_3Bi_4$ — •Shobha Singh[1], Shivam Rathod[1], Rong Chen[2], Lipika Lipika[1], Sneh Sneh[1], Rie. Y Umetsu[3,4], Yan Sun[2], and Kaustuv Manna[1] — [1]Department of Physics, Indian Institute of Technology Delhi, New Delhi 110016, India — [2]Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences 72 Wenhua Road, Shenyang 110016, China. — [3]Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan — [4]Center for Science and Innovation in Spintronics, Tohoku University, Sendai 980-8577, Japan

Here, we present the single-crystal growth, magnetization, and electrical transport characterizations of the van der Waals-like layered antiferromagnet $GdTi_3Bi_4$.The system exhibits pronounced field-induced first-order phase transitions. Comprehensive frequency, temperature, and field-dependent ac susceptibility measurements, and Hall analysis, reveal the formation of a spin-cluster-like glassy magnetic phase attributed to noncoplanar spin textures. Additionally, the system demonstrates a colossal anomalous Hall conductivity (σ_{xy} = 8652 $\Omega^{-1}cm^{-1}$ at 2 K). Detailed scaling analyses reveal the coexistence of skew scattering and intrinsic Berry-curvature contributions to the anomalous Hall effect. First-principles calculations highlight a flat band near the Fermi level, with f-electrons of the Gd ion contributing a large intrinsic Hall response.

TT 61.5 Wed 15:00 P4

Temperature and pressure dependant structural studies of $PtBi_2$ — •Esteban Aguirre García[1], Swarnamayee Mishra[1,2], and Jochen Geck[1,2] — [1]Institute of Solid State and Materials Physics, Technical University Dresden, 01062 Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Technical University Dresden, 01062 Dresden, Germany

Trigonal $PtBi_2$ is a non-centrosymmetric Weyl semimetal (space group P31m) in which strong spin-orbit coupling and broken inversion symmetry lift the degeneracy of linearly dispersing bands, providing a natural setting for topological superconductivity. While bulk $PtBi_2$ becomes superconducting only at very low temperatures of about 0.6 K, an enhanced and robust surface superconducting state with a critical temperature of 5 K or higher has been shown to emerge from the Fermi arc surface states, accompanied by a sizeable superconducting gap. In this work, high resolution single crystal X-Ray diffraction is employed as a function of temperature and pressure, which allows us to correlate structural features of the trigonal phase with the presence of surface superconductivity and to identify possible symmetry based mechanisms that can support topological pairing.

TT 61.6 Wed 15:00 P4

Nonlinear Hall effect in magnetic B_2O compounds — •Maximilian Phielepeit[1], Ivan Volkau[1], Yannis Ullrich[1,4], Marc A. Wilde[1,3], Andreas Bauer[1,3], Andreas Schnyder[4], and Christian Pfleiderer[1,2,3] — [1]Technical University of Munich (TUM) — [2]MCQST, Munich — [3]TUM Zentrum für Quantum Engineering — [4]Max Planck Institute for Solid State Research

A novel theoretical framework decomposes second-order nonlinear Hall conductivity into four quantum geometric contributions: the nonlinear Drude weight (NLD), the Berry curvature dipole (BCD), the interband quantum metric dipole (interQMD) and the intraband quantum metric dipole (intraQMD)

[1]. In systems with C_3^z-symmetry, the BCD and interQMD terms are forbidden, which allows for the selective isolation of the NLD and intraQMD contributions [1]. We seek to investigate these contributions in magnetic B_2O systems, which host a C_3^z-rotational axis along the [111] crystallographic direction [2]. In this work, we perform nonlinear Hall measurements with two different magnetic field directions.

[1] Ulrich et al., arXiv:2506.17386 (2025)
[2] Hall et al., Phys. Rev. B 104 (2021)

TT 61.7 Wed 15:00 P4

Magnetic Properties of Single Crystal $MnNb_2O_6$ — •Florian Kübelbäck[1], Leo Maximov[1], Andreas Bauer[1], and Christian Pfleiderer[1,2,3] — [1]School of Natural Sciences, Technical University of Munich, Garching, Germany — [2]Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Technical University of Munich, Garching, Germany

$CoNb_2O_6$, with effective $S = \frac{1}{2}$ Ising chains, is a benchmark system for quasi-one-dimensional magnetism and field-induced quantum phenomena [1]. Its isostructural analogue columbite $MnNb_2O_6$ contains $S = \frac{5}{2}$ Mn^{2+} ions arranged in zig-zag chains and is expected to realise a more classical regime of low-dimensional magnetism [2, 3].

We have grown high-quality $MnNb_2O_6$ single crystals using the optical floating-zone technique. Magnetization measurements reproduce the antiferromagnetic transition at $T_N \approx 4.4$ K and reveal anisotropy with the c-axis acting as the hard direction, consistent with the recently refined phase diagram [4]. Field sweeps for $H \parallel c$ show a spin-flop transition near 1.8 T.

These results establish $MnNb_2O_6$ as a clean, anisotropic antiferromagnet and a promising classical counterpart to the quantum $S = \frac{1}{2}$ chain material $CoNb_2O_6$.

[1] R. Coldea et al., Science 327, 5962 (2010)
[2] L. M. Holmes et al., Solid State Communications 11, 409 (1972)
[3] O. V. Ni elsen et al., J. Phys. C 9 (1979)
[4] R. Maruthi et al., J. Phys.: Condens. Matter 33, 345801 (2021)

TT 61.8 Wed 15:00 P4

Dirac Quantum Hall States on (Reciprocal) Curved Surfaces — •Maximilian Fürst — University of Regensburg, Regensburg, Germany

Three-dimensional topological insulator nanowires in an axial magnetic field B host peculiar Dirac-type quantum Hall surface states. Spatial variations in the wires' cross sections allow for shaping curved surfaces and hence for highlighting imprints of geometry and curvature, and their interplay, in the corresponding quantum Hall spectra [1, 2]. We discuss the peculiar spectral and magnetic properties of these systems. We show that these are composed of two classes, one asymptotically insensitive to the surface shape, scaling with B-field like regular quantum Hall states in the plane, and the other with an asymptotic B-field dependence intimately related to the wire geometry. Moreover, we demonstrate that a curved nanowire surface possesses a reciprocal partner nanowire surface such that the respective quantum Hall spectra are dual to each other upon exchanging angular momentum and magnetic flux. Notably, a cone-shaped nanowire, and the Corbino quantum Hall geometry as a limiting case, has a reciprocal partner wire with a dual quantum Hall spectrum that is B-field independent, with corresponding non-magnetic quantum Hall-type eigenstates. We support our analytical findings by numerical results for B-field ranges and wire geometries within reach of current experiment [3].

[1] R. Kozlovsky et al., Phys. Rev. Lett. 124, 126804 (2020)
[2] M. Fürst et al., Phys. Rev. B 109, 195433 (2024)
[3] I. Dusa et al., arXiv:2503.17166 (2025)

TT 61.9 Wed 15:00 P4

Andreev reflection and interferometry of fractional quantum Hall edge states — •Tom Menei, Maxime Jamotte, and Thomas L. Schmidt — Department of Physics and Materials Science, University of Luxembourg, Luxembourg

Recent experimental work has demonstrated the possibility of coupling superconductors (SCs) to quantum Hall (QH) systems at both integer and fractional filling factors. However, the theoretical modelling of such QH/SC interfaces remains challenging due to the strong magnetic fields required and the presence of disorder. In this work, we develop a theoretical framework based on fractional QH edge state theory and incorporate realistic models of the superconductor to derive the effective coupling mechanisms at the interface. We analyse the resulting normal and Andreev reflection processes, as well as correlations probed through interference between multiple edge states across the QH/SC interface, and discuss their signatures in transport experiments.

TT 61.10 Wed 15:00 P4

Topologically nontrivial phase induced by disorder in a one-dimensional system — •Lars Emmrich and Michael Potthoff — Department of Physics, University of Hamburg, Germany

The Su-Schrieffer-Heger model with additional local, uncorrelated, binary-alloy site disorder of strength W is a prototypical model for studying the phase diagrams of disordered topological band insulators. With the topological-Hamiltonian approach and with the twisted-boundary-conditions approach, we employ two complementary techniques to compute the winding number ν, a topological invariant. Starting from the topologically nontrivial phase with $\nu = 1$ in the clean limit ($W = 0$), we find that, as W increases, the system undergoes a transition to a trivial phase with $\nu = 0$, followed by a second transition to a nontrivial phase with $\nu = 1$. Importantly, the latter phase cannot be connected continuously to the clean limit and thus represents a novel, disorder-induced phase, because the nontrivial topology is carried by the zeros of the single-electron Green's function.

TT 61.11 Wed 15:00 P4

Topological phases in the bosonic Haldane-Hubbard model — •Hannah Carolina Dürschmidt, Ajesh Kumar, and Achim Rosch — Institute for Theoretical Physics, University of Cologne, Zülpicher Straße 77, 50937, Köln, Deutschland

We study the interacting bosonic Haldane–Hubbard model at half filling, using a self-consistent parton mean-field approach. Within this framework, we map out the phase diagram and identify superfluid, Mott-insulating, and topological phases. The primary focus is on the effects of long-range interactions, which can cause spontaneous breaking of lattice translation symmetry. In addition to Mott insultaing states, we investigate topological phases with a finite Hall conductivity.

TT 61.12 Wed 15:00 P4

Lattice defects in topological phases of matter — •Alexander Gavrishev[1,2], Alexander Wong[2], Henry Davenport[2], Andres Perez Fadon[2], and Frank Schindler[2] — [1]Max Planck Institute for the Physics of Complex Systems — [2]Imperial College London

The defect response of topological materials offers a potential starting point for experimental probes of topology; while many comprehensive results exist for simple lattice defects in non-interacting topological matter, an analogue for interacting topological phases is missing. As a first step in this direction, we present exact diagonalisation results for lattice dislocations in a fractional Chern insulator.

TT 61.13 Wed 15:00 P4

The influence of fluctuations on the microwave response of multiterminal topological Josephson junctions — •Gleb Seleznev and Wolfgang Belzig — Universität Konstanz, 78457 Konstanz, Germany

In recent years, it has been demonstrated that multiterminal Josephson junctions (MTJJs) can realize topological states of matter in synthetic dimensions defined by the superconducting phases. In this setting, topology is hosted by Weyl singularities in the spectrum of Andreev bound states (ABS) and is characterized by a nontrivial Chern number, which manifests itself in a quantized transconductance between two superconducting leads. Moreover, the Chern number leaves signatures in the dissipative part of the microwave response function, and can therefore be directly extracted using microwave spectroscopy.

In realistic experimental conditions, however, various types of fluctuations may obscure the observation of these topological properties. In this work, we investigate the role of thermal fluctuations and finite broadening of the ABS, which have a dominant effect in the large-gap limit, on the microwave response of MTJJs. We focus especially on the vicinity of the Weyl points, where the system is most sensitive to external perturbations. As a result, we demonstrate that the redefined Chern number is reduced, while other topological signatures become smeared by fluctuations.

TT 61.14 Wed 15:00 P4

Further Evidence of a Tomonaga-Luttinger Liquid in the Au/Ge(001) Surface Reconstruction — Nico Kubetschek, •Ulrike Kürpick, Johann Tonhäuser, Till-Jakob Stehling, Marcel Schlesag, and René Matzdorf — University of Kassel, Institute of Physics, Heinrich-Plett-Str. 40, Kassel D-34132, Germany

We investigated the Au/Ge(001) surface reconstruction using scanning tunneling microscopy (STM) and spectroscopy at 77 K and 5 K. Local density of states maps reveal quasi-one-dimensional channels, which are oriented almost perpendicular to the Au-induced nanowires visible in STM topographic images. Spectroscopic analysis shows a characteristic power-law dependence, indicative of Tomonaga-Luttinger liquid behavior [1,2]. An increased power-law exponent is measured when these channels are interrupted by embedded Co-Au-induced nanorods [3]. The results are consistent with the existence of a Tomonaga-Luttinger liquid in a deeper layer of the Au-induced surface reconstruction.

[1] S.-I. Tomonaga, Prog. Theoret. Phys. 5, 544 (1950);
[2] J. Luttinger, J. Math. Phys. 4, 1154(1963).
[3] M. Schlesag et al., Phys. Rev. B 110, 195412 (2024).

TT 62: Correlated Electrons – Poster II

Time: Wednesday 15:00–17:00 Location: P4

TT 62.1 Wed 15:00 P4

Interplay of electronic and magnetic properties of single crystal Nd — •Markus Brauner[1], Ivan Volkau[1], Lukas Bauer[1], Andreas Bauer[1,3], Christian Pfleiderer[1,2,3], and Marc A. Wilde[1,3] — [1]Technical University of Munich (TUM) — [2]MCQST, Munich — [3]TUM Zentrum für QuantumEngineering

The rare earth Neodymium hosts a wide range of multi-Q magnetic phases at temperatures below 20K and fields up to 4T [1]. Recently, Neodymium was found to exhibit a previously unknown spin glass behavior in bulk-like thick films [2]. We study the interplay of magnetism and the electronic structure of bulk single crystal samples grown with the Czochralski method and map the magnetic phase diagram of Nd using vibrating sample magnetometry. First results of Fermi surface study using Shubnikov-de Haas measurements and Density Functional Theory calculations will be presented.

[1] S W Zochowski et al., J. Phys.: Condens. Matter 3, 8079 (1991)
[2] U. Kamber et al. Science 368, eaay6757 (2020).

TT 62.2 Wed 15:00 P4

Magnetic polarons in antiferromagnetic $EuCd_2P_2$ with systematic impurities — •Dominik Hoff, Julian Beu, Sarah Krebber, Kristin Kliemt, Cornelius Krellner, and Jens Müller — Goethe-University Frankfurt, Germany

Strong interactions between charge carriers and magnetism can give important insights on the physics of correlated electron systems. The colossal magnetoresistance (CMR) is one such effect, that is promising for applications. We are investigating $EuCd_2P_2$, which shows a strong CMR-effect above its antiferromagnetic transition [1]. In previous works, it was possible to link the CMR-effect to the existence and percolation of magnetic polarons resulting in a strong increase in low-frequency resistance fluctuations at the CMR-peak caused by the onset of polaron percolation. It was also found that the CMR-effect of $EuCd_2P_2$ is strongly sensitive to the sample's growth conditions [2]. To further examine these dependencies, we investigate systematic structural differences in the form of chemical substitutions. In this work we aim to investigate behavioural changes of magnetic polarons due to the substitution of Silicon in the growth process of $EuCd_2P_2$. We analyze the Hall effect, higher-harmonic resistance and resistance fluctuations as a function of temperature and magnetic field aiming to systematically determine the impact of structural impurities on polaron dynamics.

[1] Phys. Rev. B 109 (2024) 104421
[2] arXiv2503.24059

TT 62.3 Wed 15:00 P4

Noise spectroscopy on $EuZn_2P_2$ and $Sm_{1-x}Eu_xB_6$ — •Kristijan Verusheski[1], Julian Beu[1], Sarah Krebber[1], Kristin Kliemt[1], Cornelius Krellner[1], Steffen Wirth[2], Priscila Rosa[3], and Jens Müller[1] — [1]Physikalisches Institut, Goethe Universität Frankfurt, Germany — [2]Max Planck Institute for Chemical Physics of Solids Dresden, Germany — [3]Los Alamos National Laboratory, Los Alamos, NM 87545, USA

The colossal magnetoresistance (CMR) effect is of great interest because it emerges in correlated electron systems, e.g. in Eu-based antiferromagnets such as $EuZn_2P_2$ and $EuCd_2P_2$. For these materials a set of dynamical measurements revealed that the CMR effect is most likely driven by formation and percolation of magnetic polarons [1,2,3]. While both systems exhibit a pronounced CMR effect, they differ considerably in their carrier density and resistivity behaviour, resulting in markedly different transport properties. In this work, $EuZn_2P_2$ is examined in detail where we aim to investigate how magnetic polarons form, evolve and dissolve through non-linear transport and resistance fluctuation spectroscopy measurements. Similary, magnetic polarons can be studied in $Sm_{1-x}Eu_xB_6$. The antiferromagnetic composition $Sm_{0.1}Eu_{0.9}B_6$ shows a pronounced hysteresis in the MR curve [4], which likely indicates field-induced polaron stabilization.

[1] Rev. B 108, 045116 (2023)
[2] Phys. Rev. B 109, 104421 (2024)
[3] arXiv:2503.24059
[4] Condens. Matter 9, 55 (2024).

TT 62.4 Wed 15:00 P4

Growth and Structural Characterization of $NdCo_2P_2$ Single Crystals for Site-Resolved Magnetic Studies — •Francesca Martino[1,2], Benjamin Helmer[1], Kristin Kliemt[1], Kurt Kummer[2], and Cornelius Krellner[1] — [1]Physikalisches Institut, Goethe-Universität Frankfurt, Frankfurt am Main, Germany — [2]European Synchrotron Radiation Facility (ESRF), Grenoble, France

Rare-earth intermetallics with both 3d transition-metal and 4f rare-earth magnetic moments exhibit rich and often unexpected magnetic phenomena. Indeed, different intriguing properties have been found in the $LnCo_2P_2$ family [1][2]. As a first step towards exploring these interactions in $NdCo_2P_2$, high-quality single crystals have been successfully grown. In this study, we present an optimized growth procedure, confirmed by structural characterization via X-ray diffraction (XRD) and energy-dispersive X-ray spectroscopy (EDX), which demonstrates a well-ordered $ThCr_2Si_2$-type structure with high phase purity. Thermodynamic and transport measurements have also been performed to further assess the properties of the samples. These well-prepared single crystals provide a solid foundation for forthcoming site-specific X-ray magnetic spectroscopy studies, aiming to disentangle the contributions of the Nd and Co sublattices and to explore the complex magnetic behavior inherent to the $LnCo_2P_2$ series.

[1] G. Poelchen et al., ACS Nano 16, 3573(2022).
[2] C. Thompson et al., J. Mater. Chem. C2 (2014).

TT 62.5 Wed 15:00 P4

Locally non Centrosymmetric RRh_2Ga_2 (R=Ce, La) Systems: NMR/NQR as local probe for Magnetism and Superconductivity — •I. Neme[1], A. M. Strydom[2], D. T. Adroja[3], V. K. Anand[3,4], H. Rosner[1], and M. Baenitz[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Physics Department, University of Johannesburg, South Africa — [3]ISIS Facility, Rutherford Appleton Laboratory, Chilton, UK — [4]Department of Physics, National Institute of Technology Agartala, Tripura, India

$CeRh_2Ga_2$ belongs to the class of locally non-centrosymmetric (LNC) correlated Ce Kondo systems [1] and is closely related to the recently discovered superconductor $CeRh_2As_2$ [2]. The non-magnetic reference $LaRh_2Ga_2$ is superconducting with relatively high T_c of 3.7 K, in contrast with 0.28 K for $LaRh_2As_2$. We have performed ^{69,71}Ga, ^{139}La NMR and ^{69,71}Ga NQR studies to probe the magnetism and the superconductivity. For characterization, we present magnetization and heat capacity measurements. Calculations of the band structure and the local electric field gradient at the Ga and La sites support our experimental results. We discuss the magnetic ground state of the Ce system and the occurrence of superconductivity in the La reference on basis of correlations and LNC properties.

[1] V. K. Anand et al., J. Phys. Cond. Matt. 29 (2017)
[2] S. Khim et al., Science 373 (2021)

TT 62.6 Wed 15:00 P4

Exploring the reciprocal space of $CeRh_2As_2$ at a high brilliance SwissFEL beamline — •Alexander Mistonov[1], Jakub Vonka[2], Alexander Steppke[2], Swarnamayee Mishra[1], Maël Clémence[2], Adrian Rutschmann[2], Karina Kazarian[2], Wenxiang Hu[2], Bill Pedrini[2], Simon Gerber[2], Elena Hassinger[3], Seunghyun Khim[4], and Jochen Geck[1] — [1]TU Dresden, Dresden, Germany — [2]PSI, Villigen, Switzerland — [3]KIT, Karlsruhe, Germany — [4]MPI CPfS, Dresden, Germany

$CeRh_2As_2$ hosts two superconducting (SC) phases tuned by magnetic field [1] and undergoes an additional transition at $T_0 = 0.55$ K (with $T_c = 0.35$ K) [2]. The nearly non-magnetic and strongly anisotropic nature of the T_0 phase suggests an itinerant quadrupolar order of the Ce moments [3]. Since Ce-4f electrons couple to the lattice, a lowering of the tetragonal symmetry at T_0 is anticipated.

To test this, we performed single-crystal X-ray diffraction in non-resonant mode and at the Ce L_3 edge to search for symmetry reduction and signatures of multipolar order. We examined a possible splitting of the high-q (552) Bragg reflections and conducted energy-dependent rocking-curve scans near the (π, π, 0) point.

These subtle effects were probed at ultralow temperatures using a high-brilliance SwissFEL beamline combined with a dilution refrigerator. The results are presented in this work.

[1] S. Khim et al., Science 373, 1012 (2021).
[2] K. Semeniuk et al., Phys. Rev. B 107, L220504 (2023).
[3] D. Hafner et al., Phys. Rev. X 12, 011023 (2022).

TT 62.7 Wed 15:00 P4

Pressure evolution of magnetic and electronic states in $CeAgSb_2$ — •Riley Mann, Oliver Busby, Christian de Podesta, Oliver Squires, and Malte Grosche — Cavendish Laboratory, University of Cambridge, Cambridge CB3 0US, United Kingdom

$CeAgSb_2$ is a Kondo lattice material which hosts a weak ferromagnetic ground state at ambient pressure. Through the application of pressure, ferromagnetism can be suppressed, suggesting a quantum critical point at a critical pressure $p_c \sim 34$kbar. Previous measurements have shown the emergence of new phases near this quantum critical region, two of which have been interpreted as antiferromagnetic, whereas the nature of the third phase remains unclear. Our quantum oscillation measurements at ambient pressure indicate strong quasiparticle mass enhancement, with effective masses up to 34 m_e.

We present preliminary high-pressure measurements in the vicinity of the quantum critical region and extending up to about 70 kbar. Resistivity, magnetic susceptibility, and radio-frequency tunnel diode oscillator measurements were performed in high pressure anvil cells to track phase transition signatures,

clarify the structure of the high pressure phase diagram, and investigate non-Fermi liquid signatures in transport properties. Measurements at T<1K near p_c give insight into the order of the ferromagnetic transition near the critical point and into the nature of the unknown phase.

TT 62.8 Wed 15:00 P4

Electron-phonon coupling for impurity models with flat bands in the bath — •Max Fischer[1], Emin Moghadas[2], Niklas Witt[1], Alessandro Toschi[2], and Giorgio Sangiovanni[1] — [1]Institut für Theoretische Physik und Astrophysik and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany — [2]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria

In Anderson impurity models the hybridization is typically assumed to be constant close to the Fermi level. Extensions including local vibrations coupled to the impurity site have been extensively studied. In this respect, the impact of Holstein phonons on the Kondo effect is particularly interesting, due to the subtle interplay between the exchange coupling and the phonon dynamics. Retardation effects can become particularly relevant since in addition to the bare phonon frequency and the bare kinetic energy, the correlation-induced renormalized bandwidth enters into the game. We add yet another knob, which is the flatness of the fermionic bath and study with analytical, quantum Monte Carlo and renormalization group approaches the effect of a singularity in the hybridization function, following our previous study without phonons [1].

[1] M. Fischer, A.Poli, L. Crippa, D. Călugăru, S. Ciuchi, M. Vojta, A. Toschi, and G. Sangiovanni, arXiv:2503.14326 (2025).

TT 62.9 Wed 15:00 P4

The Fate of Kondo Correlations in Superconducting Magnetic Impurities beyond Mean Field — •Kilian Münz[1], Björn Kubala[1,2], Christian Ast[3], Joachim Ankerhold[1], and Ciprian Padurariu[1] — [1]Institute for Complex Quantum Systems and IQST, Ulm University, Ulm, Germany — [2]German Aerospace Center (DLR), Institute for Quantum Technologies, Ulm, Germany — [3]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

The interplay between strong electronic correlations (Kondo effect) and superconductivity is of fundamental interest in mesoscopic physics. We investigate the superconducting single-impurity Anderson model (SIAM) with Numerical Renormalization Group methods using the NRG Ljubljana code [1]. Calculations confirm the expected emergence of Yu-Shiba-Rusinov (YSR) states within the superconducting gap.

Simulations also yield the tails of the renormalized Kondo density of states extending above the gap. We demonstrate that these above-gap features translate directly into additional contributions in the tunneling current measured by scanning tunneling microscopy. Crucially, these Kondo-rooted spectral signatures exhibit a discontinuous change across the quantum phase transition of the superconducting SIAM. These NRG predictions show excellent qualitative agreement with recent experimental results from MPI-FKF Stuttgart.

[1] Žitko, Rok: NRG Ljubljana. DOI: 10.5281/ZENODO.4841076.

TT 62.10 Wed 15:00 P4

Using $1/N$ graph expansions to explore the mesoscopic regime of strongly correlated systems — •Andreas Schellenberger[1], Lidia Stocker[2], and Kai Phillip Schmidt[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Max Planck Institute for the Physics of Complex Systems, Dresden

Finite-size effects in strongly correlated systems can generate nontrivial low-energy behavior in the mesoscopic regime, yet this regime is difficult to access with standard many-body techniques [1–3]. We present a novel graph-expansion method to systematically explore strongly correlated systems with one-to-all couplings. This approach enables controlled exploration of the corrections to the thermodynamic limit in terms of a $1/N$ expansion for light-matter systems or systems with collective bath modes.

We apply our approach to the open Kondo box model at zero temperature [4], where an Anderson impurity is coupled to a bath with finite level spacing. By computing energies, correlation functions, and entanglement measures, we investigate how the Kondo effect emerges as a function of the systems parameters, benchmarking our results against exact diagonalization and DMRG.

[1] K. Lenk, J. Li, P. Werner, M. Eckstein, arXiv:2205.05559 (2022)
[2] A. Kudlis, D. Novokreschenov, I. Iorsh, I. Tokatly, arXiv:2304.00805 (2023)
[3] P. Simon, I. Affleck, PRL 89.206602 (2002)
[4] C. Rössler et al., PRL 155.166603 (2015)

TT 62.11 Wed 15:00 P4

Low-dimensional critical behavior of correlated electrons, Mermin-Wagner theorem, and local self-energy — •Šimon Kos[1], Sunil D'Souza[1], Jan Gebel[1], Ján Minár[1], and Václav Janiš[2] — [1]University of West Bohemia, Univerzitní 8, CZ-301 00 Plzeň, Czech Republic — [2]Institute of Physics, The Czech Academy of Sciences, Na Slovance 2, CZ-182 00 Praha 8, Czech Republic

We present a theoretical treatment of low-dimensional critical behavior coming from electron correlations. The treatment is based on the Baym-Kadanoff approach, which involves one-particle self-consistency between the propagator and the self-energy, along with the bare two-particle interaction. In low dimensions, self-consistency prevents ordering in agreement with the Mermin-Wagner theorem and exhibits critical behavior as the temperature is lowered towards zero. The critical behavior enables the use of the polar approximation, which reduces the convolutive Schwinger-Dyson equation to an algebraic equation for the local propagator and self-energy, amenable to solution. We demonstrate the treatment using the example of a 1d Hubbard model with an attractive interaction, which describes the tendency toward superconductivity, in the FLEX approximation. We present various features of the algebraic Schwinger-Dyson equation and the quantities that enter it.

TT 62.12 Wed 15:00 P4

Emergent relativity and topology of interacting quadratic fermions — •Lukas Berger and Thomas C. Lang — Institute for Theoretical Physics, University of Innsbruck, Austria

We investigate the lattice realization of perfect quadratic band touching of fermions augmented by local Coulomb interactions via quantum Monte Carlo simulations. We show that due to the C_4 rotational symmetry of the lattice, interactions trigger an instability towards quantum anomalous Hall order. In contrast, once the rotational symmetry of the lattice is reduced to C_2, infinitesimally small interactions dynamically induce a topological transition from quadratic band touching to multiple Dirac cones before undergoing a Gross-Neveu transition where lattice symmetry is spontaneously broken via charge order. We directly monitor the separation of the Berry flux and the simultaneous emergence of Dirac-like excitation spectra.

TT 63: Quantum Dynamics and Many-body Systems – Poster (joint session DY/TT)

Time: Wednesday 15:00–18:00 Location: P5

TT 63.1 Wed 15:00 P5

Operator spreading through the lens of the information lattice — •Luca Gawalleck[1,2], Maxime Debertolis[1], Jens H. Bardarson[3], and David J. Luitz[1] — [1]Institut of Physics, University of Bonn, Nußallee 12, 53115 Bonn, Germany — [2]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — [3]Department of Physics, KTH Royal Insititute of Technology, Stockholm, 106 91 Sweden

We study the entanglement growth during Heisenberg time evolution by extending the framework of the information lattice to operators using the operator entanglement entropy. We focus on one-dimensional quantum spin chains and work in the tensor network formalism. The generalization of the information lattice to matrix product operators allows us to observe the spreading of initially local operators in a way that is not biased by the choice of a probing operator. We demonstrate that the operator information lattice we introduce contains all information typically provided by the out-of-time-order correlator with the additional ability to resolve the correlations on different scales. This method provides a good way to analyze systematically the time dependence of entanglement and can seamlessly be integrated into existing information-lattice-based algorithms.

TT 63.2 Wed 15:00 P5

Non-Perturbative Out-Of-Equilibrium Dynamics with Initial Four-Point-Correlations — Jürgen Berges, Louis Jussios, and •Cosima Schmitt — ITP Heidelberg

We investigate how initial correlations affect the equilibration dynamics of closed systems in quantum field theory. For interacting scalar fields with N components, we derive nonequilibrium evolution equations from a self-consistent large-N expansion to next-to-leading-order. By going beyond conventional Gaussian initial conditions, we point out the role of initial four-point correlations for the propagator evolution at early times and in the late-time approach to thermal equilibrium.

TT 63.3 Wed 15:00 P5

Nonequilibrium Green Function Simulations for Large Systems — •Erik Schroedter, Jan-Philip Joost, and Michael Bonitz — Christian-Albrechts-Universität zu Kiel, Kiel, Germany

Nonequilibrium Green Functions (NEGF) provide a powerful framework for accurately simulating the dynamics of correlated many-body systems. A major limitation of standard NEGF approaches is the cubic scaling of computational

cost with the number of time steps. Recently, the G1-G2 scheme [1] overcame this limitation, achieving linear scaling. However, it introduces its own challenges, such as numerical instabilities at strong coupling and large memory requirements, which have so far restricted simulations to small systems with fewer than 150 basis states. Here, we introduce a NEGF-based quantum fluctuations approach (NEGF-QF)[2] that builds on earlier works [3] to efficiently factorize the two-particle Green function. This method drastically reduces computational costs for advanced self-energy approximations, including GW and T-matrix, while enabling straightforward parallelization. As a result, NEGF-QF allows simulations of systems with up to ten thousand basis states. We demonstrate the approach for large Hubbard clusters and graphene nanoribbons, illustrating its effectiveness for large, strongly correlated systems.

This work was funded by the Deutsche Forschungsgemeinschaft (DFG), Project No. 464370560.

[1] Schlünzen et al., Phys. Rev. Lett. 124, 076601 (2020)
[2] Schroedter et al., to be published (2026)
[3] Schroedter et al., Cond. Matt. Phys. 25, 23401 (2022)

TT 63.4 Wed 15:00 P5

Quantum Chaos in a Classical Counterpart to the Fermi-Hubbard model through an exact Path-Integral Formalism — •Louis Renck[1], Wolfgang Hogger[2], Juan Diego Urbina[2], and Peter Schlagheck[1] — [1]IPNAS, CESAM research unit, Université de Liège, Belgium — [2]Institut für Theoretische Physik, Universität Regensburg, Germany

Understanding quantum chaos in interacting many-fermion systems remains challenging : unlike many-bosons systems - where quantum-classical correspondence can be established using semiclassical tools such as the van Vleck-Gutzwiller propagator [1] -, most interacting fermions models still lack a sensible classical limit where Hamiltonian chaos can be defined.

We propose a candidate to the first classical Hamiltonian for the Fermi-Hubbard model with integrability broken by a random onsite potential. Starting from the fermionic Hamiltonian, we apply a Jordan-Wigner transformation and switch to the Schwinger-boson representation to obtain a bosonic form. A recently developed exact bosonic path-integral formalism [2] then provides a classical Hamiltonian symbol defined over a symplectic phase space. We investigate the resulting quantum-classical correspondence by comparing the effective dynamics with the quantum evolution, and we present quantitative checks of chaos based on spectral properties and out-of-time ordered correlators.

[1]. T. Engl, J. Dujardin, A. Argüelles, P. Schlagheck, K. Richter, and J. D. Urbina, Phys. Rev. Lett. 112, 140403 (2014).
[2]. F. Bruckmann and J. D. Urbina (2018)

TT 63.5 Wed 15:00 P5

Adaptive Fermion Circuits with chiral transport — •Markus Siegl and Michael Buchhold — Department of Theoretical Physics, Universität Innsbruck, Austria

Nonequilibrium quantum transport, where coherent many-body dynamics coexist with directional motion remains a central challenge in modern quantum physics. This project investigates transport phenomena in two coupled fermionic chains designed to break chiral symmetry. Using fermionic adaptive circuits and measure-ment-feedback protocols, we aim to control nonequilibrium dynamics and induce directional motion in an other-wise symmetric quantum system. By linking classical universality, quantum many-body effects, and information transport, the research seeks to uncover new mechanisms for controlled, symmetry-broken quantum transport, establishing a model system for genuinely nonequilibrium quantum matter.

TT 63.6 Wed 15:00 P5

Absorbing-State Dynamics and Feedback Control in Quantum Many-Body Scar Systems — •Lara Schorr — University of Innsbruck

We look at quantum many-body scar states, which are special excited states in non-integrable systems that do not thermalize. To better understand their non-equilibrium dynamics, we translate the problem to a measurement-based quantum circuit equipped with feedback control. Focusing on a spin-1/2 chain with SU(2) symmetry, we show that local unitary feedback enables controlled manipulation of non-local charges, allowing the system to relax into highly entangled dark states. By analyzing the convergence towards the target state, we find that the dynamics resembles an emergent absorbing-state process, in which non-local charges diffuse and annihilate over time. Studying the scaling of convergence times allows us to identify conditions under which the dynamics may exhibit an absorbing-state phase transition.

TT 63.7 Wed 15:00 P5

Floquet-Magnus expansion for driven quantum systems and spin dynamic mean-field theory in NMR — •Antonia Joëlle Bock — TU Dortmund University, Germany

An accurate and reliable theoretical description of periodically driven quantum systems is highly relevant to many applications, such as for magic-angle spinning (MAS) in nuclear magnetic resonance (NMR) and ultracold atoms in driven optical lattices. Typically, the first step in capturing the dynamics is to determine an effective time-independent Hamiltonian, for which one can choose from a broad range of slightly different, hence often confusing, theories. Thus, I specifically investigated two widely used theories: Average Hamiltonian theory (AHT) and the Floquet-van Vleck approach (secular averaging). I was able to quantify the importance of the kick operator for the equivalence between perturbative and numerically exact approaches. This was achieved through analytical calculations and numerical evaluations of exemplary spin systems. These crucial insights then build the foundation for the second step of my project: a dynamic mean-field theory for dense spin ensembles applicable to complex couplings between three or more spins (MAS-DMFT). The recently developed spinDMFT (cp., e.g., Gräßer et al., 2024) has proven to be efficient, accurate and applicable to large spin systems yielding 2-particle interactions.

TT 63.8 Wed 15:00 P5

Phonon mediated indirect spin interaction — •Pablo Reiser and Habib Rostami — University of Bath, Bath, United Kingdom

Due to the lack of inversion symmetry in the hBN monolayer, circular polarized vibration in solids, or chiral phonons, with nonzero angular momentum are allow. These chiral phonons can couple to spins of different nature through their angular momentum. Within this context, we explored the coupling of chiral phonons with non-zero angular momentum to two impurities spins in hBN. Using field theory methods, we obtained the spin susceptibility and studied it*s properties like the mass dependence of the coupling, frequency of oscillation and rate of decay. The momentum transfer due to this coupling may opens the door for non-trivial thermal or spin transport effects.

TT 63.9 Wed 15:00 P5

Dynamical Phases and Instabilities in Periodically Driven Bogoliubov-de Gennes Superconductors — •Subhadip Chakraborty, Animesh Panda, and Ferdinand Evers — Institute of Theoretical Physics, University of Regensburg, D-93040 Regensburg, Germany

We investigate the nonequilibrium dynamics of a superconductor subjected to a periodic modulation of the interaction strength starting with Bogoliubov-de Gennes (BdG) mean field Hamiltonian. Using numerical solutions of the time-dependent Bogoliubov-de Gennes equations, we first explore several dynamical superconducting regimes. Our analysis reveals a rich variety of phases, including Rabi-Higgs oscillations, synchronized Higgs dynamics, and time-crystalline responses, and shows how their stability varies across driving parameters. In some regions of parameter space, infinitesimal initial seeds of finite momentum pairing grow exponentially during our driving protocol. By computing the momentum-resolved pairing response, we identify the instability bands associated with these finite-momentum modes, quantify their growth rates, and determine their dependence on driving frequency and drive amplitude. These results provide a comprehensive numerical characterization of the dynamical phases and instabilities that arise in periodically driven superconductors before the final steady state is reached.

TT 63.10 Wed 15:00 P5

Higher order Magnus expansion for two-level quantum dynamics — •Chen Wei and Frank Grossmann — Institut für Theoretische Physik, 01062 Dresden, Germany

This study investigates the Magnus expansion[1] for a generic time-dependent two-level system. By using its convergence condition[2], we find that elementary unitary transformations significantly extend the validity of the Magnus expansion. Furthermore, higher order terms admit particular physical interpretations. By virtue of su(2) Lie algebra, the expansion is decomposed into a commutator-free form. To illustrate its usefulness, we study the Landau-Zener[3] model, which displays a special case of non-adiabatic transitions. Using agian the Magnus expansion, Hermitian and non-Hermitian versions of the semiclassical Rabi model are systematically treated by determining the Floquet quasienergy[4] and Bloch-Siegert shift[5]. As a noteworthy by-product, the Magnus expansion provides a quantitative characterization of the adiabatic theorem[6].

[1] W. Magnus, Commun. Pure Appl. Math. 7, 649-673 (1954). [2] M. M. Maricq, J. Chem. Phys. 86, 5647-5651 (1987). [3] C. Zener and R. H. Fowler, Proc. R. Soc. Lond. A 137, 696-702 (1932). [4] J. H. Shirley, Phys. Rev. 138, B979 B987 (1965). [5] F. Bloch and A. Siegert, Phys. Rev. 57, 522-527 (1940). [6] M. Born and V. Fock, Z. Phys. 51, 165-180 (1928).

TT 63.11 Wed 15:00 P5

Distribution of complex amplitudes of chaotic resonance states — •Jan Möseritz-Schmidt and Roland Ketzmerick — TU Dresden, Institut für Theoretische Physik, Dresden, Germany

Resonance states of chaotic scattering systems have complex amplitudes in the position representation. Naively, one would expect that the phase of the complex amplitude is uniformly distributed, however, we observe significant deviations. We find that part of this is a finite-size effect which is already present in the random wave model. It is enhanced by the multifractal structure of chaotic resonance states, which follows from the factorization conjecture. We quantify these

deviations using the phase rigidity and analyze its scaling behavior in the semiclassical limit. Numerically, this is demonstrated for the paradigmatic three-disk scattering system.

TT 63.12 Wed 15:00 P5

Complex dynamics and particle-wave correspondence in anisotropic mesoscopic cavities — •Silvan Stopp, Samuel Schlötzer, Lukas Seemann, and Martina Hentschel — Technische Universität Chemnitz, 09107 Chemnitz, Germany

Mesoscopic billiard systems with different geometries are well-known model systems for investigating complex dynamics and quantum chaos. While the breaking of spatial cavity symmetries is typically considered to be the origin of chaotic dynamics, we show that anisotropies, i.e., broken symmetries in momentum space, can also cause chaotic particle dynamics. To this end, we investigate bilayer graphene systems (BLG) [1] and birefringent optical microcavities [2], both of which have preferred propagation directions. Anisotropy prevent angular momentum to be a conserved quantity, and consequently, the angles of incidence and of reflection of a particle trajectory deviate. Therefore, we implementing an advanced ray tracing algorithm that we apply to BLG and birefringent cavities. We show that the presence of anisotropies induces chaotic dynamics even in circular cavities. We investigate the interplay of the cavity shape and the Fermi line geometry and illustrate how it affects the cavity dynamics. In particular, we find that certain trajectories can be stabilized by matching the symmetry in real and momentum space. In addition, we use Kwant and transformation optics to demonstrate ray/particle-wave correspondence in real space as well as in phase space using the Husimi function.

[1] L. Seemann, A. Knothe, M. Hentschel, PRB 107, 205404 (2023)
[2] M. Hentschel, S. Schlötzer, L. Seemann, Entropy 27(2):132 (2025)

TT 63.13 Wed 15:00 P5

Periodic orbit theory approach for a non-Hermitian Riemann operator — •Sebastian Hörhold, Andreas Hötzinger, Juan Diego Urbina, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, Germany

The Riemann Hypothesis (RH) is one of the most important open problems in mathematics. Among the various approaches toward its proof is the Hilbert-Pólya (HP) conjecture, stating that there should exist a Hermitian operator whose eigenvalues t_n are given by the zeros of the Riemann zeta function $\zeta(1/2 + it_n)$. The RH would then follow from the reality of these eigenvalues.

In a recent contribution toward a proof of the RH, a non-Hermitian Hamiltonian has been introduced, referred to as a Riemann operator, whose spectrum contains the t_n, and from which one can construct an HP operator [1]. Our work focuses on a similar Hamiltonian, and we intend to make use of semiclassical tools to support earlier work by Berry and Keating, who obtained a formal asymptotic expression for the counting function of the nontrivial Riemann zeros [2]. Their results suggest a strong connection between the spectral statistics of these zeros and classically chaotic systems.

In this poster contribution, we show the emergence of the Riemann zeros within the spectrum of our non-Hermitian Hamiltonian and discuss how periodic orbit theory can be applied.

[1] E. Yakaboylu, arXiv:2408.15135
[2] M. V. Berry and J. P. Keating, SIAM Review 41.2 pp. 236-266

TT 63.14 Wed 15:00 P5

Echo state network prediction of billiard dynamics — •Anna Skopnik, Lukas Seemann, and Martina Hentschel — Institut für Physik, TU Chemnitz, Germany

Machine Learning has attracted a lot of interest recently. Here, we apply an Echo State Network (ESN) algorithm to two mesoscopic billiard systems in order to explore its usability in the prediction of the internal dynamics of ballistic cavities. First, we study the well-known Limaçon system with chaotic dynamics. Second, we study the more complex dynamics in an anisotropis system inspired by bilayer graphene (BLG) representing a mixed space dynamics with regular and chaotic trajectories. Here, we present preliminary results on the training and hyperparameter optimization for both systems, Limaçon and BLG.

TT 63.15 Wed 15:00 P5

Anomalous Dynamics in Complex Quantum Systems — •Irina Petreska[1], Pece Trajanovski[1,2], Ervin Kaminski Lenzi[3], and Trifce Sandev[1,2,4] — [1]Ss. Cyril and Methodius University in Skopje, Macedonia — [2]Macedonian Academy of Sciences and Arts, Skopje, Macedonia — [3]Universidade Estadual de Maringá, Maringá, Brazil — [4]Korea University, Seoul, Korea

We will give an overview of our recent works related to some generalizations of the Schrödinger equation. Special attention will be paid to the fractional Schrödinger equation, pointing out physical examples where the time-fractional Schrödinger equation naturally emerges under certain geometric constraints. Additionally, we include a long-range interaction term, modeled by an integral operator, which captures spatial nonlocalities. Using the Green's function approach, we derive analytical solutions and explore their implications in the time-space domain. Our findings reveal anomalous behavior arising from the interplay of fractional dynamics, nonlocal potentials and memory effects.

TT 64: BKT Physics

Time: Wednesday 16:45–18:15 Location: HSZ/0103

TT 64.1 Wed 16:45 HSZ/0103

Berezinskii-Kosterlitz-Thouless renormalization group flow at a quantum phase transition — •Matthias Thamm[1], Harini Radhakrishnan[2], Hatem Barghathi[2], Chris Herdman[3], Arpan Biswas[2], Bernd Rosenow[1], and Adrian Del Maestro[2] — [1]Leipzig University — [2]University of Tennessee, Knoxville — [3]Middlebury College, Vermont

We present a controlled numerical study of the Berezinskii-Kosterlitz-Thouless (BKT) transition in the one-dimensional Bose-Hubbard model at unit filling, providing evidence of the characteristic logarithmic finite-size scaling of the BKT transition. Employing density matrix renormalization group and quantum Monte Carlo simulations under periodic boundary conditions, together with a systematic finite-size scaling analysis of bipartite particle number fluctuations, we resolve boundary-induced complications that previously obscured critical scaling. We demonstrate that a suitably chosen central region under open boundaries reproduces universal renormalization group signatures, reconciling earlier discrepancies. Finally, leveraging a nonparametric Bayesian analysis, we determine the critical interaction strength with high precision, establishing a benchmark for BKT physics in one-dimensional quantum models.

TT 64.2 Wed 17:00 HSZ/0103

Finite-size effects in the vicinity of the BKT transition in superconducting NbN thin films — •Lea Pfaffinger[1], Alexander Weitzel[1], Sven Linzen[2], Evgenii Il'ichev[2], Ilaria Maccari[3], and Christoph Strunk[1] — [1]Department of Experimental Physics, University Regensburg, Regensburg, Germany — [2]Leibniz Institute of Photonic Technology, Jena, Germany — [3]ETH, Zurich, Switzerland

For 2D superconducting thin films, Halperin and Nelson predicted a finite resistance between the Berezinskii-Kosterlitz-Thouless temperature T_{BKT} and the mean-field critical temperature T_{c0} due to the unbinding of thermally excited vortex-antivortex pairs. Recently, we observed a sharp BKT-transition in homogeneously disordered 3nm NbN films grown by ALD, which is in very good agreement with these theoretical predictions [1]. Although the sample width was much smaller the Pearl length $\Lambda_p \approx 2mm >> w = 10\mu m$, we did not observe a size induced smearing of the transition. When further reducing the width to $w \leq 1\mu m$, we do observe a finite resistance for $T < T_{BKT}$ as expected from the cut-off of the divergence of the correlation length by the finite size. This resistance is thermally activated with an activation energy that depends logarithmically on the width. We present a systematic study of the resistance in this regime combined with an analysis based on the work of [2] and [3].

[1] A. Weitzel et al., Phys. Rev. Lett. 131, 186002 (2023).
[2] L. Benfatto et al., Phys. Rev. B 80, 214506 (2009).
[3] V.G. Kogan et al., Phys. Rev. B 83, 144526 (2011).

TT 64.3 Wed 17:15 HSZ/0103

Quasi-two-dimensional superconductivity in 1T-$Ti_{1-x}Ta_xSe_2$ — •Poulami Manna, Suhani Sharma, Tarushi Agarwal, Shashank Srivastava, Priya Mishra, and Ravi Prakash Singh — Indian Institute of Science Education and Research, Bhopal

The emergence of two-dimensional (2D) superconductivity in bulk transition metal dichalcogenides (TMDs) has sparked crucial research interest for hosting exotic quantum states. Intercalation, doping, or inserting insulating layers can significantly weaken the interlayer coupling, thereby achieving 2D behavior in bulk materials. While doped bulk crystals of TaS_2 and $NbSe_2$ show 2D superconductivity, Ti-based TMDs remain largely unexplored. Among them, non-superconducting $TiSe_2$ has been extensively studied due to its controversial electronic nature and semimetallic/semiconducting behavior.

Here, we discuss the superconducting properties of single-crystalline 1T-$Ti_{1-x}Ta_xSe_2$ for $x = 0.2$, using magnetization, resistivity, and specific heat measurements. The results reveal anisotropic bulk superconductivity with a transition temperature of 2.32(1) K. Specific heat measurements show weakly coupled, isotropic s-wave superconductivity in $Ti_{0.8}Ta_{0.2}Se_2$. Notably, the first evidence of quasi-2D superconductivity in Ti-based TMD is confirmed by angle-dependent magneto-transport measurements and observation of a BKT transition. These findings offer an opportunity to explore numerous low-dimensional quantum

phases in bulk materials and effectively broaden the new pathway for realizing 2D superconductivity.

TT 64.4 Wed 17:30 HSZ/0103

Two-dimensional multiband superconductivity in 1T-MoS_2 — •Chithra H. Sharma[1,2] and Madhu Thalakulam[2] — [1]Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]IISER Thiruvananthapuram, 695551 Thiruvananthapuram, India

van der Waals materials provide ultra-clean platforms to realise superconductivity in 2D, which is decorated by features such as Berezinskii-Kosterlitz-Thouless (BKT) phase transition and Bose metal phase owing to the vortex dynamics in the system. One interesting yet seldom-studied material is 1T-MoS_2, the metallic phase. Stable 1T-MoS_2 prepared using Ar/H_2 microwave plasma exposure shows 2D superconductivity with a critical temperature of ~920 mK. BKT phase transition, Bose metal phase and enhanced parallel critical field above the Pauli limit have been observed in the system. The low-noise differential I-V characteristics of the sample show features corresponding to multiband superconductivity.

TT 64.5 Wed 17:45 HSZ/0103

Phases of Quasi-One-Dimensional Fractional Quantum (Anomalous) Hall Superconductor Heterostructures — Steffen Bollmann[1], Andreas Haller[2], Jukka I. Väyrynen[3], •Thomas L. Schmidt[2], and Elio J. König[4,1] — [1]Max-Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]University of Luxembourg, L-1511 Luxembourg, Luxembourg — [3]Purdue University, West Lafayette, Indiana 47907, USA — [4]University of Wisconsin-Madison, Madison, Wisconsin 53706, USA

We study fractional quantum (anomalous) Hall-superconductor heterostructures in the presence of $U(1)$ order-parameter fluctuations and focus on the case of $\nu = 2/3$ quantum Hall states leading to $\mathbb{Z}_3$ parafermions. For an alternating pattern of superconductor and tunneling regions, coupled to fractional quantum Hall edge states, we use a map onto a topological Josephson junction chain involving lattice parafermions. Using DMRG simulations, we establish a phase diagram composed of Mott insulating phases and two different Luttinger liquids carrying excitations with charges $2e$ and $2e/3$. In agreement with analytical considerations using conformal field theory, we numerically find transitions of Berezinskii-Kosterlitz-Thouless (BKT) type as well as a continuous $\mathbb{Z}_3 \times U(1)$ second-order phase transition characterized by central charge $c = 9/5$. We finally extract information about a possible ground state degeneracy and comment on the stability of parafermionic edge states in the presence of order parameter fluctuations.

TT 64.6 Wed 18:00 HSZ/0103

Persistence of the Berezinskii-Kosterlitz-Thouless transition with long-range couplings — •Luis Walther[1,2], Josef Willsher[1,3,2], and Johannes Knolle[1,3,4] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany — [4]Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom

The Berezinskii–Kosterlitz–Thouless (BKT) transition is an archetypal example of a topological phase transition, which is driven by the proliferation of vortices. In this Letter, we analyze the persistence of the BKT transition in the XY model under the influence of long-range algebraically decaying interactions of the form $\sim 1/r^{2+\sigma}$. The model hosts a magnetized low temperature phase for sufficiently small σ. Crucially, in the presence of long-range interactions, spin waves renormalize the interaction between vortices, which stabilizes the BKT transition. As a result, we find that there is no direct transition from the magnetized to the disordered phase and that the BKT transition persists for arbitrary long-range exponents, which is distinct from previous results. We use both Landau–Peierls-type arguments and renormalization group calculations—including a coupling between spin wave and topological excitations—and obtain similar results. We discuss the relevance of our findings for current Rydberg atom experiments, and highlight the importance of long-range couplings for other spin models.

TT 65: 2D materials: Stacking and heterostructures – Poster (joint session O/TT)

Time: Wednesday 18:00–20:00 Location: P2

TT 65.1 Wed 18:00 P2

Unexpected Ordered Interfaces in WSe_2-$MoSe_2$ Lateral Interfaces Observed by STEM — •Matvei Kislitsyn[1], Max Bergmann[1], Julian Picker[2], Jürgen Belz[1], Robin Günkel[1], Badrosadat Ojaghi Dogahe[1], Shamail Ahmed[1], Andrey Turchanin[2], and Kerstin Volz[1] — [1]mar.quest | Marburg Center for Quantum Materials and Sustainable Technologies, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Faculty of Chemistry and Earth Sciences, Friedrich-Schiller-Universität, 07743 Jena, Germany

Two-dimensional WSe_2-$MoSe_2$ lateral heterostructures offer a platform for engineering band alignment and excitonic behavior through atomic-scale control of composition, making this material attractive for use in 2D optoelectronic devices. In this contribution, we present a systematic scanning transmission electron microscopy (STEM) study of monolayer WSe_2-$MoSe_2$ heterostructures synthesized by chemical vapor deposition (CVD) directly on SiO_2 TEM grids. While some investigated 2D flakes show atomically sharp interfaces with minimal intermixing, we also observe a highly ordered and unexpected interface configuration consisting of alternating Mo and W atomic rows. By comparing experimental observations with STEM image simulations and theoretical predictions, we analyze the structural origins of both interface types and discuss the mechanisms that may give rise to this unusual ordering. These results provide insight into interface formation mechanisms in lateral transition-metal dichalcogenide heterostructures and their potential impact on material properties.

TT 65.2 Wed 18:00 P2

Superdomains and Strain Localization in Twisted Two Dimensional Transition Metal Dichalcogenides — •Riya Patel[1], Daniel Wolf[1], Kristina Weinel[1,2], Silke Hampel[1], and Axel Lubk[1,2] — [1]IFF, IFW Dresden, 01069 Dresden — [2]Faculty of Physics, Technical University Dresden, 01069 Dresden

Bilayers of 2D transition metal dichalcogenides (TMDCs) exhibit special structural and electronic phenomena when stacked with a low-twist-angle. Particularly, they undergo lattice reconstruction, forming large triangular stacking domains, separated by domain walls that concentrate strain (soliton regime), which was shown in simulations. However, direct experimental quantification of these strain features and their correlation with electronic properties remains limited. Here we investigate low-twist-angle TMDCs using high-resolution transmission electron microscopy to visualize the reconstructed super lattice and identify the resulting superdomains structure. We employ geometric phase analysis to quantitatively map the strain distribution at the domain walls with nanometer resolution, revealing spatial maps of different strain components. We use Electron Energy Loss Spectroscopy to further probe the electronic properties of the reconstructed system. The understanding of strain localization in superdomain structures and the related electronic properties in such systems facilitate strain-engineered electronic properties in twisted TMDCs.

TT 65.3 Wed 18:00 P2

Pseudomonolayer TMDCs via organic intercalation — •Katharina Steinkirchner[1,2], Jakob Dilling[1,2], Matthias Kalläne[1,2,3], Tim Riedel[1,2], Markus Scholz[4], and Kai Rossnagel[1,2,3,4] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [4]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany

Transition metal dichalcogenides (TMDCs) are a versatile class of layered materials with tuneable electronic properties. One approach to tailoring these properties is to manipulate the material's effective dimensionality. Specifically, intercalating cationic organic molecules with different alkane carbon chain into the van der Waals gaps between the layers increases the interlayer distance of the TMDC host material. This transforms the crystal from a bulk state to a monolayer-like state, thereby altering the electronic structure [1]. Here, we present a comprehensive study of the geometric and electronic structures of intercalated and non-intercalated TMDCs, such as $NbSe_2$, using SEM, EDS, and 11eV laser-based ARPES.

[1] H. Zhang *et al.*, Nat. Phys. **18**, 1425 (2022).

TT 65.4 Wed 18:00 P2

Preparation of quasi-freestanding few-layer samples of 2D materials — •Seyedeh Helya Alaei, Hanna Shirin Pulikkal Hamza, Mashood Tariq Mir, Lukas Nöding, Ahmed Hassanien, Arne Senftleben, Jochen Mikosch, and Thomas Baumert — University of Kassel, Institute of Physics, 34132 Kassel, Germany

Two-dimensional (2D) materials have garnered significant attention in the last two decades and have been analyzed using various methods in the fields of materials science and physics. To study the dynamic behavior of 2D materials upon irradiation with femtosecond laser pulses using ultrafast electron diffraction, it is necessary to isolate few-layer structures from bulk crystals and prepare them in a quasi-freestanding manner. Due to the weak van-der-Waals forces between the layers relative to the in-plane forces of the structure, mechanical exfoliation is a commonly used method. However, the transfer is challenging, due to the thinness of the flake and the adhesive force between the flake and the surface. Our

preparation involves three major steps: (1) exfoliation using adhesive tape and viscoelastic gel, (2) isolation of 2D material nanosheets with thicknesses ranging from 3 to 50 nm, and (3) transfer onto a standard sample mesh of transmission electron microscopy with a high success rate. The transfer exploits liquid-solid phase transitions of a soluble wax-like material. In this ongoing study, the 2D ferromagnetic material Fe_5GeTe_2 has been of interest. We will discuss the different steps in detail and the challenges associated with the preparation of this material, including the fragility of the crystals due to oxidation and the partially covalent out-of-plane forces.

TT 65.5 Wed 18:00 P2

Ordering Phenomena in MoS_2 Nanocrystals on Graphite — •Lukas Nöding[1], Ahmed Hassanien[1], Mashood Tariq Mir[1], Hanna Shirin Pulikkal Hamza[1], Seyedeh Helya Alaei[1], Thomas Baumert[1], Jochen Mikosch[1], Florian Grassme[2], Claudia Backes[2], and Arne Senftleben[1] — [1]University of Kassel, Institute of Physics, Kassel, Germany — [2]University of Kassel, Institute of Chemistry, Kassel, Germany

Two-dimensional transition-metal dichalcogenides (TMDCs) such as MoS_2 offer a platform for tailoring electronic and optical properties through controlled stacking and orientation. Achieving ordered assemblies of MoS_2 nanocrystals on crystalline substrates is, therefore, of considerable interest. In this work, we study the crystallographic alignment of MoS_2 nanocrystals on a graphite substrate. The samples were prepared using the Langmuir-Schäfer technique, enabling the reproducible deposition of nanocrystals with controlled density. To probe the crystallographic alignment of the deposited nanocrystals with respect to the graphite lattice, we performed wide field static electron diffraction measurements at an acceleration voltage of 35 kV, complemented by selected area electron diffraction at 200 kV.

Our preliminary analysis reveals a pronounced localized and short-range ordered crystallographic alignment of the MoS_2 nanocrystals, extending over at least a few micrometers. A quantitative evaluation of the global ordering behavior, as well as its dependence on crystal size and deposition parameters, is currently underway and will be discussed.

TT 65.6 Wed 18:00 P2

Multiferroic Two-Dimensional Cu(CrX2)2 (X = S, Se, and Te) as Anode Materials for Lithium-Ion Batteries: A First-Principles Study — •Muhammad Fayaz[1] and Zijing Lin[2] — [1]Department of Physics, University of Science and Technology of China, Hefei 230026, China — [2]Department of Physics, University of Science and Technology of China, Hefei 230026, China

Identifying two-dimensional (2D) materials with the desired electrochemical performance for lithium-ion batteries is of great interest in developing next-generation energy devices. Motivated by the successful synthesis of multiferroic 2D materials, Cu(CrX2)2 (X = S, Se, and Te), which exhibit simultaneous ferroelectricity and ferromagnetism, we performed first-principles calculations to investigate their potential as anodes for lithium-ion batteries. We comprehensively investigate the electrochemical properties of the predicted systems and demonstrate that lithium exhibits sufficient mobility on their surface, with appreciable stability. For instance, the binding energy (Eb) of the lithium adatom on Cu(CrS2)2 is -4.034 eV, with a diffusion barrier as low as 0.212 eV. As a consequence, the maximum theoretical specific capacity for lithium adatoms reaches as high as 1089 and 666 mAhg-1, respectively, for Cu(CrS2)2 and Cu(CrSe2)2, which can be attributed to a much higher storage capacity of lithium adatoms compared to previously identified 2D anode materials. All of these remarkable properties, including high binding energy (Eb), low diffusion barrier, high specific capacity, and good electrical conductivity.

TT 65.7 Wed 18:00 P2

Valence-Band Renormalization and Spin Splitting in a Monolayer WTe2/WSe2 Heterostructure — •Daiyu Geng, Natalie Lehmann, Jiabao Yang, and Niels Schröter — Max Planck Institute of Microstructure Physics, Weinberg 2, Halle (Saale), Germany

Monolayer WTe2 (1L-WTe2) hosts a variety of broken-symmetry phases, including a quantum spin Hall insulator, a topological excitonic insulator, and several intriguing spin-ordered states. The dielectric environment and charge-carrier density play crucial roles in the competition among these electronic phases. In this work, we investigate the band structure of 1L-WTe2 interfaced with semiconducting WSe2 using laser- and synchrotron-based micro-ARPES. We observe strong valence-band renormalization accompanied by pronounced spin splitting in 1L-WTe2. Additionally, multiple replica pockets emerging in the Fermi surface indicate a substantial moiré effect in this heterostructure.

TT 66: 2D Materials: Electronic structure, excitations, etc. – Poster (joint session O/TT)

Time: Wednesday 18:00–20:00 Location: P2

TT 66.1 Wed 18:00 P2

Observation of many-body-localization in substituted 1T-TaS_2 — •Jesumony Jayabalan[1], Gael Reecht[1], Ricards Kristers Knipšis[2], Florian K Diekmann[3], Friedemann Queisser[2], Walter Schnelle[4], Ping Zhou[1], Kai Rossnagel[3], Ralf Schützhold[2], Manuel Gruber[1], and Uwe Bovensiepen[1] — [1]Uni. of Duisburg-Essen, Fakultät für Physik and CENIDE — [2]HZ Dresden-Rossendorf, — [3]CAU of Kiel and DESY — [4]MPI for Chemical Physics of Solids, Dresden

Random modulations in the potential landscape are known to localize a single quantum particle, the Anderson localization leads, to stable non-thermalizing states. Adding interaction is expected to cause delocalization and a quick thermalization of such single particles, but in a strongly disordered system, the many-body quantum state itself becomes localized, known as the Many-Body Localization (MBL). Using time-resolved photoelectron spectroscopic measurements, we show that it is possible to realize MBL states in a Tungsten substituted 1T-TaS_2 material. Electrons are excited by using a 1.51 eV, 50 fs pulses and a 6 eV probe pulse was used to photoemit electrons. In contrast to ultrafast (<20 fs) decay of doublons in pristine 1T-TaS_2[1], we observe that some of the doublons decay in hundreds of femtosecond time scale, while the rest lasts for more than few microseconds. This observation is supported by scanning tunneling microscopic measurements and Fermi-Hubbard model calculations. Funding by DFG through QUAST-FOR5249 and SFB 1242 is acknowledged. [1] M. Ligges et al., Phys. Rev. Lett., 120, 166401 (2018).

TT 66.2 Wed 18:00 P2

Exciton Transport in Monolayer TMDs — •Lifeng Ou, Alejandro Molina-Sánchez, and Alberto García-Cristóbal — ICMUV, University of Valencia, Valencia, Spain

Atomically thin transition metal dichalcogenides semiconductor emerges as promising candidates for novel optoelectronic application, displaying weak dielectric screening due to its truly two-dimension character. The optical properties are mostly related to inter-band transitions between valence and conduction bands, also called the strongly binding electron hole pair, exciton. Strain is expected to impact spatiotemporal distribution of excitons, e.g. spatially inhomogeneous strain acts as a driving force for exciton/carrier funneling, similarly to bias fields for charged particles. In this work we demonstrate the capability to manipulate exciton motion via spatially modulated strain fields, where excitonic energy especially its bandgap is largely tunable and the effective mass of electronic valleys is modified resulting in a qualitative change of the excitonic landscape and efficiency of exciton-phonon scattering channels. These transport properties are represented by the coupled two equations, continuity equation and drift-diffusion equation, which derive from zero-order and first-order moment of Boltzmann equation, respectively. In addition, the simulation diffusion coefficient and mobility in latter equation are evaluated by first-principle and experiment qualitatively, as the function of strain fields.

TT 66.3 Wed 18:00 P2

trARPES investigation electron-phonon coupling in CrSBr — •Maurits Houmes, Karl Schiller, Lasse Sternemann, Jonah Nitschke, and Mirko Cinchetti — Departement of Physics, TU Dortmund University, 44227 Dortmund, Germany

CrSBr is a magnetic, semiconducting van der Waals material that has recently attracted significant interest. It hosts both localized Frenkel excitons and delocalized Wannier-Mott-like excitons, and its excitonic properties are strongly influenced by magnetic ordering and lattice distortions. [1,2,3] These features make CrSBr a compelling platform for exploring correlated phenomena in condensed matter systems.

To advance our understanding of the interplay between excitons, magnetism, and lattice dynamics in this material, a more complete characterization is essential. In this work, we present time- and angle-resolved photoemission spectroscopy (trARPES) measurements performed on CrSBr, with particular emphasis on quantifying the electron-phonon coupling. Aiming to provide a previously missing component needed to build a comprehensive picture of the interactions in CrSBr, offering a foundation for future studies and potential technological applications of this promising material.

1. Smiertka, M. et al. Preprint at ArXiv:2506.16426 (2025). 2. Lin, K. et al. ACS Nano 18, 2898-2905 (2024). 3. Bork, S. et al. Preprint at ArXiv:2511.20268v1 (2025).

TT 66.4 Wed 18:00 P2

Probing defect-induced wave patterns and superconductivity in $2H$-NbS_2 — Werner M.J. van Weerdenburg, •Margarete Huisinga, Constantin Flommersfeld, Lisa M. Rütten, and Katharina J. Franke — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Transition metal dichalcogenides (TMDCs) host a variety of electronic phases, including superconductivity and charge-density-wave (CDW) order. Recent reports on $2H$-NbS_2 have added a coexisting pair-density-wave (PDW) order to this set, inspiring new questions about the coexistence and driving mechanisms of these phases [1]. In contrast, the closely-related superconducting compound $2H$-NbS_2 lacks a CDW phase, but has been suggested to be close to a CDW instability and sensitive to the presence of defects [2,3].

Using low-temperature scanning tunneling microscopy and spectroscopy, we probe the electronic, phononic and superconducting properties of $2H$-NbS_2. We observe wave-like modulations around intrinsic defects in differential-conductance maps and compare them to band-structure calculations. To assess the nature of these modulations, we probe the modulated regions and characterize the superconductivity spatially. These observations add to the ongoing exploration of superconducting, CDW, and PDW phases in TMDC materials.

[1] Liu et al., Science 372,1447-1452 (2021); [2] Heil et al., PRL 119, 087003 (2017); [3] Wen et al., PRB 101:241404, 6 (2020)

TT 66.5 Wed 18:00 P2

Theory of few- and many-body excitations in carbon nanotubes — •Maurice Beringuier[1,2] and Richard Schmidt[1,2] — [1]Institut für Theoretische Physik, Philosophenweg 16, 69120 Heidelberg — [2]Universität Heidelberg, Grabengasse 1, 69117 Heidelberg

Even decades after their discovery, some properties of Carbon Nanotubes (CNTs) are still not fully understood. One of the phenomena still lacking a satisfying explanation is the behaviour of the absorption spectrum of semiconducting CNTs under doping. A resonance in these spectra appears only in the presence of additional charge carriers.

This has in the past been described with phenomenological models or few body physics (using trions and excitons), but experimental data (e.g. time resolved measurements of the spectra) hint at potential signatures of many-body physics. Inspired by their abundance in 2D or 3D semiconductors and cold quantum gases, we investigate whether quasiparticles like Fermi polarons could be responsible for the observations in CNTs, which due to their interesting geometry exhibit aspects of both 1D and 2D materials.

We tackle these questions by modeling charge carriers and excitons on CNTs interacting using a combination of exact diagonalization and variational techniques to gain insight into the interplay of few- and many-body physics in these systems.

TT 66.6 Wed 18:00 P2

Spin-orbit coupling in non-van der Waals 2D materials — •Mani Lokamani[1], Gustav Bihlmayer[2], Gregor Michalicek[2], Daniel Wortmann[2], Stefan Blügel[2], and Rico Friedrich[1,3] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [2]Forschungszentrum Jülich — [3]TU Dresden

In recent years, the rising class of non-van der Waals 2D materials [1] has garnered substantial attention for their distinctive electronic and magnetic properties. In this contribution, we explore the impact of spin-orbit coupling (SOC) on the properties of these non-van der Waals 2D systems and its potential to induce topological properties. Given the presence of heavy elements like Bi and Tl in several 2D candidates, SOC effects notably influence the electronic structure. In our approach, we utilize AFLOW's standardized workflows [2] for initial screening. Subsequently, we extract metadata using AFLOW and tailor the parameters with an AiiDA-plugin [3] for precise electronic structure calculations employing the full-potential all-electron program FLEUR [4] within AiiDA. We analyze the influence of SOC on band structures and densities of states, with a particular focus on topologically protected 1D conduction edge channels.

[1] R. Friedrich *et. al.*, Nano Lett. **22**, 989 (2022).
[2] Divilov *et. al.*, High Entropy Alloys Mater. **3**, 178 (2025).
[3] G. Pizzi *et al.*, Comput. Mater. Sci. **111**, 218 (2016).
[4] The FLEUR project: https://www.flapw.de.

TT 66.7 Wed 18:00 P2

Strain Engineering Single Photon Emission in hBN and MoS2 Monolayers using First Principles — •Paulina Chodyra, Chengcheng Xiao, Johannes Lischner, and Arash Mostofi — Departments of Physics and Materials and the Thomas Young Center for Theory and Simulation of Materials, Imperial College London, London SW7 2AZ, U.K

Point defects in monolayer hexagonal boron nitride (hBN) and molybdenum disulphide (MoS_2) are promising single-photon emitters (SPEs) for quantum technologies due to their potential for room-temperature operation and high photon emission efficiency. In this work we use density-functional theory calculations to investigate the nitrogen antisite-vacancy complex (N_BV_N) and boron vacancy (V_B) in hBN, and the sulphur vacancy (V_S) in MoS_2. We calculate the defect formation energy of different charge states of these defects as a function of biaxial strain and electronic chemical potential. For the charge states that are likely candidates for SPE, we find that their stability can be enhanced via application of biaxial strain. Furthermore, the range of electronic chemical potential over which these charge states are stable can also be increased. These findings can provide predictive design rules for strain-engineered SPEs with improved resilience against electrostatic fluctuations. It also establishes our first steps toward an accelerated discovery of stable SPEs across 2D materials, where DFT-derived stability criteria combined with optical absorption and emission spectra could enable a deeper understanding of SPE operation under realistic conditions.

TT 66.8 Wed 18:00 P2

Beyond the Gamma point: Scanning tunneling spectroscopy on MoS_2/graphene/Ir(111) — Borna Pielić[1,2], Dino Novko[2], Nina Girotto Erhardt[2], Vito Despoja[2], Alice Bremerich[1], Sumanasa Begur Prakash[1], •Robin Ohmann[1], and Carsten Busse[1] — [1]Universität Siegen, Walter-Flex-Str. 3, 57068 Siegen, Germany — [2]Institute of Physics, Bijenička cesta 46, 10000 Zagreb, Croatia

Scanning tunneling spectroscopy (STS) reveals information about the band structure of surfaces by measuring the local density of states, and it also allows detection of quasiparticles. For semiconducting transition-metal dichalcogenides the conduction- and valence-band edges have been readily explored with this method. However, STS studies at higher energies than the Γ-point are limited. Here, we investigate epitaxially grown monolayer islands of MoS_2 on graphene/Ir(111) using STS at low-temperature (T=10 K). Specifically, we employ the constant-current STS method, which enables easier access to spectroscopic features with higher energies, than the more commonly used constant-height STS. We find several peaks a few hundred meV above the Γ-point. We do not see them on graphene, allowing us to exclude substrate- or tip-related effects. When measured near the step edge of an island, these peaks bend closer to the Fermi level, similar to the peak at the Γ-point. Their appearance also varies depending on tip condition and intercalation. Our observations cannot be explained in a single-particle picture. Possible many-body models, such as phonon assisted inelastic tunneling or plasmarons are discussed.

TT 66.9 Wed 18:00 P2

Band structure and Work Function in Ultrathin HfSe2 — •Young Jun Chang — University of Seoul, Seoul, Republic of Korea

Two-dimensional (2D) transition metal dichalcogenides (TMDs) exhibit significant modifications in their electronic structures when reduced from bulk to monolayer thickness. In this study, we investigated the thickness-dependent electronic properties of epitaxial 1T-HfSe2 thin films. The films were grown via molecular beam epitaxy (MBE) and monitored in situ by reflection high-energy electron diffraction (RHEED). Scanning tunneling microscopy (STM) revealed atomically flat surfaces with well-defined 1T hexagonal lattices, while scanning tunneling spectroscopy (STS) measured a bandgap of ~1.1 eV for the monolayer. Angle-resolved photoemission spectroscopy (ARPES) revealed thickness-induced band splitting in the valence band, while the valence band maximum (VBM) remained pinned regardless of thickness. In contrast, the work function increased monotonically with film thickness. Density functional theory (DFT) calculations reproduced the observed band structures and attributed the thickness-dependent work function to the screening effect of the underlying graphene substrate. These findings provide key insights into band alignment and interface engineering in 2D semiconductor-based electronic and optoelectronic devices. (RS-2023-00220471, RS-2023-00284081, RS-2024-00334854)

TT 66.10 Wed 18:00 P2

Exciton and trion dynamics of 2D transition metal dichalcogenides — •Seawoo Moon[1], Alessandro De Vita[1], Lawson T. Lloyd[2], Tania Mukherjee[1], Anh T. Nguyen[3], Dong-Wook Kim[3], Martin Wolf[2], Ralph Ernstorfer[1,2], and Tommaso Pincelli[1] — [1]Institute for Physics and Astronomy, TU Berlin, Germany — [2]Fritz Haber Institute of the Max Planck Society, Germany — [3]Department of Physics, Ewha Womans University, South Korea

Key functionalities of transition metal dichalcogenides (TMDs) are determined by excitons whose behaviour can be tweaked by interface–induced external perturbation such as proximity effects, charge transfer and local electromagnetic fields. Excitonic behaviors and band alignment of TMDs with interfacing materials are explored. We studied the band alignment of monolayer WS_2 on nanostructured Ag by Kelvin probe force microscope, a tool that can map electrical potential of sample surface. By this method, the exciton–to–trion conversion mechanisms in WS_2 could be explained, including the role of the localized surface plasmons. For a more direct approach, time and angle–resolved photoemission spectroscopy (TrARPES) with pump–probe technique is employed to directly map the equilibrium and non–equilibrium electronic structure of TMD–metal and TMD/TMD interfaces. In–situ and ex–situ techniques are required to achieve pristine TMD surfaces and interfaces, since TrARPES is a highly surface sensitive technique.

TT 66.11 Wed 18:00 P2

Ultrafast Photocarrier-Induced Ionic Rearrangement in Monolayer ReS_2 Probed with Femtosecond Electron Diffraction — •Victoria C. A. Taylor[1], Yoav W. Windsor[1,2], Samuel Lai[3], Hyein Jung[1,2], Martin Wolf[1], Fang Lui[3], and Ralph Ernstorfer[1,2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany — [2]Technische Universität Berlin, 10623 Berlin, Germany — [3]Stanford University, Stanford, CA 94305, USA

Rhenium disulphide (ReS_2) exhibits a distorted crystal structure compared to prototypical hexagonal transition metal dichalcogenides. This Peierls-like distortion results in quasi-1D chains of Re ions running in plane through each layer of ReS_2, which give rise to prominent anisotropic properties, such as polarization dependent optical absorption and anisotropic effective carrier masses.

We investigate the ultrafast lattice dynamics of monolayer ReS_2 with femtosecond electron diffraction (FED). Leveraging the strength of FED as a direct and quantitative measurement of the crystal lattice, we fit the intensities of many hundreds of Bragg peaks at each time delay to extract time resolved crystallographic information.

With this method, we not only resolve the increase in the incoherent phonon population (Debye-Waller), but also reveal a concerted atomic rearrangement within the lattice, with the ions rapidly (< 1 ps) moving away from their equilibrium atomic coordinates and returning on timescales of a few picoseconds. We associate this response with the aforementioned distortion, and discuss the physical origin.

TT 66.12 Wed 18:00 P2

Exploring Zincblende (100) Semiconductor Surfaces as Platforms for Correlated Adatom Lattices — •Olga Kashirina, Niklas Enderlein, and Philipp Hansmann — Friedrich-Alexander-Universität Erlangen-Nürnberg

Adatom lattices on (111) surfaces of zincblende structured semiconductors have proven to be versatile, experimentally realizable platforms for hosting strong electronic correlations and associated emergent behavior near the Fermi energy (see [1] and references therein). Our recent study [2] reveals transition metals adatom lattices on 3C-SiC(111) surfaces to be intriguing candidates for strongly correlated material design. In the present contribution we continue this strategy by leaving the hexagonal/triangular lattices. Specifically, we explore the (100) surfaces of silicon, diamond, and 3C-SiC which in the infinite bulk exhibit a fourfold rotoinversion symmetry enabling square/rectangular adatom lattices. As the (100) surface is prone to dimerization, an additional complication arises from dimer-derived electronic states inside the bulk gap, which - depending on the chosen adatom and substrate combination - may or may not hybridize with the adatom states. In this context, the adatom coverage is another crucial parameter as it directly influences the nature of surface reconstructions and dimerizations. To assess the structural stability of our candidate systems, we employ phonon calculations based on density-functional perturbation theory as well as molecular-dynamics simulations. [1] X. Cao, et al., PRB 97, 155145 (2018). [2] H. Menke, N. Enderlein, et al., arXiv:2410.17165.

TT 66.13 Wed 18:00 P2

Engineering correlated electrons in adatom lattices on semiconductors — •Tim Kullick[1], Niklas Enderlein[1], Henri Menke[1,2], Giorgio Sangiovanni[3], and Philipp Hansmann[1] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Max Planck Institute for Solid State Research, Stuttgart — [3]Julius-Maximilian-Universität of Würzburg

Adatom lattices on (111) surfaces of zinc-blende structured semiconductors have proven to be versatile, experimentally realizable platforms for hosting flat bands with strong electronic correlations near the Fermi energy. A recent study [1] revealed transition metals on 3C-SiC(111) surfaces to be intriguing adatom systems, showcasing the diverse nature of strongly correlated systems. Together with earlier theoretical and experimental studies on adatom lattices on the Si(111) surfaces, this recent work underlines the great potential of this material family. In the present project, we explore promising adatom lattices on semiconducting/insulating substrates such as SiC and cubic BN in order to realize one-, two-, and three-band Hubbard models at different fillings. Combined with estimates of the quasiparticle interaction via cRPA, we point out new material directions in this increasingly vivid field. [1] H.Menke, N.Enderlein, *et al.*, arXiv:2410.17165.

TT 66.14 Wed 18:00 P2

Investigation of the atomic and electronic structures of WSe2-xTex — •Ganbat Duvjir[1], Nguyen-Hoang Dang[2], Younghun Hwang[1], and Jungdae Kim[1] — [1]Department of Semiconductor Physics and Engineering, University of Ulsan, Ulsan 44610, Republic of Korea — [2]Electricity and Electronics and Semiconductor Applications, Ulsan College, Ulsan 44610, Republic of Korea

Ternary transition metal dichalcogenides (TMDs) exhibit diverse crystal structures and electronic properties depending on their composition. In this study, we systematically investigate the atomic and electronic structure of ternary WSe2-xTex as a function of Te concentration using scanning tunneling microscopy/spectroscopy (STM/S). Notably, STM topography indicates that increasing the Te content induces structural deformation of the hexagonal lattice of WSe2-xTex. This deformation manifests as the stretching of 2H structure along the zigzag direction and compression along the armchair direction. STS measurements reveal a significant reduction in the band gap of WSe2-xTex with increasing Te concentration. While the valence band maximum shifts toward the Fermi level, the conduction band minimum remains relatively unchanged.

TT 66.15 Wed 18:00 P2

STM study on tuning the Fermi level of transition metal dichalcogenides — •Nguyen-Hoang Dang[1], Mincheol Kim[2], Ganbat Duvjir[1], Young Jun Chang[2,3], and Jungdae Kim[1] — [1]Department of Semiconductor Physics and Engineering, University of Ulsan, Ulsan 44610, Republic of Korea — [2]Department of Physics, University of Seoul, Seoul 02504, Republic of Korea — [3]Department of Smart Cities, University of Seoul, Seoul 02504, Republic of Korea

Controlling the Fermi level is essential for tailoring the electronic properties of semiconductors. Here, we investigate two routes of chemical doping and defect control using scanning tunneling microscopy and spectroscopy. For V-doped $MoSe_2$, we study how substitutional V atoms influence its electronic structure. Although STM primarily probes the top Se layer and the dopants are not directly imaged, the topography exhibits defect-like features whose contrast reverses with the bias polarity: dark at positive sample bias and bright at negative bias. This is characteristic of negatively charged acceptor states, consistent with V substituting Mo. STS spectra show a Fermi-level shift toward the valence band, indicating that V doping drives $MoSe_2$ from intrinsic n-type toward p-type. For $HfSe_2$, we study defect control via thermal annealing. STS measurements under different annealing conditions show Fermi level shifts toward the conduction band, suggesting that prolonged annealing enhances Se-vacancy formation, which acts as an electron donor. These results highlight how STM/STS links local defects with electronic properties, offering microscopic insight into Fermi level tuning through doping and defect engineering.

TT 66.16 Wed 18:00 P2

Impact of Mo doping on the charge density wave in 1*T*-TaS_2 studied by laser-ARPES and LEED — •Adina Timm[1,2], Finja Schillmöller[1,2], Florian K. Diekmann[1,2], Jana Kähler[1,2], Matthias Kalläne[1,2,3], Tim Riedel[1,2], and Kai Rossnagel[1,2,3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Controlling charge density waves (CDWs) in quantum materials enables the fine-tuning of their electronic properties, paving the way for future electronic and optoelectronic devices. The layered compound 1*T*-TaS_2 exhibits various temperature-dependent CDW phases that we aim to modify through doping. We introduced the dopant molybdenum during crystal growth via the chemical vapor transport method. Using 11-eV laser-based angle-resolved photoelectron spectroscopy (ARPES), we comparatively measured the electronic band structures of pristine and Mo-doped 1*T*-TaS_2 crystals. Complementary low-energy electron diffraction (LEED) measurements revealed the structural rearrangements during the CDW transitions and partial CDW suppression at specific doping levels. Our results suggest that modest Mo doping allows for subtle adjustments to the CDW landscape of 1*T*-TaS_2, yielding different transition temperatures while preserving the underlying electronic-structural order.

TT 66.17 Wed 18:00 P2

Probing Electronic Structure Modulation in WSe_2 and $MoTe_2$ under Out-of-Plane Electric Fields via ARPES and XPS — •Sonja Reinheimer[1,2], Lukas Bruckmeier[1,2], Jakob Dilling[1,2], Jens Buck[1,2], Matthias Kalläne[1,2,3], Chithra Sharma[1,2,4], Markus Scholz[5], and Kai Rossnagel[1,2,3] — [1]IEAP, CAU Kiel, 24098 Kiel, Germany — [2]RHL, DESY, 22607 Hamburg, Germany — [3]KiNSIS, CAU Kiel, 24098 Kiel, Germany — [4]Universität Hamburg, 22761 Hamburg, Germany — [5]DESY, 22607 Hamburg, Germany

Transition metal dichalcogenides (TMDCs) are quantum materials that exhibit a broad spectrum of emergent electronic phenomena, arising from layer-dependent band structures. Owing to their tunable (opto-)electronic properties, TMDCs are promising candidates for next-generation photovoltaic devices and highly integrated electronic components. A key challenge is to systematically control charge transport and band alignment in these layered systems. Here, we investigate vertically stacked 2*H*-WSe_2/2*H*-$MoTe_2$ heterostructures using angle-resolved photoemission spectroscopy (ARPES) and X-ray photoelectron spectroscopy. By performing in-operando ARPES on a sample with an applied out-of-plane electric field during the measurements, we can directly probe field-induced modifications to the electronic band structure and the density of states. This approach enables us to identify electric-field-driven changes in the electronic and lattice structure and contribute to a deeper understanding of electric control mechanisms in TMDC heterostructures.

TT 66.18 Wed 18:00 P2

Many-body localisation in the Fermi-Hubbard model? — •Ričards Kristers Knipšis[1], Jesumony Jayabalan[2], Gael Reecht[2], Vivek Mondal[2], Florian Konstantin Diekmann[3], Friedemann Queisser[1], Ping Zhou[2], Walter Schnelle[4], Kai Rossnagel[3,5], Ralf Schützhold[1,6], Manuel Gruber[2], and Uwe Bovensiepen[2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Faculty of Physics and CENIDE, University of Duisburg-Essen, Duisburg, Germany — [3]Institute of Experimental and Applied Physics, Christian-Albrechts-University of Kiel, Kiel, Germany — [4]MPI for Chemical Physics of Solids, Dresden, Germany — [5]Ruprecht-Haensel-Laboratory, DESY, Hamburg, Germany — [6]Institute of Theoretical Physics, Dresden University of Technology, Dresden, Germany

Motivated by recent experimental results, we study the 2D Fermi-Hubbard model in the Mott insulator state under the influence of a disorder potential. Special emphasis is placed on signatures of many-body localisation.

Using the hierarchy of correlations, we find that the disorder potential can localise the effective quasi-particle wavefunctions, resulting in their spatial separation. This, in turn, can be used to explain the drastic increase in the quasi-particle lifetimes observed in experiment.

Funding by the DFG through the SFB 1242 is gratefully acknowledged.

TT 66.19 Wed 18:00 P2

Magnetic properties of V-doped WSe2 — •Jules M. Knebusch[1,2], Jana Kähler[1,2], Matthias Kalläne[1,2,3], Robert Zierold[4], Tim Riedel[1,2], Adina Timm[1,2], Robert H. Blick[4], and Kai Rossnagel[1,2,3] — [1]IEAP, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]RHL, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [4]CHyN, Universität Hamburg, 22761 Hamburg, Germany

Spintronics holds promise for highly efficient classical and quantum computing and is therefore considered a key technology for future innovation. Pristine tungsten diselenide (WSe_2), known as a semiconductor with a quasi-two-dimensional hexagonal 2*H* structure, is expected to transform into a room-temperature dilute ferromagnetic semiconductor upon vanadium doping. This makes it a highly attractive candidate for spintronic applications. Density functional theory calculations and scanning transmission electron microscopy studies support this assumption, and RKKY interactions are predicted to be the driving mechanism. Pristine WSe_2 and vanadium-doped WSe_2 crystals were synthesized in separate in-house batches using the chemical vapor transport (CVT) method. The doped samples were grown with varying nominal concentrations of V intended to induce substitutional doping at the tungsten sites. The samples were investigated using a vibrating-sample magnetometer (VSM). The results provide insight into the magnetic characteristics of the doped material compared to the pristine reference crystal.

TT 66.20 Wed 18:00 P2

Coexistence of a fully metallic antiphase boundary and the semiconducting charge density wave phase in 1T-TaS_2 — •Georg A. Traeger[1], Kai Rossnagel[2,3], and Martin Wenderoth[1] — [1]IV. Institute of Physics, University of Göttingen, Göttingen, Germany — [2]Institute of Experimental and Applied Physics, Kiel University, Kiel, Germany — [3]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

Transition metal dichalcogenides are an ideal platform for studying the interplay between charge density waves (CDWs), electronic correlations, and defect states. Using scanning tunneling microscopy and spectroscopy, we investigate a new type of intrinsic antiphase boundary (APB) in the commensurate CDW phase of 1T-TaS_2. In contrast to previous studies, we find a metallic APB extending laterally across several nanometers. We observe evanescent states spilling out from the defect into the metallic region and find that the fingerprint of the semiconducting system gradually disappears within the APB, without signs of strong interactions, suggesting the orthogonality of the two systems wave functions. Our findings highlight the crucial role of domain boundaries in the interpretation of other, especially conductivity-based, measurements. Furthermore, we propose this new type of metallic APB as a model system to study interlayer coupling in correlated layered materials.

TT 66.21 Wed 18:00 P2

Temperature-dependent VUV-ARPES of 1*T*-$Mo_xTa_{1-x}S_2$ — •Torben Petersen[1,2], Matthias Kalläne[1,2,3], Adina Timm[1,2], Tim Riedel[1,2], and Kai Rossnagel[1,2,3] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Examining the charge density wave (CDW) phase transitions of transition metal-substituted transition metal dichalcogenides (TMDCs) provides insight into tuning transition behavior by doping. To this end, we use the 1*T*-$Mo_xTa_{1-x}S_2$ reference system, comparing the pristine sample with two doped samples (x = 0.5% and x = 1%) using 11 eV laser-based VUV-ARPES. We investigate work function changes alongside doping-induced band structure changes in the temperature range of 60 K to 370 K. This allows us to observe the high- and low-temperature CDW phase transitions known from the pristine material and determine how the CDW-induced band structure changes vary with doping.

TT 66.22 Wed 18:00 P2

STM/STS Studies of Single-Atom Fe Inclusions in MBE-grown Monolayer MoS_2/Gr/Ir(111) — •Alina Drechsler, Marta Przychodnia, Maciej Bazarnik, and Anika Schlenhoff — Institute of Physics, University of Münster, Germany

Transition metal dichalcogenides (TMDs) exhibit thickness-dependent electronic properties and are highly sensitive to structural defects, which can strongly modify their density of states even at low concentrations. Defect engineering has therefore become an important route to tailor their electronic, magnetic, optical, and catalytic behaviour. While most of the current research focuses on naturally occurring defects in chemical vapour-deposited TMDs, we focus on intentional single-atom inclusions in TMDs grown by molecular beam epitaxy (MBE) to improve control in defect engineering.

We present scanning tunneling microscopy and spectroscopy (STM/STS) studies of Fe-doped monolayer MoS_2 on Gr/Ir(111), achieved by co-evaporation Fe during MBE growth. By comparing to undoped MoS_2 grown under identical UHV conditions, we identify the Fe-related defects and measure their electronic signatures. STS reveals in-gap states associated with single-atom Fe inclusions, whose spatial distributions are resolved via differential conductance mapping. Additionally, resonant tunneling spectroscopy shows that Fe inclusions modify the image potential states by locally shifting their energetic positions. Our work demonstrates the potential of single-atom substitutions for tailoring the electronic properties of two-dimensional TMDs.

TT 66.23 Wed 18:00 P2

Layer thickness dependent band gap of MBE grown single- to few-layer MoS_2 — •Maciej Bazarnik[1], Marta Przychodnia[1,2], Thorsten Deilmann[3], and Anika Schlenhoff[1] — [1]Institute of Physics, University of Münster, Germany — [2]Institute of Physics, Poznan University of Technology, Poland — [3]Institute of Solid State Theory, University of Münster, Germany

In light of the rise of transition metal dichalcogenides as 2D semiconductors for device applications, band engineering becomes very important from an application point of view. In many of these materials, such as the canonical example of MoS_2, the semiconductor band gap depends on the layer number. There is a transition from an indirect band gap semiconductor in bulk to a direct band gap for a monolayer. Interestingly, it was predicted and experimentally confirmed that, by thinning the material from bulk to a bilayer, the indirect transition blue-shifts.

Here, we present the results of scanning tunnelling spectroscopy measurements on MoS_2 that has been grown in situ via molecular beam epitaxy (MBE) on graphene on Ir(111) at thicknesses ranging from 1 to 6 layers. We observe a decrease in the band gap with increasing layer number. We also find a pinning of the conduction band, which vanishes for layer thicknesses beyond 4 layers. Comparing our experimental data with DFT and GW calculations indicates that a screening in addition to that of the substrate needs to be introduced to explain the experimentally obtained relation. We discuss possible sources of this additional screening in light of our findings.

TT 67: 2D Materials beyond graphene: Growth, structure and substrate interaction – Poster (joint session O/TT)

Time: Wednesday 18:00–20:00 Location: P2

TT 67.1 Wed 18:00 P2

In-Situ CVD growth of vertical Heterostructures of Borophene and Hexagonal Boron Nitride — •Niels Ganser[1], Marko Kriegel[1], Smruti Ranjan Mohanty[1], Karim Omambac[1], Marin Petrovic[2], Christian Brand[1], Steffen Franzka[3], Birk Finke[1], Tobias Hartl[4], Thomas Michely[4], Frank-Joachim Meyer zu Heringdorf[1,3], and Michael Horn-von Hoegen[1] — [1]Universität Duisburg-Essen — [2]Institute of Physics, Zagreb — [3]ICAN, Duisburg — [4]Universität zu Köln

Intrinsic segregation provides a promising and scalable route for the in situ fabrication of 2D heterostructures. Using UHV chemical vapor deposition (CVD)

of a single borazine ($B_3N_3H_6$) precursor [1], we demonstrate the growth of an hBN/borophene heterostructure on Ir(111). At high temperatures and low precursor pressures, boron dissolves into the Ir subsurface region, creating a boron reservoir below the surface [2]. Largely increasing the precursor dosing pressure shifts the chemical potential toward the formation of a complete hBN layer. Upon cooldown, the decreasing boron solubility of the Ir substrate drives segregation to the surface, where a borophene layer forms underneath the hBN overlayer and thus completing the heterostructure. The resulting structure and its growth kinetics were investigated using a combined low energy electron diffraction (SPA-LEED) and microscopy (LEEM) approach.

[1] K. Omambac et al., ACS Nano 17 (2023) 17946
[2] K. Omambac et al., ACS Nano 15 (2021) 7421

TT 67.2 Wed 18:00 P2

Growth of 2D molecular networks on graphene — •Haruto Shibahara and Toyo Kazu Yamada — Dept. Materials Science, Chiba Univ., Chiba, Japan

We demonstrate the engineering of qubits on solid surfaces using organic molecules and transition-metal magnetic atoms. Atomically flat and clean graphene (Gr) grown on an Ir(111) substrate was selected as the platform. Scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED) revealed the characteristic moiré pattern, while scanning tunneling spectroscopy (STS) and angle-resolved photoemission spectroscopy (ARPES) confirmed the presence of Dirac bands. Although single atoms can in principle serve as qubits, they tend to thermally diffuse on surfaces and their energy levels may remain degenerate. To overcome these issues, it is necessary to coordinate the atoms with organic ligands, whose ligand fields can lift the degeneracy. As a first approach, we attempted to employ 1,3,5-tris(4-bromophenyl)benzene (TBB) molecules to form a two-dimensional (2D) covalent organic framework. However, on the Gr surface we found that thermal activation desorbed the TBB molecules before they could undergo Ullmann coupling. As a second approach, we attempted to grow a 2D metal organic framework (MOF) on Gr. The details of this effort will be discussed.

TT 67.3 Wed 18:00 P2

Probing the Electrostatic Potential of hBN by AFM with Oxygen-Terminated Copper Tips — •Jan ter Glane[1,2], Philipp Wiesener[1,2], Thorsten Deilmann[3], Milena Merkel[1,2], Maciej Bazarnik[2], Anika Schlenhoff[2], and Harry Mönig[1,2] — [1]Center for Nanotechnology, University of Münster, Germany — [2]Institute of Physics, University of Münster, Germany — [3]Institute of Solid State Theory, University of Münster, Germany

Monolayer hexagonal boron nitride (hBN) hosts point defects with promising optoelectronic properties, yet their atomic structure remains unclear [1]. Conventional scanning tunneling (STM) and atomic force microscopy (AFM) lack elemental contrast, making it difficult to reliably distinguish B and N sites. Noncontact AFM with oxygen-terminated copper tips (CuOx-tips) has previously enabled elemental discrimination and defect identification on metal oxides [2].

Using CuOx-tip AFM, we demonstrate elemental contrast on NaCl thin films, suggesting its broad applicability to polarized surfaces. Leveraging this capability, we investigate its application to monolayer hBN. DFT-optimized electrostatic potential calculations predict clear B-N contrast. To realize these measurements, we employ in-situ chemical vapor deposition growth procedures for high-quality hBN on single-crystalline substrates. We outline the benefits of CuOx-tip AFM and present initial results towards correlating STM/STS measurements, aiming to enable atom-specific defect identification in hBN.

[1] Grosso *et al.*, Nat. Commun. **8**, 705 (2017)
[2] Wiesener *et al.*, ACS Nano **18**, 21948 (2024)

TT 67.4 Wed 18:00 P2

Pt-doped borane nanomembranes — •Martha Frey[1], Julian Picker[1], Christof Neuman[1], Jan Macháček[2], Tomáš Baše[2], and Andrey Turchanin[1] — [1]Friedrich Schiller University Jena, Institute of Physical Chemistry, Lessingstraße 10, 07743 Jena, Germany — [2]The Czech Academy of Sciences, Institute of Inorganic Chemistry, 250 68 Husinec Rez, 1001, Czech Republic

Boranes are clusters of boron and hydrogen atoms that form three-dimensional, cage-like molecules. We have recently employed them as convenient starting precursors for synthesising two-dimensional (2D) carbon-free nanomembranes. In this study, we present the preparation and characterisation of the self-assembled monolayers (SAMs) of two thiolated *syn*-$B_{18}H_{22}$ clusters on silver substrates. Subsequently, these SAMs were cross-linked laterally to form boron nanomembranes (BNMs) via low-energy electron irradiation under ultra-high vacuum (UHV) conditions. We investigated the structural and chemical properties of these 2D nanomembranes using surface-sensitive techniques such as X-ray photoelectron spectroscopy (XPS) and scanning tunnelling microscopy (STM). Both the starting SAMs and the resulting boron nanomembranes exhibited reactivity toward Pt-containing complexes. While such reactivity was expected for the SAMs, it was particularly noteworthy that the BNMs also enabled the insertion of Pt atoms. This Pt-doping positions borane-derived SAMs and BNMs as a promising 2D platform for nanoscale catalytic studies.

TT 67.5 Wed 18:00 P2

Defects and Initial Approaches to TMDC Heterostructure Growth on Pt_xTe_y films — •Isabella Stollberg, Andreas Raabgrund, and M. Alexander Schneider — Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Transition-metal dichalcogenides (TMDCs) can generally be synthesised either by co-evaporating the metal and chalcogen onto a suitable substrate [1] or by depositing only the chalcogen onto the desired metal surface. Using STM, STS, and DFT, we investigate Pt_xTe_y films on Pt(111) prepared via the latter approach. With increasing Te content, different initial growth surface telluride structures are observed, followed by the formation of Pt_2Te_2 and $PtTe_2$ layers [2]. This contribution focuses on STM and spatially resolved STS analyses of point defects in $PtTe_2$, as well as domain boundaries within a $PtTe_2$ or Pt_2Te_2 layer. Furthermore, we evaluate the suitability of these telluride films as substrates for TMDC heterostructure growth. First results on attempting to grow $TiTe_2$ and $PdTe_2$ demonstrate considerable intermixing. While $TiTe_2$ islands can be identified by their apparent height and other lattice constants, $PdTe_2$ islands cannot be distinguished from $PtTe_2$ based on topography due to their similar vertical and lateral lattice parameters.

[1] K. Lasek et al., Nano Lett. **22**, 23 (2022)
[2] T. Kißlinger et al., Phys. Rev. B **108**, 205412 (2023)

TT 67.6 Wed 18:00 P2

Boosting the Efficiency of Quantum Replica-Exchange Molecular Dynamics — •Jan-Niklas Mohr, Shubham Sharma, and Mariana Rossi — MPI for the Structure and Dynamics of Matter, Hamburg, Germany

Replica exchange molecular dynamics can be combined with path-integral techniques in order to incorporate quantum statistics in the sampled ensembles [1]. However, the efficiency in swapping replicas is decreased to a point that makes simulations extremely inefficient at lower temperatures.

We propose a new acceptance criterion for path-integral replica-exchange molecular dynamics (PI-REMD) that incorporates the path-integral spring term in the Hamiltonian and rescales it consistently. As a result, the acceptance probability is only sensitive to potential-energy differences, and the efficiency of the method is thus increased. Benchmarking on several test systems, including asymmetric double wells and glassy-like potentials, shows that our method outperforms standard PI-REMD in sampling efficiency and exchange frequency. We also show improvements for realistic materials, such as monolayer 1H-TaS_2 [2], where it is paramount to obtain an accurate description of the charge-density-wave phase transition. Our acceptance criterion therefore provides an efficient and reliable tool for studying quantum phase transitions and exploring thermodynamic ensembles under challenging conditions.

[1] Kapil *et al.*, Comput. Phys. Commun. 236, 214-223 (2019).
[2] Schobert *et al.*, SciPost Phys. 16, 046 (2024)

TT 68: Graphene: Electronic structure, excitations, etc. – Poster (joint session O/TT)

Time: Wednesday 18:00–20:00 Location: P2

TT 68.1 Wed 18:00 P2

Strong-Field Bloch Electron Interferometry for Band-Structure Retrieval — •Tamara Pröbster, Tobias Weitz, Christian Heide, and Peter Hommelhoff — Friedrich-Alexander-Universität Erlangen-Nürnberg, Department Physik, Staudtstr. 1, 91058 Erlangen

Strong optical fields drive electrons in solids far from equilibrium, enabling access to ultrafast quantum dynamics that directly reflect the underlying band structure. When Bloch electrons in graphene are exposed to an intense few-cycle laser field, they undergo coherent intraband motion during which they accumulate a quantum phase determined by the local band curvature. If this laser-driven trajectory encounters an avoided crossing between the valence and conduction bands, the electron wave packet can coherently split via a Landau-Zener transition. In our work, we exploit pairs of such transitions to realize strong-field Bloch electron interferometry, forming an interferometric sequence fully embedded in the electronic band structure. The resulting interference encodes band information in the phase-dependent photocurrent. We retrieve the Fermi velocity of

graphene near the K points as 1.07 ± 0.04 nm·fs^{-1}, in excellent agreement with theoretical expectations. Our results establish strong-field Bloch electron interferometry as a general and versatile approach for band-structure reconstruction under ambient conditions. Because the method relies solely on ultrafast optical driving and detection, it is naturally suited for tracking light-induced modifications of electronic structure with femtosecond temporal resolution.

TT 68.2 Wed 18:00 P2

Folding the electronic band structure of graphene-Bi and graphene-Pb heterobilayers — •Johanna Schurr, Alexander Korn, Andres Unigarro, Sibylle Gemming, and Nebahat Bulut — Institute of Physics, TU Chemnitz, Germany

Translational and rotational degrees of freedom in 2D material stacks open up a wealth of tunable materials properties, such as electrical conductivity, magnetism, or optical properties, in particular if heavy intercalant atoms are present. In this study, the band structure of the two hexagonal hetero-bilayer systems bismuthene-graphene and plumbene-graphene were investigated, because experiment gives evidence for a large number of structural varieties especially for plumbene.

The aim was to identify and characterise the influence of bismuthene and plumbene layers on the band structure of graphene. For this purpose a code was generated to correlate the k-path of the band structures calculated for supercells and primitive cells within their respective Brillouin zones. Subsequent folding back of the bands into the first Brillouin zone of the supercell, while maintaining the information of the original k-path in the primitive cell, provided an overview of all existing bands and the origin of their Brillouin zone.

TT 68.3 Wed 18:00 P2

A tool for folding and unfolding of electronic band structures applying it to graphene and the gold(111)-surface — •Alexander Korn, Nebahat Bulut, and Sibylle Gemming — Institute of Physics, TU Chemnitz, Germany

The electronic band structure is an important property of materials. For comparison with experiments and other studies, as well as for better readability, it is useful to display and analyse the band structure of the primitive cell rather than a supercell. Studying more complex materials with dopants or adatoms is only possible using a supercell instead. Therefore, one must unfold the band structure of the supercell into the primitive cell.

For this purpose, we offer a tool for abinit (www.abinit.org) that can be used to unfold all possible supercells. The unit vectors of the supercell can be stretched and also rotated relative to the unit vectors of the primitive cell. We also offer an additional qualitative tool for band folding that also tracks the origin of the Brillouin zone of each band at each k-point. We provide a practical example of folding and unfolding using the gold(111) surface with sulfur as an adatom.

TT 68.4 Wed 18:00 P2

Enhanced Screening in Indium Intercalated Graphene Enabled by 2D Nearly Free Electron States — •Lukas Gehrig[1,2], Cedric Schmitt[1,2], Kilian Strauss[1,2], Jonas Erhardt[1,2], Stefan Enzner[2,3], Martin Kamp[1,4], Timur Kim[5], Giorgio Sangiovanni[2,3], Jörg Schäfer[1,2], Simon Moser[6], and Ralph Claessen[1,2] — [1]Physikalisches Institut, Universität Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Germany — [3]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [4]Röntgen Center for Complex Material Systems, Würzburg, Germany — [5]Diamond Light Source, Harwell Science and Innovation Campus, Didcot, United Kingdom — [6]Experimentalphysik IV - AG Oberflächen, Ruhr-Universität Bochum, Germany

Intercalation of epitaxial graphene on SiC has been intensively explored to modify graphene's electronic properties, but previous intercalants provide only weak screening, leading to pronounced electron-plasmon coupling and the appearance of plasmaron bands in ARPES [1]. Here, we demonstrate that intercalated bilayer indium exhibits strongly Rashba-split bands, which acquire nearly free-electron-like character at the Fermi level. This induces exceptionally strong screening in graphene, significantly reducing many-body renormalization effects in the graphene bands, which arise from plasmaron coupling. This approach opens new opportunities to explore and control many-body interactions in graphene-based heterostructures.

[1] Bostwick A et al., Nat. Phys. 3, 36-40 (2007)

TT 68.5 Wed 18:00 P2

Terbium intercalation as a route to n-doping of graphene past the van Hove singularity — •Bharti Matta[1], Philipp Rosenzweig[1], Craig Polley[2], Kathrin Küster[1], and Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [2]MAX IV Laboratory, Lund, Sweden

Exotic ground states driven by many-body interactions, such as unconventional chiral superconductivity and spin-density waves, were theoretically predicted more than a decade ago for heavily n-doped graphene near the van Hove singularity (VHS). In recent years, achieving such high doping levels in epitaxial graphene on SiC via intercalation has attracted considerable interest. Intercalation of rare-earth elements such as Gd, Yb, and Er has already proven promising in reaching these regimes. Here, we demonstrate that intercalation of Tb atoms at the graphene/SiC interface provides access to extreme n-doping levels beyond the π^* VHS, without requiring any adsorbates on the graphene surface. The extended VHS is shifted by 0.07 eV below the Fermi level (E_F) as seen in angle-resolved photoemission spectroscopy. From the area enclosed by the giant hole pocket around Γ, we extract an electron density of $\approx 5\times10^{14}$ cm^{-2}. Strong renormalization of the graphene bands leads to a Dirac point about 1.55 eV below E_F, indicating that the doping cannot be described by a rigid single-particle band shift. Based on these experimental parameters, theoretical calculations predict the emergence of topological superconductivity with a critical temperature up to 600 mK (S. A. Herrera *et al.*, *ACS Nano 18* (51), 34842–34857 (2024)).

TT 68.6 Wed 18:00 P2

Vanishing Fermi velocity in Periodically Strained Graphene — •Leo-Malik Benneka[1], Taher Rhouma[2], Guy Trambly de Laissardière[2], Clemens Winkelmann[1], Mark Zelsmann[3], and Vincent Renard[1] — [1]Université Grenoble Alpes, CEA-IRIG-PHELIQS, 38000 Grenoble, France — [2]CNRS-LPTM, CY Cergy Paris Université, 95302 Cergy-Pontoise, France — [3]CNRS-LTM, 38000 Grenoble, France

Intense research has been made in engineering flat bands in twisted bilayer graphene, leading to various correlated phases [1]. An alternative route to realizing similar flat bands involves a monolayer graphene strained by a periodic triangular superlattice induced by a corrugated substrate. The height modulation h and the superlattice periodicity L serve as tuning parameters for controlling band flattening and the Fermi velocity v_F near the Dirac cones [2, 3]. Tight-binding calculations were performed by explicitly accounting for relative rotations between the graphene lattice and the superlattice, as would occur in an experimental device. These calculations not only reproduce the known decrease of the Fermi velocity with increasing h [4], but also reveal a renormalization of v_F that depends on the specific ratio $\sqrt{a_C C\, L}/h$ and on the relative lattice orientation. Remarkably, this behavior is universal for any superlattice size L. These predictions may assist in the design of experimental devices aimed at engineering flat bands. [1] Cao et al., Nature, 556 (2018) 43-50 ; [2] Mao et al., Nature, 7820 (2020) 215-220 ; [3] Yuan et al., Phys. Rev. B, 24 (2024) 245408 ; [4] S. P. Milovanović et al., Phys. Rev. B, 24 (2020) 245427.

TT 68.7 Wed 18:00 P2

Optimizing the excitation cross section for graphene phonons in inelastic electron tunnelling via intercalation. — Karl Rothe[1], •Nicolas Néel[1], Mads Brandbyge[2], and Jörg Kröger[1] — [1]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany — [2]Center of Nanostructured Graphene, Department of Physics, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark

Platinum-intercalated graphene on a (111)-oriented iridium surface gives rise to a variety of rotational domains, which exhibit characteristic moiré patterns. Independent of the twist angle subtended by the graphene and substrate lattice, inelastic electron tunnelling spectroscopy reveals elevated graphene phonon excitation only on the intercalated phases. Combining spatially resolved spectroscopy of the electronic structure with non-equilibrium Green's function simulations highlights the relevance for effective phonon creation of the balance between elastic and inelastic electron transport. The intercalation-induced shift of electron density of states from the Brillouin zone centre to its boundary enhances the inelastic channel at the expense of the elastic channel and thereby increases the phonon excitation cross section. Financial support by the Deutsche Forschungsgemeinschaft through KR 2912/18-1 is acknowledged.

TT 68.8 Wed 18:00 P2

Se-intercalation of graphene on SiC(0001) — •Susanne Wolff[1,2] and Thomas Seyller[1,2] — [1]Institut für Physik, Technische Universität Chemnitz — [2]Research Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Technische Universität Chemnitz

The epitaxial growth of graphene on SiC in an argon atmosphere is a well-established method to produce homogeneous, high quality carbon layers. The first-grown carbon layer exhibits a $\left(6\sqrt{3}\times 6\sqrt{3}\right)R30^\circ$ periodicity and is partially covalently bound to the SiC substrate. Therefore, this so-called buffer layer lacks the typical electronic properties of graphene. One pathway to decouple the buffer layer from the substrate and obtain graphene-like electronic properties is intercalation, which involves introducing a certain element at the buffer layer/SiC interface. Furthermore, the choice of intercalant influences the electronic properties of the decoupled graphene.

In this study, we investigated the intercalation of a buffer layer with selenium (Se). This process was carried out in a two-zone tube furnace, with the selenium precursor $SnSe_2$ and the buffer layer positioned in different temperature zones. The samples were characterized using X-ray photoelectron spectroscopy (XPS) and angle-resolved photoelectron spectroscopy (ARPES). XPS revealed successful decoupling of the buffer layer with intercalated Se at the interface and not-intercalated Se on the surface. ARPES measurements in the vicinity of the Dirac point of graphene showed a p-type doping of the decoupled carbon layer.

TT 68.9 Wed 18:00 P2

Mesoscopic Lateral Intercalation Dynamics of Indium Between the Epitaxial Zero-Layer of Graphene and SiC — •Benno Harling[1], Zamin Mamiyev[2], Narmina Balayeva[2], Dietrich R.T. Zahn[2], Christoph Tegenkamp[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August-Universität, Friedrich-Hund-Platz 1, 37077, Göttingen, Germany — [2]Institut für Physik, Technische Universität Chemnitz, Reichenhainer Str. 70, 09126, Chemnitz, Germany

Intercalation, the process of diffusing a material species in-between layered materials, can be utilized for both bulk and 2D systems to achieve tailored electronic properties. [1] For the 2D limit, this work investigates the lateral diffusion dynamics of indium intercalation into the epitaxial zero-layer of graphene on SiC using Kelvin Probe Force Microscopy (KPFM). For tin, material transfer across surface substrate steps is observed at local sites at the mesoscopic scale. [2] With the used experimental parameters, we find that this is not the case for indium intercalation. Instead, only terrace transport is observed. The KPFM measurements were complemented by micro-Raman spectroscopy, assessing the extent and uniformity of In intercalation. Remarkably, intercalation through the carbon layer seems to be dependent on the graphene or substrate properties that still need to be further resolved. This leads to a situation where just some of the terraces are observed to be intercalated. Financial support by the DFG within Research Unit FOR5242 is acknowledged. [1] Stark et al., Adv. Mater. 2019, 31, 1808213 [2] Harling et al., Carbon 244 (2025) 120711

TT 69: Focus Session: Nickelate Superconductivity: Insights into Unconventional Pairing and Correlation Effects II (joint session TT/DS/MA)

Time: Thursday 9:30–12:30 Location: HSZ/0003

TT 69.1 Thu 9:30 HSZ/0003

Bulk High-Temperature Superconductivity and Density Waves in Layered Nickelates — •Jun Luo[1,2], Jie Dou[1,2], Shuo Li[1], Qin Xin Shen[1,2], Xu Yang Feng[1,2], De Min Chai[1,2], Ran Sheng Jia[1,2], Jie Yang[1,2], and Rui Zhou[1,2] — [1]Institute of Physics, Chinese Academy of Sciences, and Beijing National Laboratory for Condensed Matter Physics, Beijing 100190, China — [2]School of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100190, China

The recent advances in bilayer nickelates $La_3Ni_2O_7$ have revealed fascinating high-temperature superconductivity (HTSC) under high-pressure conditions, offering a promising platform to explore unconventional superconducting mechanisms. In this talk, I will first discuss the discovery of bulk HTSC in Pr-doped $La_2PrNi_2O_7$, where Pr substitution effectively suppresses intergrowth phases, resulting in nearly pure bilayer structures. Superconducting onset temperature reaches 82.5 K at 16 GPa. Clear diamagnetic signals confirm the bulk nature of HTSC. I will also present microscopic evidence of charge and spin density wave (CDW/SDW) orders in $La_3Ni_2O_7$, revealed through 139La nuclear quadrupole resonance (NQR). Below the density wave transition temperature, we observe distinct line splitting and magnetic broadening, indicating unidirectional CDW order coupled with SDW order. By integrating insights from high-pressure and NQR studies, this work provides a comprehensive understanding of the structural and electronic mechanisms underlying HTSC in bilayer nickelates, paving the way for future experimental and theoretical investigations.

TT 69.2 Thu 9:45 HSZ/0003

ARPES spectra and the role of interstitial-*s* orbital in infinite-layer nickelates calculated by DFT+DMFT — •Leonard Verhoff[1], Liang Si[1,2], and Karsten Held[1] — [1]Institut für Festkörperphysik, Technische Universität Wien, Wien, Austria — [2]School of Physics, Northwest University, Xi'an, China

Infinite-layer nickelates, such as $NdNiO_2$, are a compelling platform to explore the microscopic origin of unconventional high-temperature superconductivity, from both theoretical and experimental perspectives.

Experimentally, infinite-layer nickelates are reduced from the stable perovskite phase, leaving an empty apical oxygen site. *Density functional theory* (DFT) calculations show that the resulting interstitial vacancy hosts localized, *s*-like states about 2 eV above the fermi level, while recent *angle-resolved photoemission spectroscopy* (ARPES) measurements of superconducting $NdNiO_2$ thin films conjectured Fermi surfaces with major *s*-like orbital character, highlighting a possible role of interstitial-*s* states in superconductivity.

We present DFT and *dynamical mean field theory* calculations of Fermi surfaces and band structures for both bulk and slab geometries, directly comparable to ARPES spectra. Our ARPES simulations explicitly include first-principles photoemission matrix elements, capturing the impact of orbital shapes on the measured intensity. We show how the correlated band structure reproduces low-energy ARPES spectra and identify the features dominated by interstitial-*s* character.

We acknowledge support through a joint German and Austrian Science Funds (DFG and FWF) project; FWF project ID I5398.

TT 69.3 Thu 10:00 HSZ/0003

A photoinduced two-dimensional electron gas (2DEG) at infinite-layer nickelate/strontium titanate interfaces — •D. Sanchez-Manzano[1], G. Krieger[2], A. Raji[3], B. Geisler[4], V. Humbert[1], H. Jaffres[1], J. Santamaria[5], R. Pentcheva[4], A. Glotter[3], D. Preziosi[2], and Javier E. Villegas[1] — [1]Laboratoire Albert Fert, CNRS, Thales, Université Paris-Saclay, France. — [2]Institute of Physics and Chemistry of Materials of Strasbourg, CNRS, University of Strasbourg, France. — [3]Laboratoire de Physique de Solides, CNRS, Université Paris-Saclay, France. — [4]Department of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, Germany — [5]6Departamento de Física de Materiales, Universidad Complutense de Madrid, Spain

We demonstrate, through experiments (transport, electron microscopy & spectroscopy) and density functional theory (DFT), that a high-mobility 2DEG can be optically switched on and off at an oxide interface where such a state does not naturally exist [1]. We show that near-ultraviolet light instantly creates a volatile 2DEG at the interface between $SrTiO_3$ (a band insulator) and infinite-layer $NdNiO_2$ (a poor metal), resulting in a conductivity increase of up to five orders of magnitude. This stems from structural and electronic reconstructions that, along with a built-in interfacial electric field, facilitate the Ti-3d band occupation by photogenerated carriers. These findings open venues for engineering photoconductance in strongly correlated systems.

[1] Sanchez-Manzano et al., Nat. Mater. (2025). https://doi.org/10.1038/s41563-025-02363-y

TT 69.4 Thu 10:15 HSZ/0003

Democratizing nickelates superconductors: Topotactic reduction induced by aluminum sputter deposition — •Lucía Iglesias[1], Dongxin Zhang[1], Aravind Raji[2,3], Luis M. Vicente-Arche[1], Alexandre Gloter[2], and Manuel Bibes[1] — [1]Laboratoire Albert Fert, CNRS, Thales, Université Paris-Saclay — [2]Laboratoire de Physique des Solides, CNRS, Université Paris-Saclay — [3]Synchrotron SOLEIL

Superconductivity in infinite-layer (IL) nickelates (ABO_2) was discovery in 2019, opening a new research frontier. However, progress remains limited by the challenging topotactic reduction needed to remove all apical oxygens from the perovskite precursor, typically achieved through a complex ex situ CaH_2 method. Although recent in situ approaches, such as metal overlayer deposition via molecular beam epitaxy and atomic hydrogen bombardment, have improved control and reproducibility, their restricted accessibility highlights the need for simpler synthesis routes. Here, we demonstrate a broadly accessible method to fabricate superconducting IL $Pr_{0.8}Sr_{0.2}NiO_2$ films via aluminum deposition using direct-current magnetron sputtering. The sputtered Al drives the reduction through a redox reaction, converting the precursor perovskite into the superconducting IL phase. Systematic optimization of Al-induced reduction yields high-quality films with a maximum transition temperatures of 17 K, consistent with the best reported values. This accessible and highly reproducible approach provides an effective alternative to existing techniques and lowers barriers to the exploration of nickelate superconductors.

TT 69.5 Thu 10:30 HSZ/0003

Two-dimensional vortex matter in infinite-layer nickelates — •David Sanchez-Manzano[1], Vincent Humbert[1], Araceli Gutiérrez-Llorente[1,2], Dongxin Zhang[1], Jacobo Santamaría[3], Manuel Bibes[1], Lucia Iglesias[1], and Javier E. Villegas[1] — [1]Laboratoire Albert Fert, CNRS, Thales, Univerisité Paris-Saclay, 91767 Palaiseau, France — [2]Escuela Superior de Ciencias Experimentales y Tecnología, Universidad Rey Juan Carlos, 28933 Madrid, Spain — [3]GFMC, Dpto. de Física de Materiales, Facultad de Ciencias Físicas, Universidad Complutense de Madrid, 28040 Madrid, Spain

Characterizing the dimensionality of the superconducting state in the infinite-layer (IL) nickelates is crucial to understanding its nature. Most studies have addressed the problem by studying the anisotropy of the upper critical fields. Yet, the dominance of Pauli-paramagnetism effects over orbital ones makes it challenging to interpret the experiments in terms of dimensionality. Here we address the question from a different perspective, by investigating the vortex phase diagram in the mixed-state. We demonstrate that superconducting $Pr_{0.8}Sr_{0.2}NiO_2$ thin films present a vortex liquid-to-glass transition of a two-dimensional nature. The obtained results suggest that bidimensionality is an intrinsic property, and that superconductivity resides in fully-decoupled NiO_2 planes. In this scenario, the coherence length along the c-axis must be shorter than the distance between those planes, while Josephson and magnetostatic coupling between them must

be negligible. We believe that these conclusions are relevant for theories on the origin of superconductivity in the IL-nickelates.

TT 69.6 Thu 10:45 HSZ/0003

Systematically Controlled Disorder to Probe Pairing Symmetry in Infinite-Layer Nickelates — •A. Ranna[1], R. Grasset[2], M. Gonzalez[3], K. Lee[3], B. Y. Wang[3], D. Zhang[4], W. Sun[5], C. Parzyck[6], Y. Wu[6], M. Konczykowski[2], M. Bibes[4], K. M. Shen[6], Y. F. Nie[5], L. Iglesias[4], H. Y. Hwang[3], A. P. Mackenzie[1], and B. H. Goodge[1] — [1]MPI CPfS, Germany — [2]LSI, Ecole Polytechnique, France — [3]Stanford University, USA — [4]CNRS Thales, France — [5]Nanjing University, China — [6]Cornell University, USA

Superconductivity in infinite-layer nickelates has expanded rapidly with advances in thin-film synthesis and reduction techniques. A central question is the symmetry of the superconducting gap in these materials. Because superconducting samples can only be stabilized as thin films and suffer surface degradation during the post-growth reduction process, some conventional probes to determine the gap symmetry remain challenging to perform and interpret. Here, we leverage high-energy electron irradiation to controllably introduce point-like defects without altering film stoichiometry or crystallinity. Tracking superconductivity with systematically increasing disorder shows a steady suppression of transition temperature and rising normal state resistivity, indicative of an unconventional, sign-changing gap [1] . Additionally, this method offers a unique way to study the effect of point defects on superconducting and electronic properties in nickelates across rare-earth compositions, doping, and strain to disentangle intrinsic behavior from synthesis-related variability.

[1] Ranna et al., *PRL* **135**, 126501 (2025).

15 min. break

TT 69.7 Thu 11:15 HSZ/0003

Correlated electronic structure of $La_3Ni_2O_6$ and $La_3Ni_2O_{6.5}$ — •Frank Lechermann, Steffen Bötzel, and Ilya M. Eremin — Theoretische Physik III, Fakultät für Physik und Astronomie, Ruhr-Universität Bochum, Bochum, Germany

There are two known superconducting nickelate families, i.e. low-valence Ni($3d^{9-\delta}$) compounds and Ruddelsden-Popper (RP) compounds with Ni($3d^{8\pm\delta}$) valence. While both families host NiO_2 square planes, key difference is given by the missing apical oxygen atoms in the low-valence nickelates. A possible route to connect both nickelate families might be given by the reduction of the $La_3Ni_2O_7$ RP bilayer compound, i.e. by removing it's apical oxygens. Complete removal results in the $La_3Ni_2O_6$ compound, while taking out only half of the apical oxygens results in the $La_3Ni_2O_{6.5}$ compound. Both reduced materials are so far only scarcely characterized experimentally, but display quite intriguing correlation physics from theory. We will discuss the results of advanced first-principles many body calculations for these two nickelates, highlighting different mechanisms of Mott criticality as well as challenging low-temperature physics.

TT 69.8 Thu 11:30 HSZ/0003

Superconductivity governed by Janus-faced fermiology in strained bilayer nickelates — •Siheon Ryee[1], Niklas Witt[2], Giorgio Sangiovanni[2], and Tim Wehling[1] — [1]University of Hamburg, Hamburg, Germany — [2]University of Würzburg, Würzburg, Germany

High-temperature superconductivity in pressurized and strained bilayer nickelates has emerged as a new frontier. One of the key unresolved issues concerns the fermiology that underlies superconductivity. On both theoretical and experimental sides, no general consensus has been reached, and conflicting results exist regarding whether the relevant Fermi surface involves a γ pocket—a hole pocket with d_{z^2}-orbital character centered at the Brillouin zone corner. Here, we address this issue by unveiling a Janus-faced role of the γ pocket in spin-fluctuation-mediated superconductivity. We show that this pocket simultaneously induces dominant pair-breaking and pair-forming channels for the leading $s_\pm$-wave pairing. Consequently, an optimal superconducting transition temperature T_c is achieved when the γ pocket surfaces at the Fermi level, placing the system near a Lifshitz transition. This suggests that superconductivity can emerge, provided the maximum energy level of the γ pocket lies sufficiently close to the Fermi level, either from below or above. Our finding not only reconciles two opposing viewpoints on the fermiology, but also naturally explains recent experiments on $(La,Pr)_3Ni_2O_7$ thin films, including the superconductivity under compressive strain, two conflicting measurements on the Fermi surface, and the dome shape of T_c as a function of hole doping.

TT 69.9 Thu 11:45 HSZ/0003

Bonding-antibonding $s_\pm$ superconductivity in bilayer nickelates: potential experimental signatures — •Steffen Bötzel, Frank Lechermann, and Ilya Eremin — Ruhr-Universität Bochum, Bochum, Germnay

The discovery of high-T_c superconductivity in Ruddelsden-Popper bilayer nickelates under applied high pressure and/or compressive strain provides a promising platform to study the interplay of multiorbital intralayer and interlayer Cooper-pairing in bilayer systems. In particular, dominant interlayer pairing may naturally lead to a bonding-antibonding $s_\pm$-gap structure, which directly reflects the bilayer geometry. Such a scenario would produce characteristic experimental signatures that differ from d-wave type gap symmetries. In this contribution, we theoretically address the possible gap structures in bilayer nickelates and discuss how a interlayer-dominated bonding-antibonding $s_\pm$-gap structure can be potentially distinguished from a d-wave type pairing using experimentally observables.

TT 69.10 Thu 12:00 HSZ/0003

Interlayer interaction-driven $s^\pm$-to-d_{xy}-wave superconductivity in $La_3Ni_2O_7$ under pressure — •Lauro B. Braz[1], George B. Martins[2], and Luis G. G. de V. D. Da Silva[1] — [1]Instituto de Física, Universidade de São Paulo, Rua do Matão 1371, São Paulo, São Paulo 05508-090, Brazil — [2]Instituto de Física, Universidade Federal de Uberlândia, Uberlândia, Minas Gerais 38400-902, Brazil

Experimental and theoretical progress on the normal-state properties of the high-temperature superconductor $La_3Ni_2O_7$ has provided evidence of strong interlayer interactions. To better understand the effects of interlayer interactions in $La_3Ni_2O_7$ under high pressure, we investigate a two-layer, two-orbital electron model that includes both intra- and interlayer Coulomb interaction terms within the framework of the matrix random-phase approximation. Our analysis reveals that interlayer interactions play a crucial role in determining the preferred superconducting pairing symmetry. Specifically, when interlayer interactions are included, a d_{xy}-wave pairing symmetry is favored over the $s^\pm$-wave symmetry, which was previously found to dominate in their absence. Furthermore, we find that interlayer interactions enhance interorbital pairing by incorporating contributions from all three electron pockets, which originate from both $d_{3z^2-r^2}$ and $d_{x^2-y^2}$ orbital characters. This results in the emergence of nodes in the superconducting gap function - features absent in the $s^\pm$-wave state - ultimately stabilizing the d_{xy}-wave pairing symmetry.

TT 69.11 Thu 12:15 HSZ/0003

Incommensurate spin-fluctuations and competing pairing symmetries in $La_3Ni_2O_7$ — •Han-Xiang Xu[1] and Daniel Guterding[2] — [1]Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing, China — [2]Technische Hochschule Brandenburg, Brandenburg an der Havel, Germany

The discovery of superconductivity in the bilayer nickelate $La_3Ni_2O_7$ under high pressure raises key questions about the pairing symmetry and microscopic mechanism. Using a three-dimensional multi-orbital Hubbard model including all Ni 3d and O 2p states, we analyze the superconducting instability within the random phase approximation. Spin fluctuations with incommensurate wave vectors $(\pi/2, \pi/2)$ and $(7\pi/10, 7\pi/10)$ coexist and compete, leading to nearly degenerate sign-changing $s_\pm$- and $d_{x^2-y^2}$-wave pairing channels. The leading symmetry depends sensitively on pressure and the ratio of Hund's rule to Coulomb interactions. Cooperative incommensurate fluctuations stabilize a $d_{x^2-y^2}$-wave state for realistic parameters, while their competition may explain the absence of magnetic order. These findings reconcile previous contradictory results and highlight the importance of careful model construction for bilayer nickelates.

[1] H.-X. Xu and D. Guterding, arXiv:2501.05254

TT 70: Correlated Electrons: Method Development III

Time: Thursday 9:30–10:45 Location: HSZ/0101

TT 70.1 Thu 9:30 HSZ/0101

Lineon Condensation in the XY toric code — •Maximilian Vieweg, Viktor Kott, Matthias Mühlhauser, and Kai Phillip Schmidt — Staudtstraße 7, 91058 Erlangen, Germany

In this work, we study the XY toric code[1] in an external magnetic field and determine its quantum phase diagram using high-order series expansions. The XY toric code is a generalization of the toric code that introduces anisotropic couplings on the star operators. The phase diagram of the XY toric code without a magnetic field is exactly solvable via duality mappings and hosts both topologically ordered and spontaneous-subsystem-symmetry-broken phases (SSSB), and therefore supports fractons and subdimensional particles as excitations in the SSSB phase. Our results for the transitions out of the SSSB in certain parameter regimes are consistent with an exotic second-order phase transition that is not described by a scale-invariant theory.

[1] M. Vieweg, K.P. Schmidt, Phys. Rev. Res. 7 (2025)

TT 70.2 Thu 9:45 HSZ/0101

Real Green functions for the Anderson disorder model — •Marcus Kollar[1], Martin Biehle[1], Yannick Schäffer[1], and Bas Lodewijks[2] — [1]Theoretical Physics III, Institute of Physics, University of Augsburg — [2]Probability Group, School of Mathematical and Physical Sciences, University of Sheffield

Green functions for the Anderson model on the Bethe lattice fulfill a recursion relation, leading to a self-consistent solution for the complex self-energy [1]. Recently a new criterion for the localization transition was introduced [2] using the susceptibility of real cavity Green functions to changes of the disorder potential at distant lattice sites, which can be expressed in terms of repeated applications of an asymmetric integral kernel corresponding to the conditional probability distribution of cavity Green functions on neighboring sites. We derive a system of equations that connects this integral kernel and the distributions of real local and cavity Green functions to an arbitrary disorder distribution. For the special case of Cauchy disorder we use it to determine the Green function distributions explicitly for all energies. Furthermore for the band center we determine the complete kernel spectrum exactly, from which typical Lyapunov exponents and Green function correlation functions are obtained. Applications to other disorder distributions are also discussed.

[1] R. Abou-Chacra et al., J. Phys. C **6**, 1734 (1973).
[2] G. Parisi et al., J. Phys. A **53**, 014003 (2019).

TT 70.3 Thu 10:00 HSZ/0101

CFET-Enhanced TDVP Simulations of Floquet Dynamics in the Driven t-V Model — •Tobias Blum[1], Karun Gadge[2], Salvatore Manmana[2], and Reinhard Noack[1] — [1]Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Georg-August-University Göttingen, 37077 Göttingen, Germany

Periodically driven interacting systems feature characteristic Floquet sidebands and frequency-dependent heating, but time evolution remains challenging for explicitly time-dependent Hamiltonians. We study the one-dimensional t-V model using the time-dependent variational principle (TDVP) combined with commutator-free exponential time propagators (CFET). We describe the integration of CFET into an already existing implementation of TDVP within the MPS framework. Its integration allows significantly reduced time-evolution errors. We compare standard TDVP and TDVP enhanced with CFET and analyze heating rates and the structure of Floquet sidebands for different driving frequencies, going from high-frequency regimes to low-frequency behavior. The results show that CFET-enhanced TDVP substantially improves the accuracy of calculated observables in explicitly time-dependent strongly correlated systems.

TT 70.4 Thu 10:15 HSZ/0101

Noninteracting tight-binding models for Fock parafermions — •Edward McCann — Department of Physics, Lancaster University, Lancaster, LA1 4YB, United Kingdom

By mapping itinerant spin-1/2 fermions to four-state Fock parafermions, we construct noninteracting tight-binding models for Fock parafermions in one dimension. They have single-particle real energy spectra consisting of a sum of single-particle energy levels each multiplied by a parafermionic occupation number. The single-particle levels may be determined by diagonalizing a square matrix whose order scales linearly with system size, and these levels are the same as those of noninteracting fermionic models. We generalize the approach to describe tight-binding models in two dimensions. We show that the thermodynamic distribution function for the occupation numbers of noninteracting four-state parafermions, the internal energy, and the heat capacity are consistent with the mapping to spin-1/2 fermions.

TT 70.5 Thu 10:30 HSZ/0101

A new take on an old method for approximating quantum many-body ground states — •Joe Crossley[1], Bruno Bertini[2], Arash Jafarizadeh[3], Molly Gibbins[1], and Adam Gammon-Smith[1] — [1]University of Nottingham, United Kingdom — [2]University of Birmingham, United Kingdom — [3]None

For decades, quantum chemists have been using so-called "post Hartree-Fock" methods to study systems of many interacting electrons moving on a fixed structural background. This set-up closely resembles many important problems from the world of condensed matter physics. However, despite the conceptual overlap, these methods have seen little adoption within the physics community. In this talk, I will discuss our recent progress on exploring the potential of post Hartree-Fock techniques applied to condensed matter problems—particularly in regimes where standard tools such as tensor networks and quantum Monte Carlo are known to struggle.

TT 71: Ultrafast Phenomena

Time: Thursday 9:30–11:15 Location: HSZ/0103

TT 71.1 Thu 9:30 HSZ/0103

Ultrafast control of competing FM and CDW orders in $SmNiC_2$ — •Chandra V Kotyada[1], Bhageerath Swaraj[1], Amon. P Lanz[1], Priyanka Yogi[1], Amir.A Haghighirad[2], Sofia. M Souliou[2], Matthieu Le Tacon[2], and Jure Demsar[1] — [1]JGU Mainz — [2]KIT

$SmNiC_2$ belongs to the rare-earth (R) transition-metal carbide family $RNiC_2$, a unique class of intermetallic compounds that crystallize in the non-centrosymmetric orthorhombic $CeNiC_2$-type structure and exhibit pronounced quasi-one-dimensional characteristics. Diffraction studies on $SmNiC_2$ reveal an incommensurate charge-density-wave (CDW) modulation with wavevector $(0.5,\ 0.5+\delta,\ 0)$ below $T_{CDW} \approx 148$ K. Upon lowering the temperature, a first-order phase transition into a ferromagnetic (FM) state occurs at $T_M \approx 18$ K, accompanied by a complete suppression of the CDW order.

Here, we apply optical pump-probe spectroscopy to investigate collective response in both symmetry-broken phases. Using CDW amplitude mode as a fingerprint of the CDW order, we then use the quench-pump-probe approach to track the dynamics of the photoinduced FM-to-CDW phase transition. We show that the buildup of the CDW after quenching the FM order is limited by the demagnetization time of 10 ps.

TT 71.2 Thu 9:45 HSZ/0103

Experimental signature of transient symmetry breaking in a cavity superconductor — •Siyu Duan[1,2], Jingbo Wu[1], Xiaoqing Jia[1], Huabing Wang[1], Ilya M. Eremin[3], Götz S. Uhrig[2], Biaobing Jin[1], and Zhe Wang[2] — [1]Research Institute of Superconductor Electronics (RISE) & Key Laboratory of Optoelectronic Devices and Systems with Extreme Performances of MOE, School of Electronic Science and Engineering, Nanjing University, Nanjing 210023, China — [2]Department of Physics, TU Dortmund University, 44227 Dortmund, Germany — [3]Institut für Theoretische Physik III, Ruhr-Universität Bochum, 44801 Bochum, Germany

Transient states of matter far from equilibrium may exhibit physical properties beyond those allowed by the equilibrium-state crystalline symmetries. We explore ultrafast and direct electronic excitations of transient states in a cavity superconductor by using time-resolved terahertz-pump terahertz-probe spectroscopy. Our results show that the strong terahertz field can transiently modify the symmetries of the electronic subsystems via the injection of a transient supercurrent, leading to high-order nonlinear dynamical responses that are not compatible with the equilibrium-state symmetries, which evidences for transient symmetry breaking on the picosecond time scale. Our study also finds that the strong coupling of the superconductor to the designed microcavities enables the sensitive detection of the nonlinear responses associated to the transient symmetry breaking.

TT 71.3 Thu 10:00 HSZ/0103

Giant Dynamical Paramagnetism in the driven fluctuating superconductors — •Marios Michael[1], Duilio De Santis[2], Eugene Demler[2], and Patrick Lee[3] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Straße 38 01187 Dresden Germany — [2]Institute for Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland — [3]Department of Physics, MIT, 77 Massachusetts Avenue, 02139 Cambridge, MA, USA

In the past decade, photo-induced superconducting-like behaviors have been reported in a number of materials driven by intense pump fields. Of particular interest is the high-Tc cuprate Y Ba2 Cu2 O(6+x) (YBCO), where such effect has been reported up to the so-called pseudogap temperature T* ~ 300-400 K. In a recent tour-de-force experiment, a transient magnetic field which is proportional to and in the same direction of an applied field has been observed outside the sample, suggestive of flux exclusion due to the Meissner effect. In this talk I will present a different explanation of these experiments, based on the model of preformed Cooper pairs in the pseudogap phase. I will demonstrate that a combination of external magnetic field and strong terahertz drive used in experiments by Fava et al. Nature 2024, results in a novel Floquet instability in the model. This instability results in currents at the edges of the bilayer formed by defects or grain boundaries, with the current flowing in the opposite direction of the equilibrium screening current, producing a giant paramagnetic magnetization in the same direction as the applied field. We show how this scenario can fit most of the available data.

TT 71.4 Thu 10:15 HSZ/0103

Two-dimensional coherent spectroscopy of multiband superconductor — •Silvia Neri — Max Planck for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart

An intriguing question in superconductivity is how to efficiently detect signatures of the collective excitations associated with the superconducting order parameter. The features associated with collective modes can indeed provide in-

sight into various aspects of the superconducting state. We address this question by theoretically modeling a 2D THz pump probe spectroscopy experiment for a two-band superconductor. Two-dimensional spectroscopy is a powerful method with wide applications, from rovibronic excitations in biomolecular systems to magnons in antiferromagnets, and it has been recently applied to superconducting collective modes [1]. To numerically compute the dynamics of our model, we adopt a pseudospin description and choose realistic parameters for both the pulses and the superconducting state, reflective of MgB_2. The numerically evaluated 2D spectrum shows, in addition to the first- and third-harmonic signals, the presence of sidebands associated with the Leggett-mode frequency of the system. We then derive an analytical expression for the nonlinear current to identify the process responsible for this numerical finding. Our results suggest that applying 2D techniques to superconductors offers a promising route for exploring their collective dynamics.

[1] A. Dutta et al., J. Phys.: Condens. Matter 37, 203002 (2025)

TT 71.5 Thu 10:30 HSZ/0103

Ultrafast coherent dynamics in open quantum systems: Auger-Meitner decay and controlled stearing of interactions in SF_6 — •Sina Shokri[1], Patrick Rupprecht[2,3], Thomas Pfeifer[3], and Maurits W. Haverkort[1] — [1]ITP, Universität Heidelberg, 69120 Heidelberg, Germany — [2]UC Berkeley Dept. of Chemistry and LBNL Chemical Sciences Division, Berkeley, CA 94720, USA — [3]MPI für Kernphysik, 69117 Heidelberg, Germany

Ultrafast x-ray pump-probe spectroscopy provides a powerful tool to study and steer quantum materials on their intrinsic time and length scales. In correlated molecules and solids, theoretical understanding remains challenging due to the interplay of competing interactions. In small molecules, quantitative modeling of the coupled electronic and vibrational dynamics is possible.

The coupling to many continuous degrees of freedom can lead to rapid loss of coherence. This results in long-time dynamics that are determined by classical equations of motion. Descriptions on the intermediate time scale that show how one goes from coherent quantum dynamics to classical equations of motion are highly non-trivial.

In this work, we employ nonlinear response theory to predict the transient dynamics and Auger-Meitner-induced lifetimes of electronic excitations in x-ray absorption spectroscopy of SF_6, following excitation by an intense infrared laser field. Based on first-principles density functional theory calculations, we show how the intense laser field can modify the Auger-Meitner decay channels and, with that, the coherent lifetimes of excitations.

TT 71.6 Thu 10:45 HSZ/0103

Charged three-particle bound states at the L_{23}-edge in $SrTiO_3$ — •Sarah L. Görlitz[1], Widad Louafi[2], Sina Shokri[1], Martin Brass[1], Marc Merstorf[1], Jonas Hoecht[1], Kevin Ackermann[1], and Maurits W. Haverkort[1] — [1]Institut for Theoretical Physics, Heidelberg University, 69120 Heidelberg — [2]Laboratory of Theoretical Physics, Faculty of Exact Sciences, University of Bejaia, 06000 Bejaia, Algeria

Few-body bound states underpin phenomena across physics-from hadronic three-body systems to excitons and trions in semiconductors-yet their formation and decay remain poorly understood.

We report analogous physics in bulk $SrTiO_3$ in Ti 2p → 3d core excitations. The XAS spectrum shows seven sharp peaks, understood from atomic physics as a Ti 2p hole interacting with a local Ti 3d electron in a cubic point group. Fluorescence and Auger-Meitner decay calculations explain the linewidth of the first four peaks but predict much sharper excitations than observed for the last two. Because these highest excited states are degenerate with the continuum, their broadening may arise if they are continuum excitations or resonances rather than bound excitons. To test this, we performed ab initio GW+BSE calculations, which agree with parameter-based atomic multiplet theory and reveal seven infinitely sharp excitons. In contrast, an Anderson-impurity model yields a finite linewidth for the highest excitons. We show that these are three-particle bound states composed of two locally bound Ti 3d electrons, one Ti 2p hole, and an additional free hole in the O 2p valence band.

TT 71.7 Thu 11:00 HSZ/0103

Study of light-induced band inversion in SnTe via Ab Initio Calculations — •Asier Ribechini[1], Álvaro R. Puente-Uriona[1], and Julen Ibañez-Azpiroz[1,2,3] — [1]Centro de Física de Materiales (CSIC-EHU), 20018, Donostia, Spain — [2]IKERBASQUE, Basque Foundation for Science, 48009 Bilbao, Spain — [3]Donostia International Physics Center (DIPC), 20018 Donostia, Spain

Modern technology enables precise control of matter through light-matter interactions. Periodically driven quantum systems, described by Floquet theory, offer a powerful framework for predicting light-induced phenomena, including topological phases and quantum phase transitions [1], though their experimental detection remains challenging.

We evaluate the method of our group [2] for computing the Floquet quasienergy spectrum of SnTe using the velocity gauge in a truncated Hilbert space to build the ab initio time-periodic Hamiltonian. From it, we construct the effective Floquet Hamiltonian and obtain the quasienergy spectrum. Our results reveal a light-induced gap opening between conduction and valence band Floquet replicas near resonant driving, as well as a band-character inversion indicative of a possible light-induced topological phase transition. We further compute the corresponding topological invariants to characterize this transition and discuss our findings in relation to recent time-resolved ARPES evidence for light-induced topological behavior[3].

[1] J. I. Inoue et al., Phys. Rev. Lett. 105, 017401 (2010)
[2] Á. R. Puente-Uriona et al., Phys Rev. B 110, 125203 (2024)
[3] F. Chassot et al., arXiv:2502.11967v1

TT 72: Correlated Magnetism – Spin Liquids I

Time: Thursday 9:30–12:00 Location: HSZ/0105

TT 72.1 Thu 9:30 HSZ/0105

Anisotropic Spin Ice on a Breathing Pyrochlore Lattice — •Gloria Isbrandt[1,2], Frank Pollmann[1,2], and Michael Knap[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany

Spin ice systems represent a prime example of constrained spin systems and exhibit rich low-energy physics. We investigate how a tunable anisotropic spin coupling modifies the classical Ising spin-ice Hamiltonian on the breathing pyrochlore lattice. Introducing sublattice-dependent anisotropy reshapes the ground-state manifold, reduces the residual entropy, and induces qualitative changes in the spin-structure factor. We theoretically uncover a rich phase diagram by varying the anisotropy and demonstrate how this modification reduces the ground state degeneracy across different phases. Using Monte Carlo simulations, we find that at low temperatures the system either crosses over into a constrained spin-ice manifold, whose entropy density falls below the Pauling value, or undergoes a transition into an ordered, symmetry-broken state. We further compute spin-structure factors for the anisotropic model and show that they are well captured by a self-consistent Gaussian approximation. Our results develop the understanding of spin ice in anisotropic limits, which may be experimentally realized by strain, providing, among others, key signatures in entropy and specific heat.

TT 72.2 Thu 9:45 HSZ/0105

The monopole plasma resonance: an opto-electronic smoking gun of 3D U(1) spin liquids — •Anish Koley, Saranyo Moitra, and Inti Sodemann Villadiego — Institut für Theoretische Physik, Universität Leipzig,04103 Leipzig, Germany

Certain 3D U(1) spin liquids, such as those arising in quantum spin ice models, have a low-energy "monopole-like" emergent particle which acts as the source of an emergent magnetic field that has the same transformations under symmetries as an electric polarization. As a consequence, these monopoles carry a polarization physical electric charge. Curiously, at finite temperatures these monopoles form a finite density plasma, but due to their coupling to emergent gauge fields, the full physical system behaves as an electrical insulator from the point of view of DC transport. Remarkably, however, we have found that when the system is probed at finite frequencies, the monopoles can display a sharp and low frequency plasma resonance analogous to a metal. This offers a new blueprint to experimentally detect these elusive but fascinating states in real materials.

TT 72.3 Thu 10:00 HSZ/0105

Spin-liquid-like ground states in the double hydroxyperovskites $CuSn(OD)_6$ and $MnSn(OD)_6$ evidenced by μSR spectroscopy — •moumita naskar[1], anton a. kulbakov[1], kaushick k. parui[1], jonas a. krieger[2], ellen häussler[3], thomas doert[3], darren c. peets[1], hans henning klauss[1], dmytro s. inosov[1,4], and rajib sarkar[1] — [1]Institut für Festkörper und Materialphysik, Technische Universität Dresden, 01062 Dresden, Germany — [2]Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzer-

land — [3]Fakultät für Chemie und Lebensmittelchemie, Technische Universität Dresden, 01062 Dresden, Germany — [4]Würzburg-Dresden Cluster of Excellence on Complexity and Topology in Quantum Matter - ct.qmat, Technische Universität Dresden, 01062 Dresden, Germany

Muon spin rotation measurements were carried out on the hydroxy perovskites $CuSn(OD)_6$ and $MnSn(OD)_6$ over the temperature range 0.053-50 K. The absence of long range magnetic order is confirmed down to 0.053 K. The temperature dependence of the muon relaxation rates show an increase with decreasing temperature, indicating that spin fluctuations remain present down to 0.053 K in both the compounds. Spin correlations results from both samples indicate homogeneous spin dynamics. These observations suggest that both compounds possess a fluctuating ground state consistent with a spin-liquid phase.

TT 72.4 Thu 10:15 HSZ/0105

Emergent magnetic order and spin dynamics in a Yb-based triangular lattice delafossite — •Arjun Unnikrishnan[1,2,3], Bishnu Prasad Belbase[1], Piyush Chhallare[1], Mohan Bikram Neupane[1], Eun Sang Choi[4], Philipp Gegenwart[2], and Arnab Banerjee[1] — [1]Department of Physics and Astronomy, Purdue University, West Lafayette, Indiana 47906, USA — [2]Experimental Physics VI, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, Augsburg 86159, Germany — [3]Solid State and Structural Chemistry Unit (SSCU), Indian Institute of Science, Bengaluru - 560012, India — [4]National High Magnetic Field Laboratory, Tallahassee, Florida - 32310, USA

We have synthesized a new member of the $AYbX_2$ (A = monovalent cation; X = O, S, Se, Te) delafossite family and investigated its magnetic properties using magnetization and heat-capacity measurements. At zero magnetic field, the system shows no evidence of long-range magnetic order down to 20 mK. When a magnetic field is applied along the *ab*-plane, multiple field-induced magnetic phases emerge above ~ 2.5 T, followed by full spin polarization near 17 T. The material exhibits stronger exchange interactions compared to other known Yb-based delafossites. We will discuss the magnetic phase transitions and the evolution of the spin dynamics under applied fields. The heat-capacity results suggest the presence of a possible quantum spin liquid (QSL) phase at low temperatures and low magnetic fields, highlighting this system as a promising platform for exploring QSL physics.

TT 72.5 Thu 10:30 HSZ/0105

Microscopic modelling of the honeycomb system $Na_3Ni_2BiO_6$ and its field-induced phases — •Amanda Anna Konieczna, Panagiotis Stavropoulos, and Roser Valentí — Goethe Universität, Frankfurt am Main, Germany

Frustration in magnetic systems has for decades provided a central testbed for the investigation of unconventional properties. Among others, frustrated systems may show magnetic-field-induced phases with characteristic magnetization plateaus, as is the case in triangular lattice and Kagome lattice spin-1/2 systems, where magnetic frustration arises due to the geometry of the lattice. Although the honeycomb lattice geometry is not geometrically frustrated, frustration may still appear due to bond-dependent magnetic exchanges, as proven by the Kitaev honeycomb model with its quantum spin liquid ground state.

Experimental evidence for a one-third magnetization plateau at intermediate magnetic fields has been reported for the spin-1 honeycomb compound $Na_3Ni_2BiO_6$. The aim of this talk is to present our approach based on an ab initio scheme in order to understand the origin of the plateau phase. The approach involves the modeling of an ab-initio-derived multiorbital relativistic Hubbard Hamiltonian and utilize projective diagonalization techniques to construct an effective spin model. The data extracted from the model is compared to and discussed in the context of experimental findings.

TT 72.6 Thu 10:45 HSZ/0105

Evolution of $Na_3Co_2SbO_6$ under pressure — •Thore Martens[1], Prashanta Mukharjee[2], Philipp Gegenwart[2], and Alexander A. Tsirlin[1] — [1]Leipzig University — [2]University of Augsburg

$Na_3Co_2SbO_6$ is a potential candidate for the Kitaev spin liquid where the high-spin S=3/2-state is turned into the J_{eff}=1/2-state under spin-orbit coupling. Recently, the impact of the trigonal field in $Na_3Co_2SbO_6$ on the formation of the spin liquid phase has been discussed and theorized that finetuning of the trigonal field by applying pressure may lead to the desired Kitaev state. Therefore, neutron diffraction experiments are performed to obtain the lattice parameters and probe the evolution of the magnetically ordered state of $Na_3Co_2SbO_6$ under pressure. Using density functional theory, new relaxed unit cells are calculated as well as the subsequent exchange couplings and trigonal field as a function of pressure.

15 min. break

TT 72.7 Thu 11:15 HSZ/0105

Low temperature thermodynamic studies on the Kitaev candidates $Na_2Co_2TeO_6$ and $Na_3Co_2SbO_6$ — •Sebastian Erdmann[1], Prashanta Mukharjee[1], Chanhyeon Lee[2], Kwang-Yong Choi[3], and Philipp Gegenwart[1] — [1]Experimental Physics VI, University of Augsburg, Germany — [2]Department of Physics, Chung-Ang University, Republic of Korea — [3]Department of Physics, Sungkyunkwan University, Republic of Korea

Cobalt-based honeycomb magnets have recently attracted considerable attention as a new class of materials that may host bond-directional Kitaev interactions [1]. Among these, $Na_2Co_2TeO_6$ and $Na_3Co_2SbO_6$ undergo antiferromagnetic ordering below 27 K and 5 K, respectively [2, 3]. We employed heat-capacity and magnetic Grüneisen parameter measurements to study the nature of the various low-temperature field-induced phase transitions, building on our previous work with the sister compound $BaCo_2(AsO_4)_2$ [4]. The phase diagrams are extended to below 2 K and the entropy $S(T, B)$ of the different field-induced phases is determined. Our results provide new insights on proposed field-induced spin liquid states and reveal commonalities and distinctions of different prototype Kitaev candidate materials.

[1] H. Liu, G. Khaliullin, Phys. Rev. B 97, 014407 (2018).
[2] E. Lefrançois et al., Phys. Rev. B 94, 214416 (2016).
[3] J.-Q. Yan et al., Phys. Rev. Materials 3, 074405 (2019)
[4] Prashanta K. Mukharjee et al., Phys. Rev. B 110, L140407 (2024).

TT 72.8 Thu 11:30 HSZ/0105

High pressure phase transition of quantum spin liquid candidate $Na_2Co_2TeO_6$ observed using Raman spectroscopy — •Ihsan Ahmed Kolasseri[1], Subhadip Das[1,2], and Yong P. Chen[1] — [1]Aarhus University, Aarhus, Denmark — [2]University of Copenhagen, Copenhagen, Denmark

Quantum spin liquids (QSL) are materials that have possible data storage applications in quantum computing. Conflicting neighbor electron spin interactions of antiferromagnetically coupled magnetic atoms on triangle-based geometries can lead to QSL phase. Two structural phases of NCTO have been reported: the hexagonal $P6_322$ phase and the monoclinic C2/m phase. The hexagonal phase of NCTO has an antiferromagnetic ordering at 27 K. An in-plane magnetic field of 7T can suppress the QSL state because of the material's structure. Understanding and discovering different structural phases of these classes of materials is crucial to learn about QSL states. In this study we applied pressures upto 20 GPa on hexagonal NCTO single crystal and observed significant changes in the Raman peak profile. We have classified the pressure evolution into four pressure regions were the Raman peak profiles change drastically. High pressure single crystal X-ray diffraction and high pressure polarization dependent Raman study could be conducted to confirm this conclusion. Those data are currently under analysis, but will be briefly mentioned.

TT 72.9 Thu 11:45 HSZ/0105

Pressure dependent ab-initio studies of the Kitaev candidate $Ag_3LiRh_2O_6$ — •Bolivar Efrain Insuasti Pazmino[1], Ramesh Dhakal[2], Shi Feng[3], Steve M. Winter[2], Johannes Knolle[3], and Alexander A. Tsirlin[1] — [1]Leipzig University, Germany. — [2]Wake Forest University, USA — [3]Technical University of Munich, Germany

$Ag_3LiRh_2O_6$ is created by substituting Li with larger Ag atoms in Li_2RhO_3 [1]. This "negative pressure" expands the lattice and distorts the RhO_6 octahedra, altering the Rh-O-Rh angle that governs proximity to the quantum spin liquid state. Under hydrostatic pressure, the compound shows a sharp reduction in Néel temperature up to 4 GPa, with a transition to a non-magnetic state only at 6.6 GPa [2].

We perform ab initio calculations on the ideal crystal. Geometry optimization and Wannier functions are obtained using DFT. Magnetic couplings are derived from second-order perturbation theory and exact cluster diagonalization. Both methods agree well on the general trends of the couplings, but also reveal differences. While a large negative off-diagonal Γ' along with the sizable trigonal crystal field may indicate deviations from the j_{eff}=1/2 state, the strong Kitaev coupling suggests the material remains close to that limit. The talk will address these questions by discussing the material's microscopic behavior. This work was supported by DFG via TRR360 (492547816).

[1] F. Bahrami et al., Sci. Adv. 8, eabl5671 (2022)
[2] P. Sakrikar, B. Shen, E. Poldi et al., Nat Com. 16:4712 (2025)

TT 73: Superconductivity: Tunneling and Josephson Junctions

Time: Thursday 9:30–12:45 Location: CHE/0089

TT 73.1 Thu 9:30 CHE/0089

Transparency-controlled multiple charge transfer in superconducting tunnel junctions at atomic scale — •Jiasen Niu[1,2,3], Yudai Sato[1,2,3], Maialen Larrazabal[4], Jian-feng Ge[5], and Milan Allan[1,2,3] — [1]Leiden Institute of Physics, Leiden University, Niels Bohrweg 2, 2333 CA Leiden, The Netherlands — [2]Fakultät für Physik, Ludwig-Maximilians-Universität, Schellingstrasse 4, München 80799, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), München, Germany — [4]Debye Institute of Nanomaterials Science, Utrecht University, PO Box 80000, 3508 TA Utrecht, The Netherlands — [5]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

Charge transport in superconducting junctions enable multi-charge transfer and can be identified through shot noise. Using shot noise STM with a newly developed amplifier, we measured Pb(111) junctions with tunable transparency. At low transparency, the effective charge is strongly suppressed (q < ne), while increasing transparency enhances AR/MAR, driving q toward 2e in SIN junctions and ne in SIS junctions. The measurements agree quantitatively with single-channel simulations. Our results track the continuous evolution from multi-electron to single-electron transport and demonstrate transparency as a key parameter in controlling superconducting quantum transport.

TT 73.2 Thu 9:45 CHE/0089

The Evolution of the Josephson Effect: From Dynamical Coulomb Blockade to Dissipationless Supercurrent — •Irena Padniuk[1], Xianzhe Zeng[1], Joachim Ankerhold[2], Juan Carlos Cuevas[3], Klaus Kern[1,4], and Christian R. Ast[1] — [1]MPI für Festkörperforschung, Heisenbergstraße 1, Stuttgart — [2]Institute for Complex Quantum Systems, University of Ulm, Albert-Einstein-Allee 11, Ulm — [3]Departamento de Física Teórica de la Materia Condensada and Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, Spain — [4]Institut de Physique, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

The Josephson effect measured with scanning tunneling microscopy (STM) offers a unique platform to study superconducting transport at the atomic scale. The tunneling of Cooper pairs in ultra-low temperature STM is typically dissipative due to the dynamical Coulomb blockade, involving energy exchange with the electromagnetic environment related to the junction's capacitance. In contrast, the well-known macroscopic Josephson effect between superconductors in planar tunnel junctions is dissipationless, allowing supercurrent to flow without energy loss. Until now, a direct connection between these two regimes has remained elusive. In my talk, I will discuss how, using our ultra-high energy resolution mK-STM, we investigate the evolution of the Josephson current over a wide range of junction transmissions. Our results provide insight into the transition between dissipative quantum transport and dissipationless Cooper pair tunneling in atomic-scale junctions.

TT 73.3 Thu 10:00 CHE/0089

Voltage fluctuations in atomic-scale Josephson junctions — •Verena Caspari[1], Werner M. J. van Weerdenburg[1], Christian Lotze[1], Clemens B. Winkelmann[2], and Katharina J. Franke[1] — [1]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin, Germany — [2]Univ. Grenoble Alpes, CEA, Grenoble INP, IRIG-Pheliqs, Grenoble, France

Phase diffusion in Josephson junctions and the switching from the superconducting to the quasiparticle branch can be explained by the dynamics of a fictitious phase particle in the tilted washboard potential. Usually, only the average voltage is measured[1].

Here, we measure the voltage fluctuations in single-atom Pb-Pb junctions with MHz-bandwidth using a scanning tunneling microscope. In the current-bias regime, the current-voltage V(I) curves show a hysteretic behavior that allows to set the junction into the phase-diffusion regime, where we observe multi-level transitions in time traces. These can be interpreted as phase-slips events leading to the finite average voltage in the superconducting state. In the voltage-bias regime, we observe bistabilities indicating the transition between the superconducting and the quasiparticle branch. Our experiments allow access to the phase-slip dynamics in the STM-based Josephson junction.

[1] R. L. Kautz, J. M. Martinis, Phys. Rev. B 42, 9903 (1990)

TT 73.4 Thu 10:15 CHE/0089

Non-Linear Response Theory of the Josephson Effect — •Christian R. Ast[1] and Juan Carlos Cuevas[2] — [1]MPI for Solid State Research, Stuttgart — [2]Universidad Autónoma de Madrid, Spain

The dissipationless supercurrent in the Josephson effect depends linearly on the junction conductance in a planar superconductor-insulator-superconductor tunnel junction, if there is no interaction with the environment. In ultrasmall tunnel junctions, such as in a scanning tunneling microscope (STM), the interaction with the environment cannot be neglected, which leads to a dissipative supercurrent that depends quadratically on the junction conductance. This dissipative supercurrent has been very successfully modeled within the dynamical Coulomb blockade and $P(E)$-theory based on Fermi's golden rule. In this talk, I will present a derivation of the dissipative supercurrent based on non-linear response theory. The result is basically identical to the existing model, although there are some distinct differences, which will be discussed.

TT 73.5 Thu 10:30 CHE/0089

Microwave mediated Cooper pair currents in single and double Josephson junctions — •Stefano Trivini[1], Leonard Edens[1], Jon Ortuzar[2], and Jose Ignacio Pascual[1,3] — [1]CIC nanoGUNE-BRTA, San Sebastian, Spain — [2]Quantronics group SPEC, CEA-Saclay — [3]Ikerbasque, Basque Foundation for Science, Bilbao, Spain

Tunnelling of Cooper pairs in STM Josephson junctions (JJs) is usually described as an incoherent process mediated by the junction's electromagnetic environment. Under microwave irradiation, photons can assist the tunnelling of quasiparticles as captured by the Tien-Gordon theory. For a current-biased, phase-coherent junction, Shapiro steps at voltages multiple of hv/2e are expected. Here, we study Pb-Pb single JJs realized in bulk Pb and in double JJs systems, formed by small Pb islands, under microwave irradiation. The microwave power maps depend on the tip-sample distance and can be described either by the TG approach or the RCSJ model. In double JJs, we observe asymmetric microwave maps whose shape reflects Coulomb-blockade processes on the Pb island.

TT 73.6 Thu 10:45 CHE/0089

Supercurrent Transport and Shapiro response in phase-pure core/shell GaAs/InAs nanowire-based Josephson junctions — •Farah Basaric[1,2], Yurii Kutovy[2,3], Alexander Pawlis[2,3], Detlev Grützmacher[1,2], and Thomas Schäpers[1,2] — [1]Peter Grünberg Institut (PGI9), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich and RWTH Aachen University, Germany — [3]Peter Grünberg Institut (PGI10), Forschungszentrum Jülich, 52425 Jülich, Germany

We investigate Josephson junctions based on epitaxially grown, phase-pure core/shell GaAs/InAs nanowires comprising closed-loop states in the InAs shell. The core/shell architecture, combined with superconducting Al, enables confined states in the InAs shell that are expected to enhance proximity coupling at the InAs/Al interface. Using shadow-wall evaporation for junction and contact definition, we are able to realize nanowire-based Josephson junctions in the short junction limit. Current-voltage characteristics measurements under radio-frequency irradiation reveal both integer as well as fractional Shapiro steps, the latter commonly associated with ballistic junctions. Additionally, magnetoconductance measurements on nanowires with normal contacts provide insight into the transport properties of the nanowire segment forming the weak link. Together, these results demonstrate that GaAs/InAs core/shell nanowires constitute a very promising platform for future quantum circuits based on hybrid devices.

15 min. break

TT 73.7 Thu 11:15 CHE/0089

Supercurrent Interference in Planar Josephson Junction Arrays Probed by Microwave Excitations — •Alexander Kirchner[1], Simon Feyrer[1], Vjeko Dimić[1], Sebastian Ramsauer[1], Johanna Berger[1], Narges Momeni[1], Francisco Jesus Matute-Cañadas[2], Davide Curcio[3], Matthias Kronseder[1], Michael Prager[1], Dieter Schuh[1], Dominique Bougeard[1], Giorgio Biasiol[3], Alfredo Levy Yeyati[2], Nicola Paradiso[1], Christoph Strunk[1], and Leandro Tosi[1,4] — [1]Institut für Experimentelle und Angewandte Physik, University of Regensburg, Regensburg, Germany — [2]Departamento de Física Teórica de la Materia Condensada, Condensed Matter Physics Center (IFIMAC) and Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, Madrid, Spain — [3]CNR-IOM Istituto Officina dei Materiali, Trieste, Italy — [4]Centro Atómico Bariloche and Insitituto Balseiro, CNEA, CONICET, San Charlos de Bariloche, Río Negro, Argentina

We present measurements of one dimensional Josephson junction arrays based on a hybrid superconductor-semiconductor quantum well heterostructure probed at microwave frequencies. The behavior of their plasma modes as a function of an applied magnetic field reveals interference patterns: an out-of-plane field results in a Fraunhofer-like pattern, from which we extract the effective transparency of the junctions; furthermore, periodic oscillations of the inductance occur when applying an in-plane magnetic field. The periodicity of these oscillations scales with the length of the island, pointing towards an orbital origin.

TT 73.8 Thu 11:30 CHE/0089

Purely even harmonic Josephson current due to crossed pair transmission across strongly spin-polarized materials — •Danilo Nikolić, Niklas L. Schulz, and Matthias Eschrig — Institut für Physik, Universität Greifswald, Felix-Hausdorff-Straße 6, 17489 Greifswald, Germany

We revisit the problem of the second harmonic generation in the current-phase relation across ferromagnetic bilayers placed between BCS superconductors. In particular, we consider a strongly spin-polarized metallic ferromagnet coupled to two superconducting leads via thin spin-active (left) and non-spin-active (right) insulating layers. The system is examined in the framework of the quasiclassical Green's function formalism both in the ballistic (Eilenberger) and the diffusive (Usadel) limit. Strong spin polarization allows for neglecting short-range mixed-spin correlations, and the Josephson supercurrent across the ferromagnet is fully mediated by long-range equal-spin triplet correlations. Using a diagrammatic technique for ballistic propagators, we describe the relevant Andreev processes responsible for the effective conversion of two spin-singlet Cooper pairs in the superconductor into two $\uparrow\uparrow$ and $\downarrow\downarrow$ pairs in the ferromagnet. Contrary to the naive picture of direct conversion, we show that the lowest order process involves four Cooper pairs in the superconductor, among which three are incoming and one is outgoing giving rise to net charge transport of $4e$ across the non spin-active interface. The self-consistent numerical treatment of the diffusive junction, typically more relevant in experiments, confirms this picture quantitatively.

TT 73.9 Thu 11:45 CHE/0089

Signatures of triplet pairing in FSF hybrid junctions — •Andreas Costa[1], Pablo Tuero[2], Cesar Gonzalez-Ruano[2,3], Yuan Lu[4], Farkhad G. Aliev[2], and Jaroslav Fabian[1] — [1]University of Regensburg, Germany — [2]Universidad Autónoma de Madrid, Spain — [3]Universidad Pontificia Comillas, Spain — [4]Université de Lorraine, France

Interfaces between ferromagnets and conventional s-wave superconductors serve as prototype systems to explore the conversion of singlet into spin-polarized triplet Cooper pairs in superconducting spintronics.

Recent experimental studies found anomalous quasiparticle conductance modulations in ferromagnet/superconductor/ferromagnet (FSF) hybrids under a rotated in-plane magnetic field. In this talk, we will report on our theoretical conductance simulations performed to unravel the physical origin of these anomalies. We will demonstrate that the experimental data show strong signatures of nonuniform magnetization and complex interfacial spin-orbit fields present in these junctions. As both are expected to induce spin-triplet Cooper pairs by rotating the spin quantization axis, we propose the observed conductance anomalies to provide a possible experimental fingerprint of unconventional triplet superconductivity.

The theory part of this work has been supported by Deutsche Forschungsgemeinschaft (DFG; German Research Foundation)—454646522; 314695032.

TT 73.10 Thu 12:00 CHE/0089

Critical current surfaces of multiterminal graphene Josephson junctions — •Paul Maier, Romain Danneau, and Detlef Beckmann — Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, D-76021 Karlsruhe, Germany

Topological states are predicted to exist in the Andreev bound state spectrum of multiterminal Josephson junction with four or more terminals [1]. Superconductor graphene hybrid structures are especially suitable to realize such devices due to the gate tunability of graphene and high contact transparencies which are necessary to form Andreev bound states. Understanding the distribution of supercurrent in graphene multiterminal Josephson junctions is one step in the search for these states. We report on the experimental investigation of transport in four-terminal graphene Josephson junctions with current control or phase control by up to two superconducting loops and flux lines. We observe magnetic interference patterns in two-terminal measurements and critical current surfaces by controlling a total of three currents or phases in multiterminal measurements, the results show excellent agreement with theoretical simulations.

[1] R.P. Riwar et al., Nat Commun 7, 11167 (2016).

TT 73.11 Thu 12:15 CHE/0089

Preserving the Josephson coupling of twisted cuprate junctions via tailored silicon nitride circuits boards — •Tommaso Confalone[1,2], Kornelius Nielsch[1,2], Golam Haider[1], and Nicola Poccia[1,3] — [1]IFW Dresden — [2]TU Dresden — [3]U. Naples

The fabrication of van der Waals (vdW) Josephson junctions (JJs) using the cuprate superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ (BSCCO) remains limited by the material's extreme sensitivity to heat and chemical processing, which hinders the integration of high-quality junctions into functional device architectures. Although the cryogenic stacking technique (CST) has enabled atomically sharp BSCCO interfaces with preserved superconducting properties [1], conventional CST-based devices rely on post-assembly contacting strategies that degrade junction performance or restrict circuit complexity. Here, we present a CST-compatible contact scheme in which electrodes embedded in a silicon nitride membrane are directly transferred onto the BSCCO junction during assembly [2]. This membrane-based transfer eliminates high-temperature or chemically aggressive steps and preserves interface integrity. Using this approach, we realize twisted BSCCO JJs exhibiting the strongest Josephson coupling reported to date. The technique is fully compatible with ultra-high-vacuum (UHV) environments, enabling integration with emerging UHV-based vdW fabrication platforms. These results underscore the critical role of contact engineering and open the path for exploring the fundamental properties of these devices.

[1] Science 382,1422 (2023)
[2] Small e06520 (2025)

TT 73.12 Thu 12:30 CHE/0089

Cooper quartets in frustrated Josephson junction arrays — •Erik Lennart Weerda[1], Matteo Rizzi[1,2], Michele Burrello[3] und Olav Fredrik Syljuåsen[4] — [1]Forschungszentrum Jülich — [2]Universität zu Köln — [3]University of Pisa — [4]University of Oslo

Josephson junction arrays in the shape of the dice lattice are the main candidates for a mesoscopic realization of superconductivity mediated by Cooper quartets of charge 4e. Here, we analyze numerical signatures of this exotic phase emerging when these superconducting arrays are frustrated by the insertion of 1/3 of a flux quantum per rhombic plaquette. Through the simulation of relaxation dynamics and two-dimensional infinite tensor network techniques, we examine the related classical XY model at finite temperature. We evaluate the characteristic properties of the supercurrent in this system, its correlation functions, and entropy. We also consider the effects of Josephson energy and flux disorder typical of Josephson junction arrays, and we address the role of charging energies in the full two-dimensional quantum model. Our results indicate that the peak of critical currents and temperatures at frustration 1/3 corresponds to a Cooper quartet phase, and the related superconducting-insulating phase transition is caused by the deconfinement of half-vortices.

TT 74: Topological Insulators

Time: Thursday 9:30–12:45 Location: CHE/0091

TT 74.1 Thu 9:30 CHE/0091

Probing the Quantized Berry Phases of an Obstructed Atomic Band in 1H-$NbSe_2$ Using Scanning Tunneling Microscopy — Dumitru Călugăru[1,2], Yi Jiang[3], Haojie Guo[3], Sandra Sajan[3], •Yongsong Wang[3], Haoyu Hu[1,3], Jiabin Yu[1], B. Andrei Bernevig[1,3], Fernando de Juan[3], and Miguel M. Ugeda[3] — [1]Princeton University, Princeton, USA — [2]University of Oxford, Oxford, United Kingdom — [3]Donostia International Physics Center, San Sebastián, Spain

Topologically trivial insulators can host obstructed atomic phases, where the electronic charge is localized at symmetry positions that do not coincide with atomic sites. Despite intense theoretical interest, such phases have lacked quantitative experimental confirmation. Here we provide direct experimental evidence that the narrow band at the Fermi level of monolayer 1H-$NbSe_2$ and $TaSe_2$ realizes an optimally compact obstructed atomic phase by means of STM/STS (1). Bias-dependent constant-height conductance maps reveal a strong redistribution of spectral weight between inequivalent high-symmetry positions within the unit cell. We identify these positions experimentally by using substitutional transition-metal alloys and chalcogen vacancies as local markers. By deconvolving the STM images with orbital-resolved wave functions from ab-initio calculations, we reconstruct the short-range inter-orbital correlations and real-space charge distribution associated with the band. The resulting pattern is centered at non-atomic positions and is uniquely consistent with an obstructed atomic insulator.

[1] Calugaru et al., Nature Physics, in press(2025).

TT 74.2 Thu 9:45 CHE/0091

Characterization of TI nanowire junctions using resonator circuits — •Lucas Marten Janssen, Jorge Esteban Bolio, Christian Dickel, and Yoichi Ando — Physics Institute II, University of Cologne, Zülpicher Str. 77, 50937 Köln, Germany

Topological insulators (TIs) are being investigated for their potential to host Majorana Zero Modes (MZMs). Specifically, TI nanowires proximitized by a conventional superconductor have shown signatures of potential topological phase transitions [1]. Microwave measurements can be used to investigate the hardness of the gap [2] and to reconstruct the current-phase relationship [3]. Additionally, high-frequency operation could be necessary to eventually realize topological

qubits. To assess the quality of our TI nanowire junctions, we design co-planar waveguide resonator circuits of NbTiN with a parallel plate capacitor to ground on one side and a connection to ground through the nanowire junction on the other side. This allows us to measure the sub-gap resistance and the current-phase relationship of the junction. In order to investigate the TI nanowire in the topological regime, an in-plane magnetic field of about 1 T needs to be applied. The resonators are engineered to be compatible with such fields.

[1] Nikodem et al., arXiv:2412.07993 (2024)
[2] Schmidt et al., Nat. Commun. 9, 4069 (2018)
[3] Uhl et al., Phys. Rev. Applied 22, 064052 (2024)

TT 74.3 Thu 10:00 CHE/0091

Growth and quantum transport analysis of high mobility Bi_2Te_3 thin films — •Jonas Buchhorn[1,2], Abdur Rehman Jalil[1,3], Detlev Grützmacher[1,2], and Thomas Schäpers[1,2] — [1]Peter-Grünberg-Institut (PGI-9), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology, Jülich-Aachen Research Alliance, Forschungszentrum Jülich and RWTH Aachen University, 52425 Jülich, Germany — [3]Institute of Experimental Physics III, Würzburg University, 97070 Würzburg, Germany

To improve future hybrid devices, underlying material properties and conduction mechanisms must be understood and controlled. In this work, we use quantum mechanical and classical models to describe the measured conductivity tensor of Bi_2Te_3 thin films. The crystals have been prepared by molecular beam epitaxy on sapphire substrates and were shaped into Hall bar structures by optical lithography and Ar-etching. At cryogenic temperatures non-linear Hall resistance and Shubnikov-de Haas oscillations were observed. A multi-channel model motivated from band structure calculations is used to extract classical carrier properties. Model residues are quantitatively analyzed to include electron-electron interaction, spin-orbit-effects and quantum oscillations of surface states. Considering these insights, we attempt to disentangle the complex conduction mechanisms of bulk and surface states of topological insulators. The proposed methods should also be applicable to the state-of-the-art ternary or quaternary compounds to identify remaining bulk-contributions.

TT 74.4 Thu 10:15 CHE/0091

Dual-gated hBN/BiSbTeSe/hBN heterostructures: fabrication and low-temperature magnetotransport — •Kirill Teslenko, Holger Mirkes, Alexandre Bernard, and Christoph Kastl — Walter Schottky Institute, School of Natural Sciences, Technical University of Munich

Topological insulators with tunable surface states provide a platform for exploring quantum transport phenomena. We present the fabrication and characterization of dual-gated hBN/BiSbTeSe/hBN (BSTS) heterostructures designed to allow controlled access to the topological surface states. The devices are fabricated via optimized optical lithography, and the heterostacks are assembled using a dry-transfer stacker operated both under nitrogen atmosphere and under ambient conditions. Two approaches are used: transferring BSTS onto prepatterned metal contacts, and assembling the full heterostack before metal evaporation. Photocurrent measurements on non-encapsulated BSTS, BTS, and SbTe flakes were carried out to assess their optoelectronic response. Furthermore, low-temperature magnetotransport measurements on the encapsulated devices are carried out to resolve characteristic signatures of topological surface states.

TT 74.5 Thu 10:30 CHE/0091

Field-induced band modification and large magnetoresistance in topological-insulator $Bi_{1-x}Sb_x$ thin films — •E. Osmic[1,2], P. Bercoff[3], F. Commeto[3], Y. Skourski[1], F. Ganss[4], J. Wosnitza[1,2], and J. Barzola Quiquia[5] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Universidad Nacional de Córdoba, Córdoba, Argentina — [4]Institut für Ionenstrahlphysik und Materialforschung, HZDR, Dresden, Germany — [5]Felix-Bloch Institute for Solid-State Physics, Universität Leipzig, Germany

We studied the magnetic-field and temperature dependence of the electrical transport in topological-insulator $Bi_{1-x}Sb_x$ ($x = 0.1, 0.15, 0.2$) thin films. The resistivity $\rho(T)$ shows a clear crossover between metallic surface transport at low temperatures and semiconducting bulk behavior at higher temperatures. Below 10 K, $\rho(T)$ exhibits a characteristic two-dimensional electron–electron interaction contribution. Magnetoresistance measurements in pulsed magnetic fields up to 69 T reveal large, nonsaturating MR values reaching 2250 % over a broad temperature range. The full MR response can be consistently described using a modified two-band bulk model with field-dependent charge-carrier concentrations, complemented by a weak-antilocalization description of the surface states. These results highlight the possible field-induced band modification and the interplay between bulk and surface transport in Bi–Sb thin films.

TT 74.6 Thu 10:45 CHE/0091

THz Signatures of Boundary-Dominated Transport in Bi_2TeI — •shuhan wang[1], Anjan N M[1], Mohammad Mehmandous[2], Michael Ruck[2], and Stefan Kaiser[1] — [1]Institute of Solid State and Materials Physic, TUD Dresden University of Technology — [2]Inorganic Chemistry II,TUD Dresden University of Technology

Bi_2TeI is a weak topological insulator made of stacked topologically nontrivial (QSH) layers separated by trivial insulating layers. Despite its weak topological indices, it still hosts symmetry-protected boundary states on specific crystal surfaces. Using terahertz time-domain spectroscopy (THz-TDS), we resolve its low-energy electrodynamics in thin films. The THz conductivity shows a low frequency Drude response dip at 15K-20 K. This behavior is consistent with dc transport measurements. Notably, these features are only seen in thin films which are absent in bulk crystals. The suppression of Drude weight points to a crossover toward boundary-dominated transport in Bi-TeI thin films.

15 min. break

TT 74.7 Thu 11:15 CHE/0091

Topological fragility and bilinear magneto-resistance in spin-momentum locked edge states — •Cosimo Gorini[1], Matthieu Bard[2], and Giovanni Vignale[3] — [1]SPEC, CEA, CNRS, Université Paris-Saclay, CEA Saclay, Gif sur Yvette, France — [2]Université Paris-Saclay, CNRS, Laboratoire de Physique des Solides, 91405 Orsay, France — [3]Institute for Functional Intelligent Materials, National University of Singapore

Time-reversal symmetric and topologically non-trivial electronic systems generally host one-dimensional (1D) spin-momentum locked states at their edges/hinges. Such 1D states are in principle fully protected against backscattering, and thus referred to as perfectly conducting: disorder cannot induce backscattering – not even via spin-orbit coupling – unless time-reversal is broken. We show however that such protection hides a remarkable fragility, yielding a bilinear magneto-resistance much stronger than in standard 2D systems. The mechanism we propose is fundamental and general, being based on spin-orbit interaction with the ever-present disordered background. It should thus be relevant in any system hosting 1D Dirac-like states with linear dispersion. Our theory compares favourably with transport measurements in high-order topological hinge states in Bi.

TT 74.8 Thu 11:30 CHE/0091

Procrustean symmetrization formalism for statistical topological matter — •Johanna Zijderveld[1], Adam Yanis Chaou[2], Isidora Araya Day[1,2,3], and Anton Akhmerov[1] — [1]Kavli Institute of Nanoscience, Delft University of Technology, Delft, The Netherlands — [2]Donostia International Physics Center, San Sebastian, Spain — [3]QuTech, Delft University of Technology, Delft, The Netherlands

The standard approach to characterizing topological matter, computing topological invariants, is known to be problematic when the symmetry protecting the topological phase only holds on average in a disordered system. Because of reliance on making the symmetry exact, the topological invariants identify more topological phases than are present in the system. Alternatively, in the recently discovered intrinsic statistical topological insulators [1], making the symmetry exact is guaranteed to destroy the topological phase. We define a procedure of symmetry embedding that solves both problems and provides a unified framework for describing disordered topological matter.

[1] Phys. Rev. Lett. 134, 226601

TT 74.9 Thu 11:45 CHE/0091

Topological invariants for the SSH model coupled to a single mode cavity — •Anna Ritz-Zwilling and Olesia Dmytruk — CPHT, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France

Coupling electronic systems to cavity photons offers a promising route to probe and control material properties through light-matter interactions. In particular, coupling to light might enable manipulation of topological phases of matter, which have gained significant attention due to their potential applications in quantum technologies. Yet, while the topological classification of non-interacting fermionic systems is well understood within the tenfold way, much less is known about how to identify topological protection when photonic operators enter the problem. In this work, we consider the Su-Schrieffer-Heeger (SSH) model as a paradigmatic one-dimensional topological insulator. In its topological phase, the SSH model exhibits zero-energy edge states protected by chiral symmetry. When the system is coupled to a cavity, however, it remains unclear whether chiral symmetry and topological protection survive. To address this question, we use a recently developed high-frequency expansion of the light-matter Hamiltonian, which traces out photonic degrees of freedom and yields an effective fermionic model. Light-matter coupling then manifests as additional interaction terms, allowing us to apply known results for interacting topological insulators. We discuss the symmetries of this effective model, compute observables such as the electronic polarization as potential topological invariants and analyze the fate of edge states.

TT 74.10 Thu 12:00 CHE/0091

Z_2 topological invariants from the Green's function diagonal zeros — Florian Simon[1] and •Corentin Morice[2] — [1]Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden — [2]Laboratoire de Physique des Solides, Université Paris Saclay, CNRS, Orsay, France

We investigate the relationship between the analytical properties of the Green's function and Z_2 topological insulators, focusing on three-dimensional inversion-symmetric systems. We show that the diagonal zeros of the Green's function in the orbital basis provide a direct and visual way to calculate the strong and weak Z_2 topological invariants. We introduce the surface of crossings of diagonal zeros in the Brillouin zone, and show that it separates TRIMs of opposite parity in two-band models, enabling the visual computation of the Z_2 invariants by counting the relevant TRIMs on either side.

TT 74.11 Thu 12:15 CHE/0091

Volkov-Pankratov states in shaped topological insulator nanowires — •Lilian Seyve and Cosimo Gorini — SPEC, CEA, Gif-Sur-Yvette, France

Topological insulators (TIs) host robust electronic states at interfaces where the bulk topological invariant changes, giving rise to protected Dirac surface modes. Beyond these gapless states, Volkov and Pankratov showed that smooth band inversions can also generate massive interface modes, now known as Volkov-Pankratov (VP) states. These states coexist with the topological zero mode and interpolate continuously between topological and bulk physics. While VP states have been studied in planar structures, how they behave in curved systems, such as nanowires, is still very much unknown.

In this work, we explore analytically and numerically how VP states appear in nanowires with cylindrical symmetry, where geometry and confinement strongly influence the electronic structure. Using a Dirac-model description with a smoothly varying mass at the wire's edge, we show how curvature, angular momentum, and longitudinal motion combine to create a set of quantized interface states. We obtain analytical expressions for their energies and spatial profiles and describe how interface curvature affects the physical properties of our system.

TT 74.12 Thu 12:30 CHE/0091

Accessing buried topological states: Revealing Dirac cones with ferromagnetic resonance — Laura Pietanesi[1], •Magdalena Marganska[2,3], Thomas Mayer[2], Michael Barth[3], Lin Chen[1], Ji Zou[4], Adrian Weindl[2], Alexander Liebig[2], Rebeca Diaz-Pardo[1], Dhavala Suri[1,5], Florian Schmid[2], Franz Giessibl[2], Klaus Richter[2], Yaroslav Tserkovnyak[4], Matthias Kronseder[2], and Christian Back[1] — [1]Technical University of Munich, Germany — [2]University of Regensburg, Germany — [3]Wrocław University of Science and Technology, Poland — [4]University of California, Los Angeles, USA — [5]Indian Institute of Science, Bengaluru, India

Ferromagnetic resonance is used to reveal features of the buried electronic band structure at interfaces between ferromagnetic metals and topological insulators [1]. The evolution of magnetic damping in a hybrid ferromagnet/3D topological insulator structure reveals a clear fingerprint of the Dirac point with additional features. The high energy resolution of this method allows us to resolve the energetic shift of the local Dirac points due to local variations of the electrostatic potential. The underlying spin-pumping mechanism relies on the dissipation of angular momentum by topological surface states (TSSs). Tuning of the Fermi level within the TSS was verified both by varying the stoichiometry of the 3DTI layer and by electrostatic backgating with a remarkable agreement. Calculations based on the chiral tunneling process naturally occurring in TSSs agree well with the experimental results.

[1] PRB 109, 064424 (2024)

TT 75: Many-body Quantum Dynamics I (joint session DY/TT)

Time: Thursday 9:30–12:45 Location: HÜL/S186

TT 75.1 Thu 9:30 HÜL/S186

Nonequilibrium transport in adaptive fermionic circuits — •Paul Weiss[1], Karim Chahine[2], and Michael Buchhold[1] — [1]Department of Theoretical Physics, Universität Innsbruck, Austria — [2]Institute for Theoretical Physics, University of Cologne, Germany

We investigate nonequilibrium dynamics in one-dimensional adaptive fermionic circuits, where monitored fermions undergo local unitary evolution conditioned on measurement outcomes. By tuning the measurement strength and the duration of the unitary gates, the dynamics can be continuously interpolated between incoherent, classical transport and coherence-dominated quantum transport. In the classical limit, we recover the asymmetric simple exclusion process (ASEP), while in the quantum regime we uncover a coherent analogue of the Burgers equation along with coherence-enhanced Kardar-Parisi-Zhang (KPZ) transport. Our analytical approach, based on transport equations and Keldysh field theory, is supported by numerical simulations.

TT 75.2 Thu 9:45 HÜL/S186

Frustration-Free Control and Absorbing-State Transport in Entangled State Preparation — •Tobias Dörstel[1,2], Thomas Iadecola[3,4,5], Justin H. Wilson[6,7], and Michael Buchhold[1,2] — [1]Department of Theoretical Physics, University of Innsbruck, Austria — [2]Institute for Theoretical Physics, University of Cologne, Germany — [3]Department of Physics, The Pennsylvania State University, USA — [4]Institute for Computational and Data Sciences, The Pennsylvania State University, USA — [5]Materials Research Institute, The Pennsylvania State University, USA — [6]Department of Physics and Astronomy, Louisiana State University, USA — [7]Center for Computation and Technology, Louisiana State University, USA

We study frustration-free control, a measurement-feedback protocol for quantum state preparation that extends the concept of frustration-free Hamiltonians to stochastic dynamics. The protocol drives many-body systems into highly entangled target states, common dark states of all measurement projectors, through minimal local unitary corrections that realize an absorbing-state dynamics without post-selection. We show that relaxation to the target state is governed by emergent transport of nonlocal charges, such as singlet excitations in SU(2)-symmetric dynamics. While measurement-feedback annihilates compatible charge configurations, both measurement and scrambling unitaries induce charge transport and thus determine the convergence time. Mapping a baseline model of SU(N) SWAP measurements with local corrections to a solvable absorbing random walk yields a runtime scaling $t \sim L^z$ with transport exponent $z = 2$.

TT 75.3 Thu 10:00 HÜL/S186

Quantum typicality approach to energy flow between two spin-chain domains at different temperatures — Laurenz Beckemeyer[1], •Markus Kraft[1], Mariel Kempa[1], Dirk Schuricht[2], and Robin Steinigeweg[1] — [1]University of Osnabrück, Department of Mathematics/Computer Science/Physics,D-49076 Osnabrück, Germany — [2]Institute for Theoretical Physics, Utrecht University, 3584CC Utrecht, The Netherlands

We discuss a quantum typicality approach to examine systems composed of two subsystems at different temperatures. While dynamical quantum typicality is usually used to simulate high-temperature dynamics, we also investigate low-temperature dynamics using the method. To test our method, we investigate the energy current between subsystems at different temperatures in various paradigmatic spin-1/2 chains, specifically the XX chain, the critical transverse-field Ising chain, and the XXZ chain. We compare our numerics to existing analytical results and find a convincing agreement for the energy current in the steady state for all considered models and temperatures.

[1] Beckemeyer et al. arXiv:2507.23439

TT 75.4 Thu 10:15 HÜL/S186

Revisiting boundary-driven method for transport: Finite-size effects and the role of system-bath coupling — •Mariel Kempa[1], Markus Kraft[1], Sourav Nandy[2], Jacek Herbrych[3], Jiaozi Wang[1], Jochen Gemmer[1], and Robin Steinigeweg[1] — [1]University of Osnabrueck, Osnabrueck, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]Wroclaw University of Science and Technology, Wroclaw, Poland

Understanding transport in interacting quantum many-body systems is a central challenge in condensed matter and statistical physics. Numerical studies typically rely on two main approaches: Dynamics of linear-response functions in closed systems and Markovian dynamics governed by master equations for boundary-driven open systems. While the equivalence of their dynamical behavior has been explored in recent studies, a systematic comparison of the transport coefficients obtained from these two classes of methods remains an open question. Here, we address this gap by comparing and contrasting the dc diffusion constant $\mathscr{D}_{\mathrm{dc}}$ computed from the aforementioned two approaches. We find a clear mismatch between the two, with $\mathscr{D}_{\mathrm{dc}}$ exhibiting a strong dependence on the system-bath coupling for the boundary-driven technique, highlighting fundamental limitations of such a method in calculating the transport coefficients related to asymptotic dynamical behavior of the system. We trace the origin of this mismatch to the incorrect order of limits of time $t \to \infty$ and system size $L \to \infty$, which we argue to be intrinsic to boundary-driven setups.

TT 75.5 Thu 10:30 HÜL/S186

Synchronized Aharonov-Bohm Motifs via Engineered Dissipation — •Christopher Wächtler and Gloria Platero — ICMM-CSIC, Madrdi, Spain

The interplay between external gauge fields and lattice geometry can induce extreme localization dynamics through complete destructive interference. We show that combining this flux-induced localization with engineered dissipation leads to robust spin synchronization in rotationally symmetric spin geometries, referred to as Aharonov-Bohm motifs, with cyclic symmetries of any order. The synchronized dynamics is independent of initial conditions and features entanglement among spins within each motif. We further demonstrate that multiple motifs can fully synchronize when coupled, which is achieved by applying additional collective dissipation acting on all intra-motif spins. These results reveal a direct connection between flux-induced localization, dissipative engineering, and collective quantum synchronization.

TT 75.6 Thu 10:45 HÜL/S186

Krylov space dynamics of ergodic and dynamically frozen Floquet systems — •Luke Staszewski[1], Asmi Haldar[2], Pieter Claeys[1], and Alexander Wietek[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Laboratoire de Physique Theorique - IRSAMC, Toulouse

In isolated quantum many-body systems periodically driven in time, the asymptotic dynamics at late times can exhibit distinct behavior such as thermalization or dynamical freezing. Understanding the properties of and the convergence towards infinite-time (nonequilibrium) steady states however remains a challenging endeavor. We propose a physically motivated Krylov space perspective on Floquet thermalization which offers a natural framework to study rates of convergence towards steady states and, simultaneously, an efficient numerical algorithm to evaluate infinite-time averages of observables within the diagonal ensemble. The effectiveness of our algorithm is demonstrated by applying it to the periodically driven mixed-field Ising model, reaching system sizes of up to 30 spins. Our method successfully resolves the transition between the ergodic and dynamically frozen phases and provides insight into the nature of the Floquet eigenstates across the phase diagram. Furthermore, we show that the long-time behavior is encoded within the localization properties of the Ritz vectors under the Floquet evolution, providing an accurate diagnostic of ergodicity.

15 min. break

TT 75.7 Thu 11:15 HÜL/S186

Chaotic many-body quantum dynamics, spectral correlations, and energy diffusion — •Dominik Hahn and John Chalker — Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford OX1 3PU, United Kingdom

We present results on the quantum dynamics of a minimal model with spatial structure and local interactions. The model features a time-independent Hamiltonian, in contrast to the widely studied quantum circuits, and is analytically tractable in the limit of large local Hilbert space dimension and weak intersite coupling. In this regime, we show that the energy dynamics are governed by a classical master equation exhibiting diffusive behavior. Furthermore, we demonstrate that the spectral form factor can be expressed exactly in terms of the solution to this master equation, demonstrating how the linear ramp emerges at long times, while locality gives rise to an additional enhancement at short times.

TT 75.8 Thu 11:30 HÜL/S186

Dissipative diffusion in quantum state preparation — •Tim Pokart[1], Lukas König[1], Sebastian Diehl[2], and Jan Carl Budich[1,3,4] — [1]Institute of Theoretical Physics, Technische Universität Dresden — [2]Institut für Theoretische Physik, Universität zu Köln, 50937 Cologne, Germany — [3]Würzburg-Dresden Cluster of Excellence ct.qmat, 01062 Dresden, Germany — [4]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany

Dissipative quantum protocols that engineer a desired state as their dark state provide a powerful route to preparing quantum many-body states. We investigate a number conserving variant of such a dissipative protocol which is able to stabilize a topologically nontrivial phase. We show that the protocol admits a unique and stable dark state. Furthermore, we find that the cooling is diffusive in nature, supported by both analytical arguments and numerical simulations.

TT 75.9 Thu 11:45 HÜL/S186

First principles simulation of spin diffusion using dynamic mean-fields — •Timo Grässer[1], Matthias Ernst[1], and Götz S. Uhrig[2] — [1]Institute of Molecular Physical Science, ETH Zurich, 8093 Zurich, Switzerland — [2]Condensed Matter Physics, TU Dortmund University, 44227 Dortmund, Germany

The transfer of a globally conserved polarization among a homogeneous spin ensemble is called spin diffusion and one of the most important phenomena in the broad field of magnetic resonance. Describing spin diffusion theoretically is a notoriously difficult task due to the large number of spins involved. We use a description through dynamic mean-fields (dubbed spinDMFT [1]) to derive an effective model for spectral spin diffusion. The approach is benchmarked for two crystalline test samples, malonic acid and dipotassium α-D-glucopyranose-1-phosphate dihydrate, yielding a remarkable agreement with experimental data and requiring only little computational effort. This strongly supports the use of spinDMFT, which may be extended in future works to understand spin diffusion in dynamic nuclear polarization (DNP) experiments [2].

[1] T. Gräßer et al., Phys. Rev. Research 3, 043168 (2021), DOI 10.1103/PhysRevResearch.3.043168

[2] J. Eills et al., Chem. Rev. 123, 1417 (2023), DOI 10.1021/acs.chemrev.2c00534

TT 75.10 Thu 12:00 HÜL/S186

Simulating universal long-time dynamics in integrable quantum spin chains — •Angelo Valli[1], Catalin Pascu Moca[2], Miklos Antal Werner[3], Marton Kormos[1], Doru Sticlet[6], Balazs Dora[1], Ziga Krajnik[4], Tomaz Prosen[5], and Gergely Zarand[1] — [1]Budapest University of Technology and Economics, Budapest (Hungary) — [2]University of Oradea, Oradea (Romania) — [3]Wigner Research Centre for Physics, Budapest (Hungary) — [4]New York University, New York (USA) — [5]University of Ljubljana, Ljubljana (Slovenia) — [6]National Institute for R&D of Isotopic and Molecular Technologies, Cluj-Napoca (Romania)

We introduce a novel tensor-network approach to calculate cumulants of the full counting statistics to unprecedentedly long times. We investigate spin-transfer in quantum spin chains, where the superdiffusive transport with dynamical exponent z=3/2 has been conjectured to fall within the Kardar-Parisi-Zhang (KPZ) universality class of classical interface growth. Recent experimental evidence on quantum simulators challenged this hypothesis. Our results extend far beyond the experimental timescales and provide unambiguous evidence that spin transfer in integrable quantum spin chains is indeed incompatible with KPZ universality. However, spatio-temporal fluctuations of the spin analogue of surface roughness exhibit a self-similar Family-Vicsek (FV) scaling, relating roughness, growth, and dynamical exponents in all transport regimes and across models with SU(N) symmetry. Our results shed light on how classical universal scaling laws extend to the quantum many-body realm.

TT 75.11 Thu 12:15 HÜL/S186

Few-body structures of Quantum impurity problems in the Heisenberg picture — •Maxime Debertolis — University of Bonn

Quantum impurity problems are known to exhibit a simplified representation of their ground state or for quench protocols when an optimized single-particle basis is chosen. This work extends the study of single-particle rotations taylored to operators in the Heisenberg picture. We present the concept of natural super-orbitals for many-body operators, defined as the eigenvectors of the one-body super-density matrix associated with a vectorized operator. These objects are related to measures of non- Gaussianity of operators associated to the occupations of the natural super-orbitals. We perform a numerical investigation of the natural super-orbitals corresponding to both the time-evolution operator and a time-evolved local operator in the t-V model and in a quantum impurity model using tensor network simulations. In the quantum impurity model, occupations of the natural orbitals for both operators decay exponentially at all times. More surprisingly, the non-Gaussianity of the local operator saturates in time. This indicates that only a small number of orbitals contribute significantly to quantum correlations, enabling a compact matrix-product-operator representation. This framework opens the door to future research that leverages the compressed structure of operators in their natural super-orbital basis, enabling for instance the computation of out-of-time-order correlators in large interacting systems over extended time scales.

TT 75.12 Thu 12:30 HÜL/S186

Propagating the Hierarchical Equations of Motion (HEOM) using the Multi-Configurational Time-Dependent Hartree method (MCTDH) — •Luisa R. Grether[1], Uwe Manthe[2], Samuel L. Rudge[1], and Michael Thoss[1] — [1]Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg im Breisgau, Deutschland — [2]Theoretische Chemie, Fakultät für Chemie, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Deutschland

The Hierarchical Equations of Motion (HEOM) are a powerful, numerically exact approach for simulating the time evolution of an open quantum system. Over the past decade, several tensor-train- and tensor-network-based approaches have been suggested and realized to make the HEOM applicable to ever larger model systems [1,2].

In this contribution, we build upon the existing twin-space formulation of the HEOM [2] and introduce a novel approach employing the Multi-Configurational Time-Dependent Hartree method (MCTDH) [3] for the time propagation of the HEOM. We demonstrate the applicability of the resulting HEOM+MCTDH method by presenting electron transport calculations for a nanojunction model, for which fully quantum results have not been available previously.

[1] Q. Shi *et al.*, J. Chem. Phys. **148**, 174102 (2018).

[2] Y. Ke *et al.*, J. Chem. Phys. **156**, 194102 (2022).

[3] H.-D. Meyer *et al.*, Chem. Phys. Lett. **165**, 73 (1990).

TT 76: Focus Session: Curvilinear magnetism: Magnetics with nanoscale curved geometries (joint session MA/TT)

The behaviour of any physical system is determined by the order parameter whose distribution is governed by the geometry and topology of the physical space of the object, in particular its dimensionality and curvature. Specifically, spin textures, static and dynamic magnetic responses become sensitive to bends and twists in physical space. In this respect, curvature effects emerged as a novel tool to tailor magnetic properties and responses relying on geometric deformations. In magnetism, coupling between geometry of a magnet and magnetic order parameter brings about novel responses of curved thin films, nanowires and nanoparticles and enforces topological constraints on the number and type of magnetic solitons living in a curved space. Curvatures can force a geometry-driven local interactions like Dzyaloshinskii-Moriya interaction (DMI) and anisotropy as well as novel non-local chiral symmetry breaking effects, which were confirmed experimentally using electron holography studies of magnetic cap-shaped structures. Advances in experimental techniques (fabrication and tomographic characterization) allow validating theoretically predicted effects and apply them for functional devices as was demonstrated with geometrically twisted 3D racetracks. Recent highlights of the community include experimental proof of curvature stabilised skyrmions, explorations of curvilinear altermagnets, tailoring magnetic solitons in curvilinear 2D magnets, curvilinear magnetoelectrics, use of curvilinear magnetic architectures to tune superconducting transport, and magnetoionic manipulation of magnetic states in nanostructures to name just a few representative topics, which will be covered at the focused symposium.

Organizers: Denys Makarov, d.makarov@hzdr.de; Paola Gentile, paola.gentile@spin.cnr.it

Time: Thursday 9:30–13:00 Location: POT/0151

Invited Talk TT 76.1 Thu 9:30 POT/0151

2D and 3D racetracks: Interplay of geometric and magnetic chiralities — •Stuart Parkin — Max Planck Institute for Microstructure Physics, Halle (Saale), Germany — Martin Luther University Halle-Wittenberg

Magnetic Racetrack Memory (RTM) is a unique memory-storage device that relies on the current driven motion of multiple domain walls along magnetic conduits that can be arranged either horizontally (2D) or vertically (3D). It has great potential as a high performance, non-volatile memory that has enormous data storage capacity compared to today*s memory technologies. Atomically engineered 2D magnetic racetracks in the form of synthetic antiferromagnets allow for very high current induced motion of nanoscopic chiral domain walls[1]. Recently we have shown that 2D RTM can be scaled to dimensions that are technologically relevant with widths of just ~50 nm[2]. 3D racetracks would allow for the highest density memories. Using a state-of-the-art multi-photon superresolution lithography system we form 3D scaffolds of arbitrary shapes on which the racetracks can be subsequently deposited. We discuss 3D racetracks that are formed with clockwise and anticlockwise chiral twists and curved cross-sections. The interplay between the geometrical chirality and the spin chirality of the individual domain walls allows for domain wall diode devices [3]. [1] S. S. P. Parkin, S.-H. Yang, Nat. Nanotechnol. 2015, 10, 195. [2] J.-C. Jeon, A. Migliorini, J. Yoon, J. Jeong, S. S. P. Parkin, Science 2024, 386, 315. [3] A. M. A. Farinha, S.-H. Yang, J. Yoon, B. Pal, S. S. P. Parkin, Nature 2025, 639, 67.

Invited Talk TT 76.2 Thu 10:00 POT/0151

Combined MFM/KPFM at the Ultimate Sensitivity Limit for Probing Curvature-Engineered Micromagnetic States — •Emily Darwin[1], Reshma Peremadathil Pradeep[1,2], Luca Berchialla[3], Daniel Rotthardt[1,2], Ales Hrabec[3], and Hans Hug[1,2] — [1]Empa, Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland — [2]Department of Physics, University of Basel, 4056 Basel, Switzerland — [3]aul Scherrer Institut PSI, 5232 Villigen, Switzerland

Curved substrates offer a promising route for tailoring the magnetic properties of multilayer systems, potentially stabilizing topologically non-trivial spin textures such as skyrmions. However, local variations in surface inclination can significantly affect growth conditions, altering crystallographic orientation or even disrupting the multilayer architecture.

In this study, we investigate a Pt/Co/Ru multilayer deposited on a polymer substrate patterned with nanoscale semispherical bumps using a combined single-pass Magnetic Force Microscopy (MFM) and Frequency-Modulated Kelvin Probe Force Microscopy (FM-KPFM) technique. Our system achieves unprecedented sensitivity to both magnetic and electrostatic interactions. We find that steep, near-vertical walls at the perimeter of hemispherical features locally disorder the multilayer stack, resulting in distinct changes in the contact potential difference. This disruption facilitates magnetic flux return and enables the formation of circular magnetic domains aligned with the external magnetic field on the dome tops.

Invited Talk TT 76.3 Thu 10:30 POT/0151

Curvilinear magnetism in superconducting spintronics — •Sol Jacobsen — Center for Quantum Spintronics, Norwegian University of Science and Technology NTNU, Trondheim, Norway

Replacing semiconductor-based computational components with superconducting elements can give an energy saving of two orders of magnitude. To harness this, we need precise control of the interaction between superconducting and magnetic components. Geometric curvature controls the superconducting transition by affecting spin relaxation and precession in superconductor-magnet heterostructures [1]. To functionalize this in devices, we can dynamically alter the curvature by inducing bending-strain. This can for example lead to electrically controlled superconducting spin-valves, current-reversal, and chirality-dependent ground states in triplet-SQUIDs [1-3]. In this presentation, I will discuss how real-space geometric curvature provides new pathways for manufacturing and controlling the interaction between superconductivity and magnetism in wires and thin films, and anticipate future developments in the field.

[1] Salamone et al, Phys. Rev. B 104 (2021) L060505; 105, (2022) 134511. [2] Salamone et al, Appl. Phys. Lett. 125 (2024) 062602. [3] Skarpeid et al, J.Phys.:Condens.Matter, 36 (2024) 235302.

15 min break

Invited Talk TT 76.4 Thu 11:15 POT/0151

Advanced Control of Magnetic Nanostructures via Metasurface Engineering and Voltage-Driven Functionalities — •Anna Palau — Institut de Ciència de Materials de Barcelona (ICMAB-CSIC)

Understanding and manipulating magnetic micro- and nanostructures are fundamental to advancing technologies in data storage, spintronics, and magnetic sensing. Magnetic metasurfaces have recently attracted significant interest for their ability to locally configure magnetic field distributions and overcome limitations of traditional magnetic imaging techniques. In this work, we demonstrate how metasurfaces enable precise control of vortex motion, coercive fields, and saturation behaviour in magnetic nanostructures without altering their intrinsic anisotropy [1]. We show that metasurfaces can overcome magnetic field constraints in X-ray Photoemission Electron Microscopy (XPEEM), enabling high-resolution imaging of magnetisation states under conditions previously inaccessible. Additionally, we explore electric-field-driven ionic migration as a complementary route for voltage-controlled, non-volatile modulation of magnetic and superconducting properties [2], highlighting new opportunities for energy-efficient control and advanced characterisation. [1] Barrera et al. ACS Nano 19, 10461 (2025), [2] Günkel et al. Small 2411908 (2025), Spasojević et al. Nat. Commun. 16, 1990 (2025)

Invited Talk TT 76.5 Thu 11:45 POT/0151

Magnetic tomography of noncollinear spin textures in curvilinear geometries — •Sandra Ruiz-Gomez — ALBA Synchrotron, Barcelona, Spain

Three-dimensional nanomagnetic systems offer a unique platform for discovering and controlling complex spin textures. Recent advances in 3D nanofabrication, magnetic characterization techniques, and micromagnetic modeling are now enabling precise control of curvature, torsion, and geometry at the nanoscale, opening new routes for engineering spin textures in three-dimensional architectures.

In this talk, I will present our latest results on how geometrical design and 3D architecture can be exploited to tailor the energy landscape of domain walls, manipulate their topological properties, and guide their motion from straight

nanowires to more complex curved cylindrical and tubular geometries. By combining state-of-the-art fabrication techniques with high-resolution imaging and theoretical analysis, we identify how curvature can be harnessed to stabilize complex spin textures, enabling deterministic control over their dynamics.

Overall, this work highlights how 3D nanomagnetism can be leveraged to access new regimes of topological control, with implications for next-generation spintronic devices, robust information carriers, and reconfigurable magnetic architectures.

TT 76.6 Thu 12:15 POT/0151

Transferred magnetic nanomembranes for curvilinear magnetism and spintronics — •Olha Bezsmertna[1], Oleksandr Pylypovskyi[1], Rui Xu[1], Mykola Vinnichenko[2], Andrea Sorrentino[3], Daniel Wolf[4], Axel Lubk[4], Peter Fischer[5,6], and Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [2]Institute for Ceramic Technologies and Systems IKTS, 01277 Dresden, Germany — [3]Alba Light Source, MISTRAL beamline, Cerdanyola del Vallès 08290, Spain — [4]Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany — [5]University of California, Santa Cruz, United States — [6]Lawrence Berkeley National Laboratory, Berkeley, United States

The functionality of the magnetic nanomembranes can be extended through controlled transfer processes and geometric design. We show that advanced giant magnetoresistive thin films can be reliably transferred onto various substrates using green chemistry, preserving their structural integrity and magnetic performance, thus enabling mechanically conformal devices for applications where low weight, flexibility, and durability are essential [1]. With the developed technique, we demonstrate fabrication of curvilinear hierarchical magnetic nanotemplates and their subsequent transfer to an appropriate handling support enabling high-resolution transmission microscopy investigations (electron- and x-ray-based) of the impact of geometric curvature on complex magnetic states [2].

References: [1] Bezsmertna et al. Adv. Funct. Mater. 35, 2502947 (2025). [2] Bezsmertna et al. Nano Lett. 24, 15774 (2024).

TT 76.7 Thu 12:30 POT/0151

Magnetic solitons in spherical maghemite nanoshells — •Oleksandr V. Pylypovskyi[1], Gaspare Varvaro[2], Davide Peddis[2,3], Priyanka Mishra[4], Carmine Autieri[4], Filipp N. Rybakov[5], Denis D. Sheka[6], and Denys Makarov[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf e.V., 01328 Dresden, Germany — [2]CNR-Istituto di Struttura della Materia, 00015 Roma, Italy — [3]Universitá degli Studi di Genova, 1-16146 Genova, Italy — [4]International Research Centre Magtop, Institute of Physics, Polish Academy of Sciences, 02668 Warsaw, Poland — [5]Uppsala University, Uppsala SE-751 20, Sweden — [6]Taras Shevchenko National University of Kyiv, 01601 Kyiv, Ukraine

Topology of the shape of magnetic nanoarchitecture makes a major impact on global properties of its magnetic textures [1,2]. Here, we present a fabrication of maghemite spherical shells and a theoretical analysis of magnetic solitons they host in equilibrium. The ferrimagnetic shells with a radius and shell thickness of about 4 nm and 1.4 nm have a radial easy axis that favors skyrmionic textures. Their ground state corresponds to a 3D onion state with the change of the radial component of magnetization at the equator. In this presentation, we will also report on the localization of magnetic solitons on spherical shells.

[1] V. P. Kravchuk et al., PRB **94**, 144402 (2016); [2] O. M. Volkov, O. V. Pylypovskyi et al., Nat. Commun., **15**, 2193 (2024).

TT 76.8 Thu 12:45 POT/0151

Coherent Spin Waves in Curved Ferromagnetic Nanocaps of a 3D-printed Magnonic Crystal — •Kilian Lenz[1], Huixin Guo[2], Mateusz Golebiewski[3], Ryszard Narkowicz[1], Jürgen Lindner[1], Maciej Krawczyk[3], and Dirk Grundler[2] — [1]Inst. of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Germany — [2]School of Engineering, Institute of Materials,Laboratory of Nanoscale Magnetic Materials and Magnonics, École Polytechnique Fédérale de Lausanne, Switzerland — [3]Institute of Spintronics and Quantum Information, Adam Mickiewicz University, Poznań, Poland

In this work we present ferromagnetic resonance measurements and simulations of a 3D magnonic crystals embedded in an on-chip microresonator. It was realized by two-photon lithography of a 3D woodpile structure and atomic layer deposition of a 30-nm-thin Ni film. Operated near 14 and 24 GHz, the microresonator output revealed numerous coherent magnons with distinct angular dependencies reflecting the underlying face-centered cubic lattice. The micromagnetic simulations show that some of the edge modes are localized at the curved nanocaps and that they remain robust against changes of the field orientation. These cap modes exhibit an unexpected phase evolution. The findings advance the development of functional microwave circuits with 3D magnonic crystals and strengthen their visionary prospects for edge-dominated magnon modes.

TT 77: Topical Talk Bibes (joint session O/TT)

Time: Thursday 9:30–10:15 Location: TRE/PHYS

Topical Talk TT 77.1 Thu 9:30 TRE/PHYS

Oxide interfaces as platforms for emergent quantum phenomena — •Manuel Bibes — Laboratoire Albert Fert, CNRS, Thales, U. Paris-Saclay, Palaiseau (France)

Oxide surfaces and heterointerfaces host electronic phases that emerge from the combined effects of broken inversion symmetry, orbital reconstruction, and electrostatic boundary conditions. In this overview, I will discuss how two-dimensional electron gases (2DEGs) formed at oxide surfaces and interfaces give rise to large and tunable spin-orbit interactions, interfacial magnetism, and ferroic control of transport properties.

The focus will be on Rashba-type spin-orbit coupling in oxide 2DEGs and its interplay with ferromagnetism and ferroelectricity, leading to effects such as electrically tunable Anomalous Hall effect, spin and orbital Edelstein effects, and spontaneous non-reciprocal charge transport. Angle-resolved photoemission spectroscopy (ARPES) and X-ray photoelectron spectroscopy (XPS) play a central role in elucidating the electronic structure, orbital character, and electrostatic landscape underlying these phenomena, and in establishing clear links between interface chemistry, symmetry breaking, and transport behavior.

Finally, I will discuss how these engineering 2DEGs enables new routes toward low-power spin-orbitronic and ferroelectric device concepts compatible with silicon technology. The talk will highlight open challenges and opportunities at the interface between surface science, correlated electron physics, and oxide electronics.

TT 78: Quantum Dots and Point Contacts (joint session TT/HL)

Time: Thursday 11:00–12:45 Location: HSZ/0101

TT 78.1 Thu 11:00 HSZ/0101

Mapping dissipation in a quantum dot junction — •Johannes Höfer[1], Subhomoy Haldar[2], Ville Maisi[2], Hervé Courtois[1], and Clemens B. Winkelmann[1,3] — [1]Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, 25 rue des Martyrs, Grenoble, France — [2]NanoLund and Solid State Physics, Lund University, 22100 Lund, Sweden — [3]Univ. Grenoble Alpes, CEA, Grenoble INP, IRIG-Pheliqs, Grenoble, France

Characterization of quantum devices relies primarily on electrical properties. It is usually assumed that all parts of the device remain at the same temperature, but the inevitable presence of local dissipation can lead to significant deviations and degrade device performance [1].

Here, we present simultaneous measurement of the current through a quantum dot junction as well as the dissipation generated by the current. To this end, we thermally isolate the drain contact of an epitaxially defined quantum dot in an InAs nanowire. The electron temperature is measured via the zero-bias conductance of a Josephson junction [2]. Due to the energy-selective transport through a single quantum level, we can tune the dissipation solely with a gate voltage, while keeping both the current and voltage across the dot constant.

The presented device enables future investigations of local dissipation in nanoscale devices, e.g. for mitigation of detrimental heating effects, as well as implementations of proposed experiments in the field of quantum thermodynamics.

[1] S.G.J. Philips et al., Nature 609 (2022) 919
[2] B. Karimi, & J.P. Pekola, Phys. Rev. Applied 10 (2018) 054048

TT 78.2 Thu 11:15 HSZ/0101

Lindblad-based linear response of hybrid semiconductor-superconductor devices — •Tobias Kuhn, Raffael L. Klees, and Monica Benito — Augsburg University, Augsburg, Germany

The field of hybrid semiconductor-superconductor quantum dots is pushing towards the development of functional devices that harness the advantages of both worlds. Their complexity calls for a complete theoretical framework to under-

stand responses to different probe fields and dissipation induced by the environment. We present a Lindblad-based linear response formalism, built upon the framework introduced in Ref. [1]. It captures not only the inherently multi-level nature of these devices but also their probe-readout flexibility and non-unitary effects of the finite-frequency response. We exemplify the framework using quantum dot based Kitaev chain setups which are promising candidates for topologically protected qubits [2,3].

[1] L. Peri, M. Benito, C. J. B. Ford, and M. F. Gonzalez-Zalba, npj Quantum Inf **10**, 1 (2024)
[2] M. Leijnse and K. Flensberg, Phys. Rev. B **86**, 134528 (2012)
[3] D.M.Pino, R.S.Souto, R.Aguado, Phys. Rev. B**109**, 075101 (2024)

TT 78.3 Thu 11:30 HSZ/0101

Dynamics of strong correlations of a hybrid quantum dot system with superconducting and ferromagnetic electrodes — •Antoni Jankiewicz, Kacper Wrześniewski, and Ireneusz Weymann — Institute of Spintronics and Quantum Information, Adam Mickiewicz University, Poznań, Poland

We theoretically explore the non-equilibrium dynamics of a quantum dot coupled to superconducting and ferromagnetic electrodes. This hybrid setup offers a rich platform to investigate the interplay between strong correlations, superconductivity, and ferromagnetism at the nanoscale. To perform the analysis we employ the numerical renormalization group and its time-dependent extension. These methods enable us to capture the subtle nature of dynamical quantum phase transitions induced by abrupt changes in Hamiltonian parameters, known as quantum quenches. Such transitions are crucial for understanding the stability and evolution of many-body states in response to external perturbations.

The aim of this work is to examine the competition between the superconducting pairing and the dot's spin. For that, we determine the time dependence of key observables, including the dot's spin and the on-dot pairing correlations. We demonstrate that these quantities reveal the competing character of correlations as they oscillate in counter-phase. Furthermore, we also analyze the dynamical quantum phase transitions in the system by determining the Loschmidt echo and the return function, which provide direct measures of the system's sensitivity to quenches.

TT 78.4 Thu 11:45 HSZ/0101

Tunneling resonances through periodically driven quantum dots — •Jan Mathis Giesen, Daniel Weber, and Sebastian Eggert — RPTU University Kaiserslautern-Landau, D-67663 Kaiserslautern, Germany

We consider a general setup of transport through a time-periodically driven quantum dot using Floquet theory. An analytic non-equilibrium solution of the problem is developed which allows the analytic prediction and analysis of the tunneling amplitudes as a function of frequency, driving amplitude, and energy levels on the dot. One main result is the discovery of a previously unknown resonant switching effect, where a very small control signal on a weakly connected quantum dot can induce perfect transmission. This opens the door for the design of novel efficient nano-electronic devices. The results are also relevant for corresponding setups using magnonic systems, photonic waveguides, or ultra-cold gases in optical lattices.

TT 78.5 Thu 12:00 HSZ/0101

Spectroscopic-imaging Coulomb blockade microscopy — Junho Bang[1], Byeongin Lee[1], Hankyu Lee[1], •Jianfeng Ge[2], and Doohee Cho[1] — [1]Department of Physics, Yonsei University, Seoul 03722, Republic of Korea — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

We use scanning tunneling microscopy (STM) to directly visualize Coulomb blockade (CB) phenomena in the double-barrier tunnel junction formed between the STM tip and crystalline indium nanoislands on semiconducting black phosphorus. Spatially resolved tunneling spectra reveal bias-dependent dispersions of CB peaks across individual nanoislands. Strikingly, the trajectories of CB peaks exhibit two-fold asymmetries: (i) their curvatures reverse sign across a nonzero bias offset, and (ii) the trajectories lack mirror symmetry about this bias offset. Simulations based on orthodox theory faithfully reproduce both asymmetries, which we trace to work-function mismatches at (i) the island-tip and (ii) the island-substrate interfaces, respectively. These results establish spectroscopic-imaging Coulomb-blockade microscopy as a quantitative probe of junction parameters, offering a pathway for diagnosing and optimizing single-electron charge sensors relevant to quantum-computing architectures.

TT 78.6 Thu 12:15 HSZ/0101

Electromigrated palladium nano-contacts: formation of atomic contacts and non linear current-voltage characteristics — •Samanwita Biswas[1], Thomas Hultzsch[1], Marcel Strohmeier[2], Elke Scheer[2], and Regina Hoffmann-Vogel[1] — [1]Institute of Physics and Astronomy, University of Potsdam — [2]Department of Physics, University of Konstanz

We investigate the electronic transport properties of atomic-size Pd contacts fabricated by electromigration (EM) of lithographically defined nano-constrictions, at room temperature in different environments. In particular we study changes in the conductance upon EM with a focus on possible shell effects [1]. By systematic analysis of a large number of data sets in the conductance range up to $\sim 10G_0$ (with the conductance quantum $G_0 = 2e^2/h$), we identify preferential conductance values and compare these with the ones expected for shell closure in multivalent metals. For contacts with $G \lesssim 5G_0$, the current-voltage characteristics often become nonlinear on a scale of few 100mV; we discuss this observation with respect to structural changes during the thinning process of EM. By monitoring the smallest conductances, we often identify a decrement of resistance inside a cycle, opposite to the overall trend, indicating the transition to the ballistic regime. Our results suggest that metallic few atomic contacts of Pd, despite being more reactive than noble metals, can be stabilized even at room temperature.

[1] Mares & van Ruitenbeek, Phys. Rev. B 72, 205402 (2005)

TT 78.7 Thu 12:30 HSZ/0101

Readout of multi-level quantum geometry from electronic transport — •Raffael L. Klees and Mónica Benito — Institute of Physics, University of Augsburg, D-86159 Augsburg, Germany

The quantum geometric tensor (QGT) of a quantum system in a given parameter space captures both the geometry of the state manifold and the topology of the system [1]. While the local QGT elements have been successfully measured in various platforms, the challenge of detecting them in electronic transport systems – such as tunnel or molecular junctions – has yet to be resolved. To fill this gap, we propose a measurement protocol based on weak and resonant parameter modulations [2], and theoretically demonstrate how the local QGT in such systems can be directly probed from changes of the tunnel conductance [3]. This approach enables the measurement of both geometrical and topological features of quantum states in a broad class of transport-based quantum systems.

[1] M. Kolodrubetz *et al.*, Phys. Rep. **697**, 1 (2017)
[2] T. Ozawa and N. Goldman, Phys. Rev. B **97**, 201117(R) (2018)
[3] R. L. Klees and M. Benito, arXiv:2508.08239 (2025)

TT 79: Correlated Magnetism – Transport

Time: Thursday 11:30–12:45 Location: HSZ/0103

TT 79.1 Thu 11:30 HSZ/0103

Spin Dynamics Approach to Thermal Hall Conductivity — •Ignacio Salgado-Linares[1,2], Alexander Mook[3], Léo Mangeolle[1,2], and Johannes Knolle[1,2,4] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, TQM, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany — [3]Department of Physics, Johannes Gutenberg University Mainz, 55128 Mainz, Germany — [4]Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom

In recent years, the thermal Hall effect has emerged as a powerful tool for probing topological phenomena of magnetic systems. At low temperatures, the thermal Hall transport of long-range ordered magnets can be described in the framework of linear spin-wave theory (LSWT). However, how to treat regimes with increased thermal fluctuations or non-linearities beyond LSWT is an outstanding question. Therefore, within this project, we developed a novel numerical technique to extract the thermal Hall transport properties, which intrinsically includes non-linear effects. In particular, we use semi-classical spin dynamics simulations to compute thermal currents in the Kitaev model in a field. The results are expected to shed new light on the topological thermal transport in Kitaev spin liquid candidate materials.

TT 79.2 Thu 11:45 HSZ/0103

Extrinsic contribution to bosonic thermal Hall transport — •Léo Mangeolle[1,2] and Johannes Knolle[1,2,3] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany — [3]Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom

Bosonic excitations like phonons and magnons dominate the low-temperature transport of magnetic insulators. Similar to electronic Hall responses, the thermal Hall effect (THE) of charge neutral bosons has been proposed as a powerful tool for probing topological properties of their wavefunctions. For example, the intrinsic contribution of the THE of a perfectly clean system is directly governed by the distribution of Berry curvature. However, disorder is inevitably present in

any material and its contribution to the THE has remained poorly understood. Here we develop a rigorous kinetic theory of the extrinsic side-jump contribution to the THE of bosons. We show that the extrinsic THE is always relevant for bosonic systems and can be of the same order as the intrinsic one but sensitively depends on the type of local imperfection. We study different types of impurities and show that a THE can even arise as a pure impurity-induced effect in a system with a vanishing intrinsic contribution. We discuss the importance of our results for the correct interpretation of THE measurements and provide a ready-to-use formula for comparison to experimental data.

TT 79.3 Thu 12:00 HSZ/0103

Giant thermopower changes due to secondary gradients of electronic properties — •Ulrike Stockert[1,2,4], Judith Grafenhorst[1], Sarah Krebber[3], Kristin Kliemt[3], Cornelius Krellner[3], and Elena Hassinger[4,1,2] — [1]Technische Universität Dresden, 01062 Dresden, Germany — [2]MPI for Chemical Physics of Solids, 01187 Dresden, Germany — [3]Physikalisches Institut, Goethe-Universität Frankfurt, 60438 Frankfurt/M, Germany — [4]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

The diffusion thermopower S_{diff} of conventional metals and semiconductors is typically small, being of the order of 10-100 μV/K. It arises from changes of the number and velocity of mobile charge carriers with temperature T due to the energy dependence of the density of states and the T dependence of the Fermi distribution. In simple models for the thermopower, these changes are assumed to be weak, and the materials behave homogeneous. However, if electronic properties as the chemical potential or the charge-carrier mobility exhibit strong T dependencies, any temperature gradient induces also significant gradients of these properties. In our presentation we will show that such a secondary gradient of the electrical conductivity σ may induce giant values of the diffusion thermopower. Using a simple drift-diffusion model and allowing explicitly for gradients of σ, we are able to predict the correct magnitude, shape, and field dependence of the thermopower. Our results open a new route to large thermopower values via gradients of electronic properties.

TT 79.4 Thu 12:15 HSZ/0103

Observation via spin Seebeck effect of macroscopic magnetic transport from emergent magnetic monopoles — •Nan Tang[1], Josef Willsher[2], Stephan Glamsch[3], Aisha Aqeel[3], Ludwig Scheuchenpflug[1], Michael Schulze[4], Christoph Liebald[5], Daniel Rytz[5], Christo Guguschev[4], Manfred Albrecht[3], Roderich Moessner[2], and Philipp Gegenwart[1] — [1]Experimentalphysik VI, Universität Augsburg, Augsburg, Germany — [2]Max-Planck-Institut für Physik komplexer Systeme, Dresden, Germany — [3]Experimentalphysik VI, Universität Augsburg, Augsburg, Germany — [4]Leibniz-Institut für Kristallzüchtung (IKZ), Berlin, Germany — [5]EOT GmbH-Coherent, Idar-Oberstein, Germany

Magnetic monopoles, elusive in high-energy physics, have been realised as emergent quasiparticles in solid-state systems, where topological defects act as effective magnetic charges. They have been proposed in diverse platforms, including skyrmion lattices, chiral magnets, soft ferromagnets, and artificial nanomagnets, yet their role in magnetic transport has remained unconfirmed. Here, we demonstrate such transport via the spin Seebeck effect in the insulating pyrochlore $Dy_2Ti_2O_7$. A thermal gradient applied perpendicular to a [111]-oriented magnetic field yields a spin Seebeck voltage showing a dominant peak at monopole proliferation, alongside a secondary feature and frequency-dependent behavior. These results establish a direct link between monopole dynamics and magnetic transport in an insulator and provide a route to probing fractionalized excitations and spintronic functionalities.

TT 79.5 Thu 12:30 HSZ/0103

Unconventional Magnetotransport and Magnetic Anisotropy in van der Waals Ferromagnet Fe_4GeTe_2 — •Riju Pal[1,2,3], Joyal J. Abraham[1,2], Buddhadeb Pal[3], Suchanda Mondal[4], Prabhat Mandal[3,4], Atindra Nath Pal[3], Bernd Büchner[1,2,5], Vladislav Kataev[1], and Alexey Alfonsov[1] — [1]Leibniz IFW Dresden, D-01069, Germany — [2]Institute for Solid State and Materials Physics, TU Dresden, D-01062, Germany — [3]S. N. Bose National Centre for Basic Sciences, Kolkata, 700106, India — [4]Saha Institute of Nuclear Physics, Calcutta, 700064, India — [5]Würzburg-Dresden Cluster of Excellence ctd.qmat, Dresden, D-01062, Germany

Magnetic van der Waals (vdW) materials, with their intrinsic two-dimensionality and tunable exchange interactions, magnetocrystalline anisotropy, and electron correlations, are promising candidates for realizing non-trivial magnetic states. Combining transport measurements and electron spin resonance (ESR) spectroscopy, we studied the quasi-2D vdW ferromagnet Fe_4GeTe_2, which has a near-room-temperature $T_C \sim 270$K and an unusual spin-reorientation transition near $T_{SR} \sim 120$K. Transport experiments reveal two electronic transitions near T_{SR} and $T_Q \sim 40$-50K marked by sign reversal in Hall effect and magnetoresistance. ESR study further quantifies the non-trivial temperature evolution of magnetic anisotropy, with characteristic temperatures coinciding with those found in transport studies, indicating strong magneto-electronic coupling relevant for spintronic applications.

TT 80: Focus Session: High-Temperature Superconductivity in Hydride Materials at High Pressures (joint session TT/DS)

Superconductors with record transition temperatures up to 250 K have been discovered and confirmed in hydride materials at high pressures over the last decade, enabled by major advances in both computational and experimental approaches. Density functional theory, combined with structure search algorithms and machine learning methods, enables high-throughput predictions of novel high-pressure phases. Ab initio microscopic theories, including Eliashberg theory and superconducting density functional theory, successfully predict transition temperatures of identified phases, with several predictions now confirmed experimentally. The synthesis of novel hydrides has revealed the importance of including hydrogen quantum fluctuations in theoretical predictions. Experimentally, advances in high-pressure synthesis techniques have enabled the preparation of novel hydride phases, while electrical transport measurements, tunneling spectroscopy, and magnetic studies have established a strong body of evidence for superconductivity by probing zero resistance, the superconducting gap, and magnetic response. This focus session will emphasize these breakthroughs, highlight ongoing challenges in both experiment and computation, and provide an outlook for finding high-temperature superconductors at lower and ambient pressures.

Coordinators: Philipp Gegenwart (Universität Augsburg), Matthias Vojta (TU Dresden)

Time: Thursday 15:00–18:45 Location: HSZ/0003

Topical Talk TT 80.1 Thu 15:00 HSZ/0003

Computational searches for conventional high temperature superconductivity — •Chris Pickard — University of Cambridge

First principles methods for the prediction of the structure of materials have delivered a powerful tool for generating candidate structures for comparison with experimental analytical methods. Early studies focused on the exotic properties and structures of relatively simple systems, typically the elements and binary compounds. The promise of discovering materials with extreme properties relies on the ability of screen a wide variety of compounds.[1] I will reflect on why ab initio random structure searching (AIRSS) is particularly suited to these challenges, focussing on the dramatic acceleration that ephemeral data derived potentials (EDDPs) afford,[2] and their role in the uncovering of Mg_2IrH_6 as a feasible ambient pressure high temperature superconductor.[3]

[1] A.M.Shipley, M.J Hutcheon, R.J.Needs, Ch.J.Pickard, Phys. Rev. B 104, 054501 (2021)
[2] Ch.J.Pickard, Phys. Rev. B 106, 014102 (2022)
[3] K.Dolui, L.J.Conway, Ch.Heil, T.A.Strobel, R.Prasankumar, Ch.J.Pickard, Phys. Rev. Lett. 132, 166001 (2024)

Topical Talk TT 80.2 Thu 15:30 HSZ/0003

High-pressure synthesis of hydrides and their characterisation by single-crystal X-ray diffraction — •Natalia Dubrovinskaia[1] and Leonid Dubrovinsky[2] — [1]Material Physics, University of Bayreuth; Bayreuth, Germany — [2]Bayerisches Geoinstitut, University of Bayreuth, Germany

The sulfur-hydrogen, lanthanum-hydrogen, and yttrium-hydrogen systems have attracted significant interest following reports of near-ambient-temperature su-

perconductivity in some of their high-pressure phases. Here, we present single-crystal X-ray diffraction studies of these systems, supported by density functional theory calculations, which reveal an unexpected chemical and structural diversity in S, La, and Y hydrides synthesised at 50*200 GPa. Syntheses were carried out in diamond anvil cells by laser heating S, La, LaH3, or Y together with hydrogen-rich precursors-ammonia borane or paraffin oil. The arrangements of heavy atoms in newly formed phases were determined from SCXRD data, while hydrogen contents were estimated using empirical relationships and ab initio calculations. Our study also uncovers the formation of previously unreported metal allotropes, carbides, and ternary compounds at high pressure. The complex phase diversity, variable hydrogen stoichiometries, and metallic nature of these high-pressure hydrides, as revealed by theory, highlight the challenges in identifying the superconducting phases and understanding electronic transitions in materials synthesised under extreme conditions.

Topical Talk TT 80.3 Thu 16:00 HSZ/0003

Electrical Transport Studies in bulk and thin-film hydride high-temperature superconductors — •Sven Friedemann[1], Sam Cross[1], Owen Moulding[1], Israel Osmond[1], Xiaojiao Liu[2], Annette Kleppe[2], Oliver Lord[3], and Jonathan Buhot[1] — [1]HH Wills Physics Laboratory, University of Bristol, UK — [2]Diamond Light Source Ltd., Didcot, UK — [3]School of Earth Sciences, University of Bristol, UK

Superconductivity is not restricted to low temperatures! Indeed, transition temperatures up to 260 K have been demonstrated by multiple groups in H_3S, LaH_{10}, and YH_9, at very high pressures. This is a success story of both theory and experiment. Theory has mastered accurate predictions of new superconductors and has been crucial to guide experimental efforts. Experiments have mastered many technical challenges. Together, these efforts open pathways to realise higher transition temperature at low pressures.

We present combined structural and electrical transport studies of hydride high-T_c superconductors based on our development of *in situ* synthesis, x-ray diffraction, and transport measurements in diamond-anvil pressures cells including thin-film methods for electrodes and superconducting samples. We present the characterisation of clean-limit superconductivity in H_3S and the discovery of the new superconductor La_4H_{23}. We demonstrate superconductivity in thin films of LaH_{10} with a T_c = 250 K consistent with bulk LaH_{10}. Our results open new avenues to study hydride high-T_c superconductors with thin-film methods.

15 min. break

Topical Talk TT 80.4 Thu 16:45 HSZ/0003

Near room-temperature conventional superconductivity in hydrogen-rich compounds at high pressures: Experimental evidences — •Vasily Minkov — Max Planck Institute for Chemistry, Mainz, Germany

The pioneering discovery of superconductivity in hydrogen sulfide (H3S) with a record Tc of 203 K at 150 GPa by M. Eremets et al. had a profound impact on the field. It validated the concept of high-Tc conventional superconductivity in hydrides and triggered an intense wave of research. Subsequent studies revealed that other hydrides - such as LaH10 and YH9 - exhibit Tc values approaching 250 K, bringing the field closer than ever to room-temperature superconductivity. Despite the experimental challenges associated with micrometer-sized samples confined in diamond anvil cells, superconductivity in these compounds has been demonstrated using multiple independent techniques. Electrical four-probe measurements provide clear resistive transitions, while recent advances in high-pressure magnetometry enable direct detection of magnetic field screening and flux expulsion. We have further developed a method to probe trapped magnetic flux in hydrides at high pressure. The distinct behavior of trapped flux generated under ZFC and FC conditions provides strong evidence for superconductivity. Furthermore, the recent adaptation of electron tunneling spectroscopy to extreme pressures offers microscopic insight into the pairing mechanism and enables direct characterization of the superconducting gap structure in the high-temperature hydride superconductors.

Topical Talk TT 80.5 Thu 17:15 HSZ/0003

Predictive T_c Calculations in Hydride Superconductors — •Christoph Heil — Institute of Theoretical and Computational Physics, Graz University of Technology, Graz, Austria

The discovery of high-T_c superconductivity in compressed hydrides has sparked a surge of theoretical predictions, yet reported critical temperatures for identical structures can differ by tens of Kelvin or more. These discrepancies reflect differences in how lattice dynamics, electronic structure, and Coulomb repulsion are treated. In this talk, we will present first-principles workflows designed to make Tc calculations both more transparent and more predictive.

We combine anharmonic lattice dynamics with full-bandwidth isotropic and anisotropic Migdal-Eliashberg calculations (IsoME and EPW) that retain the full electronic density of states, and we incorporate Coulomb repulsion via screened interactions obtained from first principles rather than an empirical μ^*. This framework allows us to systematically compare different approximation levels and to quantify how each approximation affects T_c.

Using case studies from high-pressure hydrides, we will demonstrate when simplified treatments remain adequate and when anharmonic effects, full-bandwidth electrons, and first-principle determination of Coulomb screening become essential for quantitative accuracy. I will provide practical guidelines for reliable, reproducible T_c predictions and discuss how rigorous superconductivity calculations complement crystal-structure prediction efforts in the search for new superconductors.

TT 80.6 Thu 17:45 HSZ/0003

^{1}H-NMR investigations of bulk superconductivity in superhydrides using Lenz lenses — •F. Bärtl[1,2], D. Zhou[3], T. Helm[1], S. Luther[1], H. Kühne[1], J. Wosnitza[1,2], and D. Semenok[3] — [1]HLD-EMFL, HZDR, Dresden — [2]IFMP, TUD, Dresden — [3]HPSTAR, Beijing

The discovery of near-room-temperature superconductivity at ultrahigh pressures in superhydrides has kindled intensive research activities in the past years. However, the need to use diamond-anvil cells (DACs) for the synthesis and study of such superconductors limits the number of available experimental techniques. Nuclear magnetic resonance (NMR) spectroscopy is a key technique to study the bulk properties of superconducting materials, but it usually requires sample masses of several milligrams. Here, we present our ^{1}H NMR measurements of several superhydride preparations, using Lenz lenses, which act as magnetic-flux transformers in the NMR experiment and enable the investigation of samples with masses in the microgram range in the sample chamber of DACs. We observe several features that evidence the bulk nature of the superconducting transition in the superhydrides, the most prominent being the suppression of the ^{1}H nuclear spin-lattice relaxation rate $1/T_1T \propto D(E_F)^2$. Furthermore, we report on the systematic occurrence of a rate enhancement in the regime of the superconducting transition, which is reminiscent of a Hebel-Slichter-like peak.

TT 80.7 Thu 18:00 HSZ/0003

Above-room-temperature superconductivity in substituted LaH_x superhydride — •Stanley Tozer and Audrey Grockowiak — Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden, 01069 Dresden, Germany

We have synthesized a higher order La-based superhydride with initial superconducting transition temperature of 294 K that, when heated, morphed into a higher order system with a T_c^{onset} of 556 K and a transition width of approximately 120 K [1]. The x-ray and the electrical transport data support one another with regard to the pressure measured, and the inhomogeneous nature of the synthesis that resulted in a substituted higher order La-based superhydride in close proximity to FIBed electrodes with a broad multi-phase, irreversible transition and non-zero background resistance below T_c. The electric leads embedded in our 'crucible' probe a pathway through this inhomogeneous growth, a very small portion of which is the superconductor of interest. We have used informed growth to reproduce the initial result in a range of pressures lower than allowed for the binary LaH_{10}. A multi-probe approach is being implemented to address growth-to-growth variations and follow the transformation of the initial 294 K superconductor. This will provide an understanding of this new class of superconductor that begs the question as to the upper limit of superconductivity in the superhydrides and whether BCS theory can describe them.

[1] A.D. Grockowiak et al., Electronic Materials 2, (2022)
[2] doi.org10.3389/femat.2022.837651

TT 80.8 Thu 18:15 HSZ/0003

Search for Room-temperature Superconductivity in the La-Sc-H System — •Dmitrii V. Semenok[1], Ivan A. Troyan[2], Di Zhou[1], and Viktor V. Struzhkin[1,3] — [1]Center for High Pressure Science & Technology Advanced Research, Bldg. 8E, 10 Xibeiwang East Rd, Beijing, 100193, China — [2]private — [3]Center for High Pressure Science & Technology Advanced Research, 1690 Cailun Rd, Bldg 6, Shanghai 201203, China

One of the highlights of 2025 in the field of hydride superconductivity was the announcement of the experimental discovery of room-temperature superconductivity in the fully ordered ternary polyhydride P6/mmm-$LaSc_2H_{24}$ at around 260 GPa [1]. We performed a DFT analysis of intermetallic compound formation in the La-Sc system with a view to modifying the synthetic procedure, and calculated parameters of the superconducting state of the isostructural P6/mmm-La_3H_{24} and P6/mmm-Sc_3H_{24} at 300 GPa. Attempts to experimentally reproduce the synthesis of $LaSc_2H_{24}$ from the $LaSc_2$ alloy (with a careful selection of the homogeneity region of this alloy's composition) at 264-280 GPa have not yet resulted in the detection of any traces of superconductivity between 255 K and 295 K in the corresponding hydride. In my report, I will show the results of additional experimental attempts to reproduce [1], planned for January-February 2026.

[1] Y. Song et al., arXiv: 2510.01273 (2025).

TT 80.9 Thu 18:30 HSZ/0003

Computational modeling of disordered hydride superconductors — •Pedro Nunes Ferreira[1], Luiz Tadeu Fernandes Eleno[2], and Christoph Heil[1] — [1]Institute of Theoretical and Computational Physics, Graz University of Technology, NAWI Graz, 8010, Graz, Austria — [2]Departamento de Engenharia de Materiais, Escola de Engenharia de Lorena, Universidade de São Paulo, Lorena, Brazil

Designing and optimizing novel hydride superconductors requires methods that accurately treat realistic chemical disorder. In this talk, I will present an ab initio thermodynamic framework, the extended generalized quasichemical approximation (EGQCA), tailored to the modeling of superconducting alloys, especially high-T_c superhydrides. EGQCA enables the prediction of any computationally accessible property, such as T_c and electron-phonon coupling, as a function of composition using only a small set of supercell calculations, making it particularly well suited for complex hydrogen-rich materials. I will illustrate its capabilities with applications to high-T_c superhydrides at high pressure, as well as defective hydrides stabilized at ambient pressure. Finally, I will discuss how EGQCA opens the door to high-throughput design and screening of disordered superconductors, with the potential to significantly advance hydride superconductivity research.

TT 81: Correlated Electrons: Other Materials

Time: Thursday 15:00–17:15 Location: HSZ/0101

TT 81.1 Thu 15:00 HSZ/0101

Built-in Electric-Field-Driven Rashba Spin-Orbit Interactions in $AlO_x/Sr_{1-x}Ca_xTiO_3$ Interfaces — •Janine Gückelhorn[1], Sergi Plana-Ruiz[2,3], Gyanendra Singh[1], Saul Estandia Rodriguez[1], Roger Guzman[1], Fernando Gallego[4], Luis M. Vicente-Arche[4], Joaquim Portillo[5], Thanos Galanis[5], Manuel Bibes[4], Jaume Gázquez[1], and Gervasi Herranz[1] — [1]Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Bellaterra, Spain. — [2]Scientific & Technical Resources, Universitat Rovira i Virgili, Tarragona, Spain. — [3]LENS-MIND, Department of Electronics and Biomedical Engineering, Universitat de Barcelona, Spain. — [4]Laboratoire Albert Fert, CNRS, Thales, Université Paris Saclay, France. — [5]NanoMEGAS SPRL, Brussels, Belgium.

Two-dimensional electron gases (2DEGs) at oxide interfaces exhibit strong Rashba spin-orbit coupling (SOC), arising from broken inversion symmetry and the resulting built-in electric field. However, the microscopic origin of Rashba SOC remains under debate. Density functional theory points to two key mechanisms as origin: polar lattice displacements and electric-field-driven orbital polarization. We show that the Rashba coefficient in $AlO_x/Sr_{1-x}Ca_xTiO_3$ 2DEGs increases significantly with Ca substitution, which enhances polarizability and induces ferroelectricity. Separating lattice and electrostatic effects reveals that modest structural changes accompany a near-tenfold rise in the built-in field. Our results demonstrate that nonlinear polarizability, not just structural asymmetry, dictates Rashba SOC strength, establishing polarizability as a key control of SOC in oxide 2DEGs.

TT 81.2 Thu 15:15 HSZ/0101

Non-quasiparticle states at a ferromagnetic oxide interface — Dylan Jones[1,2], Andreas Östlin[1,2], and •Liviu Chioncel[1,2] — [1]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany — [2]Augsburg Center for Innovative Technologies, University of Augsburg, 86135 Augsburg, Germany

We propose a minimal tight-binding model for the electronic interface layer of the $LaAlO_3/SrTiO_3$ heterostructure with oxygen vacancies. In this model, the effective carriers are subject to oxygen vacancy-induced magnetic impurities. Both the effects of random on-site potentials and Zeeman-like exchange interactions between correlated carriers and magnetic impurities are taken into account. By applying the combined coherent potential approximation (CPA) and dynamical mean field theory (DMFT) for a ferromagnetic state, we analyze how magnetic impurities generate incoherent non-quasiparticle spectral weight near the Fermi level and introduce a low-energy scale that is expected to be relevant for electronic transport at the interface.

TT 81.3 Thu 15:30 HSZ/0101

Transport properties of the metal to insulator transition in Ca_2RuO_4 nanoflakes — •Roman Hartmann[1], Rosalba Fittipaldi[3], Antonio Vecchione[3], Elke Scheer[1], and Angelo Di Bernardo[1,2] — [1]FB Physik, Universität Konstanz, Konstanz, Germany — [2]Dipartimento di Fisica, Università di Salerno, Fisciano, Italy — [3]CNR-Spin, Salerno, Italy

The Mott insulator calcium ruthenate Ca_2RuO_4 (CRO) has attracted considerable attention due to its insulator to metal transition (IMT) with a transition temperature of 357 K (insulating below, metallic above) and the ability to trigger the IMT using pressure, current or an electric field of just 40 V/cm [1,2]. Unfortunately, stress from a structural transition (orthorombic to tetragonal) during the IMT combined with an increase in unit cell volume [1] generally breaks bulk crystals.

To overcome this limitation we have developed a method to fabricate submicron CRO flakes from bulk single crystals (despite it not being a layered material) that we can contact using standard lithographic and thin film techniques.

In these flakes we can reversibly trigger the IMT thousands of times by passing current without breaking the sample. The robustness of the devices enables us to switch at high frequencies paving the way for potential applications and enabling us to to gain further insight into the nature of the IMT [3].

[1] F. Nakamura et al., Sci. Rep. 3, 2536 (2013)
[2] R. Okazaki et al., JPSJ 82, 103702 (2013)
[3] V. K. Bhartiya et. al., arXiv:2504.17871 (2025)

TT 81.4 Thu 15:45 HSZ/0101

Many body effects in Li-ion cathode materials: how Coulomb interactions drive the redox profile — •Francesco Cassol and Silke Biermann — CPHT, Ecole Polytechnique, Palaiseau, France

In the last decades, a rising demand for energy storage has spurred consistent efforts into the design of high energy density cathode materials.

Crystallizing in layered structures, these compounds alternate lithium and transition-metal oxide planes, facilitating Li mobility during charge and discharge. Most of the battery properties are intimately related to the electronic structure, which governs the cyclic charge redistribution via oxidation and reduction of transition metal ions.

In this talk, we investigate the effects of Coulomb interactions on the corresponding redox mechanism upon delithiation, focusing on complex Li-based alloys studied within the dynamical mean-field theory (DMFT). Our results reconcile the charge profile with experiments and emphasize the importance of many-body effects for an accurate description of battery compounds.

15 min. break

TT 81.5 Thu 16:15 HSZ/0101

Separating magnetic bulk and surface properties of Czochralski-grown FeSi — •Gilles Gödecke[1], Philipp Herre[1], Markus Etzkorn[2,3], Musfira Aqeel[2,3], Alexander Frantz[4], Dirk Baabe[4], Stefan Süllow[1], and Dirk Menzel[1,2] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [2]Laboratory for Emerging Nanometrology, TU Braunschweig, Germany — [3]Institut für Angewandte Physik, TU Braunschweig, Germany — [4]Institut für Anorganische und Analytische Chemie, TU Braunschweig, Germany

The narrow-gap semiconductor FeSi has been extensively discussed regarding its low-temperature electronic transport and magnetic properties, ranging from Kondo-insulating behavior to the emergence of conducting and magnetic surface states. We present resistivity measurements on FeSi single crystals grown by the Czochralski method. To separate bulk and surface contributions, the sample thickness is continuously decreased by polishing. In addition, we conduct magnetization measurements of FeSi powder samples with decreasing grain sizes prepared by ball milling. The increase of the surface-to-volume ratio leads to enhanced surface contributions in the conductivity and magnetization. The results enable us to distinguish between the electrical and magnetic bulk and surface contributions and further estimate the dimensions of the surface states.

TT 81.6 Thu 16:30 HSZ/0101

Flat phonons in Eu_2AuGe_3 — •Aleksandr Sukhanov[1], Oleg Utesov[2], Artem Korshunov[3], Vinicius Frehse[1], and Marein Rahn[1] — [1]Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg, 86159 Augsburg, Germany — [2]Center for Theoretical Physics of Complex Systems, Institute for Basic Science (IBS), Daejeon, Korea, 34126 — [3]Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal, 20018 San Sebastian, Spain

We employed inelastic x-ray scattering (IXS) to study the lattice dynamics in a single crystal of Eu_2AuGe_3 (orthorhombic, space group *Fmmm*). Within its crystal structure, a structural motif consisting of one Au atom and three Ge atoms plays a special role. Its atomic displacements can be effectively mapped out to the well known electronic cross-stitch model, which is a toy model for the electronic flat bands. We show that the same simple model can be applied to predict a flat phonon mode in Eu_2AuGe_3. In our experimental IXS spectra, we resolve the flat mode and show that it softens on cooling and leads to a charge density wave transition. Our first-principle calculations of the lattice dynamics further support the experimental findings.

TT 81.7 Thu 16:45 HSZ/0101

Tuning through a tetragonal collapse in $Ca_{1-x}Sr_xCo_2As_2$ single crystals investigated by thermal expansion — •Sven Graus[1], Adrian Valadkhani[2], N. S. Sangeetha[1], Markus Garst[3], Roser Valentí[2], Andreas Kreyssig[1], and Anna E. Böhmer[1] — [1]Experimental Physics IV, Ruhr University Bochum, Bochum, Germany — [2]Institute for Theoretical Physics, Goethe University Frankfurt, Frankfurt am Main, Germany — [3]Institute of Theoretical Solid State Physics, Karlsruhe Institute of Technology, Karlsruhe, Germany

$Ca_{1-x}Sr_xCo_2As_2$ crystallizes in the tetragonal $ThCr_2Si_2$-type structure and undergoes a rare substitution-driven crossover from a collapsed tetragonal to an uncollapsed tetragonal structure. The resulting rich magnetic and electronic phase diagram provides an interesting platform to investigate the complex interplay between lattice, magnetic and electronic degrees of freedom.

High-resolution thermal-expansion measurements reveal strong anisotropy between in-plane and out-of-plane directions and identify a critical region near $x \approx 0.48$, where the thermal expansion coefficients α_a/T and α_c/T diverge at low temperatures. Analysis of the temperature dependence of the c/a ratio shows an accumulation of entropy in this region. The thermal-expansion behavior is well captured by a simple model of a pressure-tuned Van Hove singularity which is supported by density-functional theory calculations.

We acknowledge support from the Deutsche Forschungsgemeinschaft (DFG) under CRC/TRR 288 (Project A02).

TT 81.8 Thu 17:00 HSZ/0101

Synthesis of $CsMn_2P_2$ single crystals and study of their low temperature properties — •Martin Kostka, Ashiwini Balodhi, Matthias Kroll, N. S. Sangeetha, Sven Graus, Maik Golombiewski, Andreas Kreyssig, and Anna E. Böhmer — Experimental Physics IV, Ruhr-University Bochum, Bochum, Germany

$CsMn_2P_2$ is an intriguing material because it exhibits unusual dynamic magnetic behavior not present in other AMn_2P_2 compounds, likely related to a mixed Mn^{2+}/Mn^{3+} valence state and enhanced magnetic fluctuations [1]. However, the synthesis of $CsMn_2P_2$ single crystals is a challenge due to the high reactivity of Cs, the high vapor pressure of Cs and P, and the high melting point of Mn. We succeeded in optimizing the growth conditions for reproducible synthesis of ~1 mm sized $CsMn_2P_2$ single crystals by systematically studying various growth techniques. The resulting samples were characterized by x-ray diffraction, electron microscopy, energy-dispersive x-ray spectroscopy, and electrical-transport measurements. The electrical resistance shows multiple intriguing phase transitions. However, it is sample dependent and varies with synthesis parameters. A relation with the lattice parameter c is observed.

We acknowledge support by the Deutsche Forschungsgemeinschaft (DFG) under CRC/TRR 288 (Project A02).

[1] F. Hummel, Magnetism and superconductivity in layered manganese and iron pnictides, Diss. LMU (2015)

TT 82: Cryogenic Detectors and Sensors

Time: Thursday 15:00–16:30 Location: HSZ/0103

TT 82.1 Thu 15:00 HSZ/0103

2D germanium-based micro-bolometers for quantum information readout — •Julius Werner, Martina Trahms, Johannes Höfer, Frederic Gustavo, Jean-Luc Thomassin, Clemens Winkelmann, and Boris Brun — Univ. Grenoble Alpes, CEA, Grenoble INP, IRIG-Pheliqs, Grenoble, France

We develop and investigate micron-scale bolometers based on a two-dimensional hole gas (2DHG) in a Ge/SiGe semiconducting heterostructure. Such devices have promising applications for quantum sensing and the readout of quantum communication signals. The high-transparency interfaces formed between germanium and superconducting aluminum leads allow using the proximity Josephson effect in the 2DHG for thermometry, which is sensitive down to 50 mK. To enable time-resolved thermometry and bolometry with MHz-bandwidth operation, the Josephson inductance is read out via its contribution to a radio-frequency resonant circuit. We present a full thermal balance investigation of the 2DHG-based bolometer at millikelvin temperatures, allowing us to determine the thermal equilibration mechanisms at play and showcase the potential of the Ge 2DHG for quantum heat-detector applications.

TT 82.2 Thu 15:15 HSZ/0103

High-Resolution Spectroscopy of Muon Induced X-ray Emission on a Prehistoric Human Tooth using Metallic Magnetic Calorimeters — •Hendrik Hadenfeldt, Andreas Abeln, Daniel Hengstler, Daniel Kreuzberger, Andreas Reifenberg, Daniel Unger, Andreas Fleischmann, Loredana Gastaldo, and Christian Enss — Kirchhoff-Institute for Physics, Heidelberg University, Germany

High-resolution X-ray spectroscopy of muonic atoms provides a powerful tool for probing nuclear and elemental properties. Muon-induced X-ray emission (MIXE), developed at the Paul-Scherrer-Institute (PSI), enables non-destructive elemental analysis. Using metallic magnetic calorimeters (MMCs), we aim to improve the precision of MIXE measurements of light muonic atoms. MMCs are low-temperature photon detectors operated at a few tens of mK. When a photon is absorbed, its energy causes an increase in the temperature of the absorber. This temperature increase leads to a change in magnetization of a paramagnetic Ag:Er sensor, which is then read out by SQUID magnetometers.

In this talk, a newly developed MMC detector setup for high-resolution muonic X-ray spectroscopy used during beamtime at PSI is presented. The detector achieved an unprecedented energy resolution of better than 50 eV full width at half maximum (FWHM) at photon energies around 120 keV. Data collected during measurements performed on a prehistoric human tooth have been analyzed to demonstrate the applicability of this detector technology to non-destructive elemental analysis.

TT 82.3 Thu 15:30 HSZ/0103

High resolution measurement of the ^{65}Zn spectrum with magnetic microcalorimeters (MMCs) — •Michael Paulsen[1], Philipp Ranitzsch[2,3], Jörn Beyer[1], Alexander Göggelmann[2], Sebastian Kempf[4,5], Karsten Kossert[2], Ole Nähle[2], Constantin Schuster[1,2], Mariia Sidorova[1,2], and Mathias Wegner[5,4] — [1]Physikalisch-Technische Bundesanstalt (PTB) Berlin — [2]PTB Braunschweig — [3]DLR e.V., Hamburg — [4]IMS, Karlsruhe Institute of Technology (KIT) — [5]IPE, KIT

MMCs have proven to be among the best spectrometers for beta transitions and electron capturing (EC) radionuclides. To achieve a high energy resolution, the sensor and absorber heat capacities are kept as low as possible. Thus, the absorber dimensions are very small, yet simultaneously large enough to ensure that a sufficient detection efficiency is achieved. This is challenging when studying EC radionuclides, such as ^{65}Zn since the emission energies range from 0 to over 1 MeV for high-intensity gamma rays. We present a high-resolution spectrum of ^{65}Zn featuring K, L and M peaks below 10 keV. For the β^+ branch (E_{max} = 329.9 keV), additional complications arise. Each emitted positron typically annihilates with an electron in the absorber and generates gamma rays with a combined energy of 1022 keV. These additional events cannot be time resolved by the detector due to the very short lifetimes of the positrons (~ 100 ps). This yields a distorted beta spectrum with a substantial number of counts above E_{max}. We consider how this relates to the issue of detector efficiency and how to unfold such spectra using Monte-Carlo based simulation methods.

TT 82.4 Thu 15:45 HSZ/0103

A novel dilution refrigerator based microwave impedance microscopy — •Yizhou Wei and Berthold Jäck — The Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong

Microwave Impedance Microscopy (MIM) is an advanced imaging technique that offers remarkable sensitivity in detecting spatial variations of the electric conductivity with a spatial resolution of between 10 and 100 nanometers. This makes it a powerful tool for investigating 2D materials, especially in the context of topological and many-body physics of moiré materials. Despite its scientific potential, several technical challenges hinder the broader application of MIM for the study of quantum materials at cryogenic temperatures. Major issues are the pervasive noise introduced by dry cryogenic systems, particularly due to the pulse tube, and the thermalization of the microscopy module to temperatures below 100 mK. To address these challenges, we have designed and realized a novel MIM system that is both noise-resistant and capable of operating at ultra-low temperatures. In this talk, we will present key design considerations as well as first results from test measurements that validate the performance of our experimental setup.

We gratefully acknowledge funding by the Croucher Foundation (Grant No.CIA22SC02).

TT 82.5 Thu 16:00 HSZ/0103

Detecting single itinerant microwave photons by stroboscopic measurement — •Hanna Zeller[1], Lukas Danner[1,2], Max Hofheinz[3], Ciprian Padurariu[1], Joachim Ankerhold[1], and Björn Kubala[1,2] — [1]ICQ and IQST, Ulm University, Ulm, Germany — [2]German Aerospace Center (DLR), Institute of Quantum Technologies, Ulm, Germany — [3]Institut Quantique, Université de Sherbrooke, Sherbrooke, Québec, Canada

Josephson-photonics devices have predominantly been used to create microwave radiation in a process where a Cooper pair tunneling across a dc-biased Josephson junction creates photonic excitations in a microwave cavity connected in series. In scenarios where incoming photons are required to enable Cooper pair transfer and trigger subsequent photon emission, their use as amplifiers [1] or single (microwave-) photon detectors [2] has also been investigated.

Here, we present a scheme utilizing a Josephson-photonics device with two cavities as a microwave detector of itinerant photons, where the Josephson-photonics effect implements a stroboscopic projective measurement. Using recently developed techniques to describe the incidence of generic traveling pulses of quantized radiation onto a quantum device [3,4], we optimize the device and find promising performance numbers.

[1] R. Albert, et al. Phys. Rev. X **14**, 011011 (2024).
[2] L. Danner et al., arXiv:2510.08030
[3] A. H. Kiilerich et al., Phys. Rev. Lett. **123**, 123604 (2019).
[4] A. H. Kiilerich et al., Phys. Rev. A **102**, 023717 (2020).

TT 82.6 Thu 16:15 HSZ/0103

Vortex Energy Barriers in Meandering Superconducting Nanowires: Controlling Jitter in SNSPDs via magnetic field and bias currents — •Carlos Alberto Diaz Lopez[1], Joachim Ankerhold[1], Björn Kubala[1,2], and Ciprian Padurariu[1] — [1]Institute of Complex Quantum Systems, University of Ulm, Ulm, Germany — [2]German Aerospace Center (DLR), Ulm, Germany

We present a theoretical and computational study of vortex dynamics in meandering superconducting nanowires (e.g., SNSPDs). Building upon established methods for computing vortex energies in non-conventional geometries, our work incorporates the effect of screening currents induced by an external magnetic field. We calculate the total Gibbs free energy landscape to determine sets of parameters (B_z, I_{bias}) to engineer a tunable energy barrier for vortex crossing events. We seek barriers high enough to suppress spontaneous vortex-crossing (the mechanism underlying dark counts and timing jitter) yet remain low enough to permit crossing upon localized perturbations (e.g., a hotspot following single-photon absorption)

This analytical approach is benchmarked against a heuristic approach via simulations of the generalized time-dependent Ginzburg-Landau (gTDGL), performed using the open-source package py-TDGL. Our findings offer a design principle for optimizing operating conditions of SNSPDs to achieve maximal timing resolution and dark-count suppression.

TT 83: Topology: Quantum Hall Systems

Time: Thursday 15:00–18:30 Location: HSZ/0105

TT 83.1 Thu 15:00 HSZ/0105

Many-body Euler topology — •Axel Fünfhaus[1], Titus Neupert[2], Thilo Kopp[3], and Roser Valentí[1] — [1]Goethe Uni Frankfurt, Frankfurt am Main, Germany — [2]University of Zurich, Zurich, Switzerland — [3]University of Augsburg, Augsburg, Germany

Chern insulators exhibit an anomalous nonzero Hall conductivity due to a spontaneous breaking of time-reversal symmetry. To identify nontrivial topology in their time-reversal symmetric many-body spectra, we identify many-body Euler numbers as a counterpart to many-body Chern numbers. Exemplarily, we perform calculations in a topological Hubbard model that can realize Chern and fractional Chern insulating phases. Furthermore, we lay out a classification scheme to realize different topological phases using symmetry indicators in analogy to topological band theory.

TT 83.2 Thu 15:15 HSZ/0105

Topological signatures in the electrostatics of Chern junctions — •Robin Durand[1,2], Pascal Simon[1], and Ion Garate[2] — [1]Laboratoire de Physique des Solides, Université Paris-Saclay, CNRS, Orsay 91405, France — [2]Département de physique, Institut quantique and Regroupement Québécois sur les Matériaux de Pointe, Université de Sherbrooke, Sherbrooke, Québec J1K 2R1, Canada

Electrostatic control in topological materials is a key challenge for next-generation electronic and quantum devices. We investigate how topological properties, especially Berry curvature and Chern number, reshape electrostatic equilibrium in Chern-insulator junctions under magnetic field. We show that Berry curvature corrections to the modified Landau quantization significantly modify both the built-in potential and the intrinsic chemical-potential profile at the junction.

Using a Landau-level framework combined with a semiclassical expansion, we derive an analytical expression revealing that the built-in potential becomes directly governed by spectral asymmetry, and therefore by the Chern number on each side. Large-scale tight-binding simulations of the half-BHZ model validate this prediction quantitatively.

Our results show that topological properties can directly influence electrostatic profiles in Chern junctions. By linking the built-in potential to spectral asymmetry and Chern number, we reveal how Berry curvature affects charge redistribution and electrostatic equilibrium at topological interfaces.

TT 83.3 Thu 15:30 HSZ/0105

Non-Hermitian topology of transport in the quantum Hall phases in graphene — •Raghav Chaturvedi[1,2], Ewelina M. Hankiewicz[2], Jeroen van den Brink[1], and Ion Cosma Fulga[1] — [1]Leibniz Institute for Solid State and Materials Research, IFW Dresden, Germany — [2]Institute for Theoretical Physics and Astrophysics, Julius-Maximilians-Universität Würzburg, Germany

Signatures of non-Hermitian topology can be realized in a conventional quantum Hall device connected to multiple current sources. These signatures manifest as robust current-voltage characteristics, dictated by the presence of a nontrivial, non-Hermitian topological invariant of the conductance matrix. Chiral edge states are believed to be responsible for this non-Hermitian response, similar to how they lead to a quantized Hall conductivity in the presence of a single current source. Here, we go beyond this paradigm, showing that multiterminal conductance matrices can exhibit non-Hermitian topological phase transitions that cannot be traced back to the presence and directionality of a boundary-localized chiral mode. By performing quantum transport simulations in the quantum Hall regime of graphene, we find that when the chemical potential is swept across the zeroth Landau level, unavoidable device imperfections cause the appearance of an additional non-Hermitian phase of the conductance matrix. This highlights graphene as an ideal platform for the study of non-Hermitian topological phase transitions, and is a first step towards exploring how the geometry of quantum devices can be harnessed to produce robust, topologically-protected transport characteristics.

TT 83.4 Thu 15:45 HSZ/0105

Superconducting Beam Splitting of Quantum Hall Edge States for HOM Interference — •Maxime Jamotte[1], Tom Menei[1], Alexander Zyuzin[2], Manohar Kumar[2], and Thomas L. Schmidt[1] — [1]University of Luxembourg, Luxembourg, Luxembourg — [2]Aalto University, Aalto, Finland

Electron interferometers have proven to be important tools for characterizing the exchange statistics of quantum Hall edge states. Moreover, it has recently become possible to proximitize quantum Hall edge states using superconductors. This opens a new avenue for interferometers based on the particle-hole degree of freedom. We propose a Hong-Ou-Mandel interferometer in which an s-wave type-II superconductor is located between two graphene systems in a magnetic field, with chiral edge states serving as the interferometer arms. Local and crossed Andreev processes hybridize electron and hole edge excitations, producing delocalized electron-hole pairs. Using a microscopic tight-binding Bogoliubov-de Gennes model, we simulate the injection of subgap electrons and compute anti-bunching probabilities and current cross-correlations, revealing how normal and Andreev processes shape the interferometric signatures of this new hybrid geometry.

TT 83.5 Thu 16:00 HSZ/0105

Plasma mapping for the Moore-Read state in ideal Chern bands — •Qi Hu[1], Saranyo Moitra[1], Inti Sodemann Villadiego[1], and Victor Gurarie[2] — [1]Institut für Theoretische Physik, Universität Leipzig, 04103 Leipzig, Germany — [2]Department of Physics, CB390, University of Colorado, Boulder, Colorado 80309, USA

We construct an improved short distance regularization of the plasma mapping for the Moore-Read fractional quantum Hall state and also extend it from Landau levels to Aharonov-Casher ideal Chern bands, which are relevant in moire materials. This allows us to map correlations of the Moore-Read wave-function onto those of a classical statistical plasma with two components which in addition are coupled to a non-uniform neutralizing background. We exploit this to understand not only the universal topological properties of the Moore-Read state but also other details of their correlation functions. We will discuss the possibility of a phase transition from the plasma into novel dielectric states that can occur when the effective magnetic field in the Chern band becomes increasingly non-uniform.

TT 83.6 Thu 16:15 HSZ/0105

Universal Transport Theory for Paired Fractional Quantum Hall States in the Quantum Point Contact Geometry — •Eslam Ahmed[1], Ryoi Ohashi[2], Yukio Tanaka[1], and Kentaro Nomura[2] — [1]Nagoya University, Nagoya, Japan — [2]Kyushu University, Fukuoka, Japan

Even-denominator fractional quantum Hall (FQH) states can be viewed as topological superconductors of composite fermions, supporting a charged chiral mode and $|C|$ neutral Majorana modes set by the Chern number C. Distinguishing the many competing paired phases remains an open problem. We develop a unified theory of transport through a quantum point contact (QPC) for arbitrary C by analyzing quasiparticle and electron tunneling within the edge CFT $SO(|C|)_1 \otimes U(1)$. Using an instanton expansion, we show that strong quasiparti-

cle tunneling is dual to weak electron tunneling for all even-denominator states. This duality yields universal scaling dimensions and identifies a stable insulating fixed point. The resulting transport exponents provide experimentally accessible signatures capable of distinguishing different paired FQH states.

TT 83.7 Thu 16:30 HSZ/0105

Quantum Hall Effect without Chern Bands — •Benjamin Michen[1] and Jan Carl Budich[1,2] — [1]TU Dresden, 01062 Dresden, Germany — [2]MPIPKS, 01187 Dresden, Germany

The quantum Hall effect was originally observed in a two-dimensional electron gas forming Landau levels when exposed to a strong perpendicular magnetic field and was later generalized to Chern insulators without net magnetization. In this talk, further extending the realm of the quantum Hall effect, we report on the robust occurrence of an integer quantized transverse conductance at the onset of disorder in a microscopic lattice model, all bands of which are topologically trivial (zero Chern number). We attribute this phenomenon to the energetic separation of nonquantized Berry fluxes within those bands. Adding disorder then nudges the system into a quantum Hall phase from an extended critical regime obtained by placing the Fermi energy within a broad window inside a trivial band. This natural integer-rounding mechanism manifests as the mobility-gap-induced quantization of a nonuniversal Hall conductance. Our results are corroborated by numerical transport simulations and the analysis of two complementary topological markers.

15 min. break

TT 83.8 Thu 17:00 HSZ/0105

Hollow Topological Matter and Dual Fractional Quantum Hall Effect — •Ram Mummadavarapu and Roman-Pascal Riwar — Peter Gruenberg Institute, Theoretical Nanoelectronics, Forschungszentrum Juelich, D-52425 Juelich, Germany

The Integer Quantum Hall Effect (IQHE) at filling factor m and the Fractional Quantum Hall Effect (FQHE) at 1/m are commonly viewed as distinct phases of matter. We propose various chiral/non-chiral heterostructures that effectively pin m co-propagating IQHE edge states to a synchronised single mode. This setup thus realizes the Dual Fractional Quantum Hall Effect (DFQHE), a phase where fractionalization is reversed, that is, fundamental excitations retain integer electric charge but carry fractional magnetic flux. While the transconductance remains integer quantized, the edge correlations nonetheless exhibit anyonic power-law scaling. We show that this is a physical manifestation of Hollow Topological Matter: due to pinning, the edge no longer corresponds to the original physical bulk, but rather to a virtual bulk that may be bosonic or fermionic independent of the microscopic exchange statistics.

TT 83.9 Thu 17:15 HSZ/0105

Fractional Statistics in Anyon Colliders: A Keldysh-Instanton Approach — •Julian Kälber, Matthias Thamm, Felix Puster, and Bernd Rosenow — Universität Leipzig

The observation of fractional statistics in fractional quantum Hall (FQH) systems remains a central goal of modern condensed-matter physics. In recent collider-type experiments, dilute anyon beams are injected through quantum point contacts (QPCs) into unbiased edges, and signatures of anyonic exchange statistics are extracted from current cross-correlations. A quantitative description of these experiments, however, requires an accurate treatment of the QPCs, which act as dynamical tunnelling gates and introduce non-equilibrium effects that are not captured by simple Poissonian models.

In this work we develop an approximation scheme that incorporates the QPC dynamics within the Keldysh formalism. From the full action we derive an effective tunnelling action and obtain real-time instanton solutions of the free chiral-edge theory. The resulting non-equilibrium prefactor for tunnelling-operator correlation functions has the same structure as the Poissonian averaging employed in dilute-beam models, it reproduces the correct long-time asymptotics, and naturally generates oscillatory short-time features absent in previous treatments. Using this formalism we calculate a generalized Fano factor for a balanced anyon collider. The predicted values agree with theoretical expectations and with experimental measurements in the limit of small QPC transparencies, and remain consistent with experimental results at finite transparencies.

TT 83.10 Thu 17:30 HSZ/0105

From hidden order to skyrmions: Quantum Hall states in an extended Hofstadter-Fermi-Hubbard model — Fabian J. Pauw[1], Ulrich Schollwöck[1], Nathan Goldman[2,3], Sebastian Paeckel[1], and •Felix A. Palm[2] — [1]LMU Munich & MCQST, Munich, Germany — [2]Université Libre de Bruxelles, Brussels, Belgium — [3]Laboratoire Kastler Brossel, Collège de France, Paris, France

The interplay between topology and strong interactions gives rise to a variety of exotic quantum phases, including fractional quantum Hall (FQH) states and their lattice analogs - fractional Chern insulators (FCIs). Such topologically ordered states host fractionalized excitations, which for spinful systems are often accompanied by ferromagnetism and skyrmions. Here, we study an extended Hofstadter-Hubbard model of spinful fermions on a square lattice. Using DMRG simulations, we demonstrate the emergence of a spin-polarized 1/3-Laughlin-like FCI phase, characterized by a quantized many-body Chern number, a finite charge gap, and hidden off-diagonal long-range order. In contrast to systems at filling factor ν=1, we do not find skyrmionic excitations upon doping, thereby disentangling spin physics and topological order. The diagnostic toolbox presented in this work, based on local densities, correlation functions, and spin-resolved observables, is directly applicable in quantum gas microscopy experiments. Our results open new pathways for experimental exploration of FCIs with spin textures in both ultracold atom and electronic systems.

TT 83.11 Thu 17:45 HSZ/0105

The fate of the Laughlin state in ideal Chern bands — •Saranyo Moitra and Inti Sodemann Villadiego — Universität Leipzig, Leipzig, Germany

Ideal Chern bands are believed to be crucial to realizing the recently discovered fractional quantum Hall states at zero magnetic field. However, the nature of even the most archetypical Laughlin states and its competition with other phases remains poorly understood in this setting. We rigorously demonstrate that the Laughlin wave-function in ideal Chern bands is unstable to a novel gapless dielectric phase. Even the celebrated filling 1/3 state crystallizes into a correlated phase with continuously tunable power-law exponents, and quasiparticles with fractional charges varying smoothly below e/3. Remarkably, this state remains gapless without spontaneous symmetry breaking, exemplifying a form of beyond-Goldstone gaplessness. Our results bridge the physics of fractional quantum Hall and Coulomb gases, and we will discuss potential implications of this finding for moiré materials and its possible connections to critical states in other settings.

TT 83.12 Thu 18:00 HSZ/0105

Parafermions emerging from spin-polorized $\nu = 2/3$ fractional quantum Hall state — •Steffen Bollmann[1], Andreas Haller[2], Jukka I. Väyrynen[3], Thomas L. Schmidt[2], and Elio J. König[4] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]University of Luxembourg, Luxembourg — [3]Purdue University, West Lafayette, Indiana, USA — [4]University of Wisconsin*Madison, Madison, Wisconsin, USA

We study the theoretical realization of Z_3 parafermions in the spin-polarized $\nu = 2/3$ fractional quantum Hall (FQH) state, motivated by recent experimental advances in materials such as rhombohedral graphene or twisted $MoTe_2$. We discuss how parafermions can emerge in FQH-superconductor heterostructures, unlike earlier proposals that rely on spin-unpolarized systems. Disorder-induced backscattering of FQH edge states drives the system toward the Kane-Fisher-Polchinski fixed point, where the edge theory decouples into a charged mode carrying charge $2e/3$ and an electrically neutral mode. Inter-edge interactions in the neutral sector lead to a strong-coupling regime that gaps the neutral modes entirely. This reduction leaves an effective low-energy description governed by lattice parafermion modes.

TT 83.13 Thu 18:15 HSZ/0105

Quantized and nonquantized Hall response in topological Hatsugai-Kohmoto systems — •Thibaut Desort, Mark Oliver Goerbig, and Corentin Morice — Laboratoire de physique des solides, Université Paris-Saclay, Orsay, France

The Hall conductivity of insulators is well-known to be quantized, including in interacting systems [1]. The Hatsugai-Kohmoto (HK) interaction [2], a type of Hubbard model diagonal in reciprocal space, is now widely studied in the context of topology, owing to the fact that its eigenstates, eigenenergies and Green's functions can be computed exactly. Using the Kubo formula, it is possible to access the Hall conductivity which has, even in the presence of the HK interaction, been reported to be quantized because it coincides with a Chern number [3]. In this work, using Zeeman fields, we lift the many-body degeneracy induced by the Hatsugai-Kohmoto interaction in the topological Kane-Mele model. This selects specific states within the ground-state manifold that reveal a surprising non-quantized Hall response.

[1] Q. Niu, D. J. Thouless, Y.-S. Wu, Phys. Rev. B 31, 3372 (1985)
[2] Y. Hatsugai, M. Kohmoto, J. Phys. Soc. Jap. 61, 2056 (1992)
[3] P. Mai, B. E. Feldman, P. W. Phillips, Phys. Rev. 5, 013162 (2023)

TT 84: 2D Materials: Electronic structure, excitations, etc. III (joint session O/HL/TT)

Time: Thursday 15:00–17:45 Location: HSZ/0204

TT 84.1 Thu 15:00 HSZ/0204

Linearized augmented plane waves for low-dimensional materials — •Andris Gulans, Ernests Jansons, and Janis Uzulis — University of Latvia, Riga, Latvia

We address the challenge of efficient yet highly precise density-functional theory calculations of low-dimensional materials and present a set of tools and algorithms specific to linearized augmented plane waves (LAPW) that is implemented in the electronic-structure code `exciting`. First, we discuss our iterative eigensolver compatible with local and hybrid functionals. It is an extension of Davidson*s algorithm and does not require explicit Hamiltonian construction while overcoming difficulties associated with high condition numbers. The second important ingredient is the adaptively compressed exchange that represents the non-local (screened) Fock exchange via a low-rank approximation. This approach enables computational complexity as low as $O(N^3 \log N)$ floating-point operations (FLOPs) with N being the number of atoms. It is a novel feature in hybrid functional calculations using LAPW as the standard approaches require $O(N^4)$ FLOPs. Finally, we introduce a cylindrical cutoff for the Coulomb interaction for handling the $q = 0$ singularity.

TT 84.2 Thu 15:15 HSZ/0204

Graphene-Enabled Mott–Metal Transition in Silicon Dangling Bonds — •Niclas Tilgner[1], Siheon Ryee[2], Zamin Mamiyev[1], Philip Schädlich[1], Christoph Tegenkamp[1], Tim O. Wehling[2], and Thomas Seyller[1] — [1]Institute of Physics, Chemnitz University of Technology, Germany — [2]I. Institute of Theoretical Physics, University of Hamburg, Germany

Controlling emergent electronic phases in materials with strong Coulomb interactions remains a central challenge in condensed matter physics. Adatom lattices on semiconducting surfaces provide prototypical platforms for exploring such correlated phenomena. Recent advances have facilitated the synthesis of 2D Mott insulators in proximity to graphene (N. Tilgner et al 2025 2D Mater. 12 045022). Here, we demonstrate that alkali adsorption on a graphene/Si/SiC(0001) heterostructure – where the Si layer hosts correlated dangling bonds – enables controlled charge transfer to the Mott insulator. Beyond a critical carrier concentration, we observe a sudden collapse of the Mott gap, indicating a transition to a correlated metallic phase. Our results point to a finite proximity coupling between the Mott layer and graphene, as recently suggested by a theoretical study (N. Witt et al 2025 arXiv:2503.03700), which gives rise to nonlocal dynamical screening beyond simple electrostatics and provides a natural pathway for the observed phase transition.

TT 84.3 Thu 15:30 HSZ/0204

From self-consistent DFT+DMFT to the two-particle level: Magnetic phase diagram of X:SiC(111) — •Lukas Bongardt[1,2], Niklas Enderlein[3], Giorgio Sangiovanni[4], Philipp Hansmann[3,5], and Henri Menke[1] — [1]Max Planck Computing and Data Facility — [2]Technical University of Munich — [3]FAU Erlangen — [4]Universität Würzburg — [5]University of Iceland, Reykjavík

Recently we have proposed a novel and versatile platform to realize a two-band Hubbard model with massless Dirac fermions and flat bands hosting strong correlations by depositing three different species of transition-metal adatoms on semiconductor surfaces (arXiv:2410.17165). Using state-of-the-art DFT+DMFT calculations we investigated the spectral properties of X:3C-SiC(111) (X = Ti, V, Cr). Due to the presence of well-defined Dirac cones and flat bands, indicating the potential for realizing topological and correlated phases, we identify transition-metal adatoms on SiC as a possible platform for exploring the interplay of correlations, topology, and magnetism in two-dimensional materials.

In this work, we explore the magnetic phase diagram of these systems within DMFT by calculating the generalized two-particle vertex and using it to solve the Bethe-Salpeter equation for the generalized susceptibility. This gives us a fully orbital-, spin-, and most importantly momentum-dependent susceptibility which carries the information about the ordering wave vector and is experimentally accessible through various techniques.

TT 84.4 Thu 15:45 HSZ/0204

Cr 3*d* Orbital Hybridization and Electronic Structure in the Layered Magnetic Semiconductor $CrPS_4$ — •Lasse Sternemann[1], David Maximilian Janas[1], Richard Leven[1], Eshan Banerjee[2], Jonah Elias Nitschke[1], Marco Marino[1], Leon Becker[3], Ahmet Can Ademoglu[1], Frithjof Anders[1], Stefan Tappertzhofen[3], and Mirko Cinchetti[1] — [1]TU Dortmund University, Department of Physics, 44227 Dortmund, Germany — [2]Department of Materials, Imperial College London, London, SW7 2AZ, United Kingdom — [3]TU Dortmund University, Department of Electrical Engineering and Information Technology, 44227 Dortmund, Germany

Despite its promising spintronic and magneto-optical characteristics, the electronic band structure of the van der Waals magnetic semiconductor $CrPS_4$ is still unknown. Here, we report angle-resolved photoemission spectroscopy measurements of its band structure in the para- and antiferromagnetic phase, complemented by DFT+U calculations. Theoretical results reveal dominating Cr 3d and S 3p contributions to the valence band and a ligand-to-metal charge-transfer band gap. Crystal field split Cr 3d orbitals display distinct hybridization regimes with S 3p orbitals: t_{2g} orbitals are only weakly affected by hybridization, while e_g states experience a 4 eV anti-bonding/bonding splitting with S-mixing relaxing dipole selection rules, otherwise darkening optical d-d transitions. These findings establish the ground state electronic and orbital structure of $CrPS_4$ and provide essential benchmarks for understanding its optical and magnetic responses.

TT 84.5 Thu 16:00 HSZ/0204

Spectroscopic Investigation of the Ni Valence States in $NiTe_2$ — •Tassaphon Tirasutt[1], Sheng-Huai Chen[1], Alexander C. Komarek[1], Chun-Fu Chang[1], Yu-Chieh Ku[2], Po-Yu Cho[3], Chun Sum Brian Pang[4], Mizuki Furo[5], Naoki Ito[5], Ulrich Burkhardt[1], Simone G. Altendorf[1], Atsushi Hariki[5], and Liu Hao Tjeng[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]National Yang Ming Chiao Tung University, Hsinchu, Taiwan — [3]National Synchrotron Radiation Research Center, Hsinchu, Taiwan — [4]The University of British Columbia, Vancouver, Canada — [5]Osaka Metropolitan University, Osaka, Japan

Nickel-based transition metal compounds exhibit a wide range of properties arising from the strongly correlated d electrons. In this study, we investigate $NiTe_2$, a layered transition-metal dichalcogenide with reported type-II Dirac semimetallic properties. While its topological nature has been the focus of interest, the fundamental question of the properties of the Ni ions in $NiTe_2$ has rarely been discussed. We address this issue using soft X-ray core-level and valence-band photoelectron spectroscopy, as well as Ni-$L_{2,3}$ absorption spectroscopy, combined with a theoretical approach using LDA+DMFT. Our findings provide insights into the Ni 3d occupation and degree of correlation of the Ni in a metallic ligand bath of the $NiTe_2$ system.

TT 84.6 Thu 16:15 HSZ/0204

TMDC surfaces as scattering targets in spin-polarization detectors: A case study of MoS_2 — •Christoph Angrick[1], Annika Henriksen[1], Nicole Edossa[1], Andre Reimann[1], Moritz Ewert[2,3], Lars Buss[2,3], Jens Falta[3], Jan Ingo Flege[2,3], and Markus Donath[1] — [1]University of Münster, Germany — [2]Brandenburg University of Technology Cottbus-Senftenberg, Germany — [3]University of Bremen, Germany

Spin-polarization detectors are employed in photoemission experiments to reveal the spin texture of electronic states. One well-proven approach is based on the VLEED process, where the spin-dependent electron reflection from targets influenced by exchange and/or spin-orbit interaction is used. The suitability of a target must be investigated beforehand [1,2]. In this talk, a first impression of TMDC-based detectors is given [3]. The spin-dependent electron reflectivity of spin-orbit-influenced MoS_2 is measured over a wide range of incident energies and angles for the following samples: a single layer of MoS_2 on Au(111) and cleaved MoS_2 single-crystal surfaces. On the basis of the resulting maps for the electron reflectivity, Sherman function, and figure of merit, promising features of MoS_2 for use in spin-polarization detection are discussed.

[1] Thiede *et al.*, Phys. Rev. Applied **1**, 054003 (2014).
[2] Angrick *et al.*, J. Phys.: Condens. Matter **33**, 115001 (2020).
[3] Angrick *et al.*, Phys. Rev. B, accepted for publication (2025).

TT 84.7 Thu 16:30 HSZ/0204

Efficient GW calculations for metals from an accurate ab initio polarizability: the case of doped MoS2 monolayer — •Giacomo Sesti[1], Pino D'Amico[1], Alberto Guandalini[2], Claudia Cardoso[1], Andrea Ferretti[1], and Daniele Varsano[1] — [1]CNR-NANO, Modena, Italy — [2]Università di Roma La Sapienza, Roma, Italy

Many-body perturbation theory in the GW approximation has proved very successful for the calculation of quasiparticle (QP) band structures of semiconductors. QP corrections are less significant in metals and are typically disregarded for the computational cost involved. Also, GW calculations of metals suffer of specific methodological challenges to properly treat the screening. This is typically solved under the addiction of a Drude term, that however is inadequate at low dimensionalities[1]. Furtherly, even for metals, QP corrections become more relevant at lower dimensionalites.

Here, we present GW calculations of QPs for doped MoS_2 monolayer showing excellent agreement with experimental ARPES measurements[2]. Such an unprecedented agreement has been possible thanks to the W-av method, which combines a Monte Carlo integration with interpolation approaches. This technique originally developed for 2D semiconductors[3] is here extended to the metallic case.

1) Champagne et al. NanoLett. 23.10 (2023)
2) Liu et al. PRL. 122 (2019)
3) Guandalini et al., npj Computational Materials, 9 (2023)

TT 84.8 Thu 16:45 HSZ/0204

Ultrafast Momentum Dependent Relaxation Dynamics in $TbTe_3$ — •Florian Denizer[1], Noah Meyer[2,3], Anisha Singh[3], Ian R. Fisher[3], Uwe Bovensiepen[1], Zhi-Xun Shen[2,3], and Patrick S. Kirchmann[2] — [1]Fakultät für Physik, Universität Duisburg-Essen — [2]Department of Physics, Applied Physics and Stanford Synchrotron Radiation Laboratory, Stanford University — [3]Geballe Laboratory for Advanced Materials, Departments of Physics and Applied Physics, Stanford University

Rare-earth tritellurides (RTe_3) form charge density waves (CDW) due to electronic instabilities at the Fermi-surface, because of an anisotropy of the crystal lattice between the two major in-plane crystal axes *a* and *c*. Unoccupied electronic states can be populated by ultrafast laser excitation. Electronic relaxation and coherent vibrational modes including the amplitude mode have been investigated by time and angle resolved photoelectron spectroscopy (*tr*-ARPES). Among the manifold of laser-driven processes, the one that is responsible for the electronic instability has not yet been identified. With this objective in mind we perform a *tr*-ARPES experiment on $TbTe_3$ and investigate the momentum transfer along the a- and the c-axis as a function of excitation strength. At sufficiently low pump fluence below $F = 0.3$ mJ/cm^2 we identify (quasi-)elastic scattering in the vicinity of the Fermi surface. In the talk we will discuss isotropic defect-induced elastic scattering and directed quasi-elastic scattering determined by the nesting vector. Funding through the DFG within SFB 1242 and through the DOE is gratefully acknowledged.

TT 84.9 Thu 17:00 HSZ/0204

Unconventional Topological Superconductivity in CrCl3/NbSe2 heterostructures — •Souvik Das[1], Benjamin Zhou[2,3], Anshuman Padhi[1], Jing-Rong Ji[1], Niclas Heinsdorf[2,3], Prajwal Rigvedi[1], Tianzhe Chen[1], Weibin Li[4], Pierluigi Gargiani[4], Manuel Valvidares[4], Marcel Franz[2,3], Banabir Pal[1], and Stuart S.P. Parkin[1] — [1]Max Planck Institute of Microstructure Physics, Halle, Germany — [2]Quantum Matter Institute, University of British Columbia, Vancouver, Canada — [3]Department of Physics and Astronomy, University of British Columbia, Vancouver, Canada — [4]ALBA Synchrotron Light Source, Barcelona, Spain

Topological p-wave superconductors can host non-Abelian particles useful for fault-tolerant quantum computing. Here we report experimental evidence of unconventional topological superconductivity in a heterostructure of monolayer, in-plane ferromagnetic CrCl3 islands on superconducting NbSe2. STM measurements show that, despite CrCl3 being ferromagnetic, the interfacial superconducting gap is more robust against out-of-plane magnetic fields than the s-wave gap of NbSe2, indicating unconventional pairing. We also find enhanced zero-energy states along CrCl3 island edges, consistent with the presence of edge modes. Theory suggests these features arise from an intrinsic helical p-wave state stabilized by interfacial Rashba spin-orbit coupling. This demonstrates a new route to create topological superconductivity via interface engineering.

TT 84.10 Thu 17:15 HSZ/0204

Structural and Electronic Properties of CrSBr Nanoribbons: Insights from First-Principles Calculations — •Daniil Kruklinskii, Mahdi Ghorbani-Asl, and Arkady Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany

Experiments show that exfoliated CrSBr flakes naturally form nanoribbons along a specific crystallographic direction, and similar structures can be fabricated using an electron beam in the TEM as a cutting tool. Here, we employ density functional theory calculations to systematically investigate the stability as well as electronic and magnetic properties of CrSBr nanoribbons. Our results indicate that nanoribbons oriented along one of the two major crystallographic directions are the most stable under typical growth and exfoliation conditions and remain semiconducting, exhibiting pronounced electron-hole separation between the VBM and CBM. In contrast, nanoribbons in the perpendicular direction display a substantially reduced band gap due to strongly localized edge states. Both orientations retain strongly spin-polarized band-edge states near the Fermi level and show only a weak dependence of the band gap on ribbon width. Using *ab initio* molecular dynamics simulations, we further demonstrate that electron-beam irradiation with energies of at least 200 keV can facilitate the fabrication of nanoribbons directly from pristine monolayer CrSBr, favouring the formation of diagonal nanoribbons. These diagonal ribbons are metallic, in contrast to the monolayer, and host a high density of majority-spin edge states, giving rise to pseudo-half-metallic transport.

TT 84.11 Thu 17:30 HSZ/0204

Band-selective coherent phonon-driven band renormalization in 1T-$MoTe_2$ — •Carl Jensen[1], Christopher Emeis[2], Stephan Jauernik[1], Petra Hein[1], Fabio Caruso[2], and Michael Bauer[1,3] — [1]nstitute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Institute of Theoretical Physics and Astrophysics, Kiel University, 24098 Kiel, Germany — [3]Kiel Nano, Surface and Interface Science KiNSIS, Kiel University, 24118 Kiel, Germany

Understanding the coupling between coherent phonons and the electronic system is crucial for controlling nonequilibrium properties in solids. Here, we investigate mode- and band-selective electron-phonon coupling in centrosymmetric 1T-$MoTe_2$ using time- and angle-resolved photoemission spectroscopy combined with frequency-domain analysis (FDARPES). Femtosecond near-infrared pulses excite coherent Ag-symmetric phonon modes at 2.34 THz, 3.34 THz, and 3.86 THz, which manifest as oscillatory modulations in photoemission intensity and binding energy across the valence bands. Pixel-wise Fourier analysis, based on a recently developed methodology [1], reveals pronounced band selectivity with distinct coupling strengths for different electronic states and phonon modes, enabling the evaluation of band-renormalization amplitudes in the few-meV range. Ab initio calculations using DFT/DFPT qualitatively reproduce the experimentally observed coupling patterns and relative trends, demonstrating the capability of combined experimental and theoretical approaches to resolve ultrafast electron-phonon interactions in quantum materials.

[1] N. Gauthier, H. Soifer, J.A. Sobota, H. Pfau, E. J. Sie, A. M. Lindenberg, Z.-X. Shen, P. S. Kirchmann, Rev. Sci. Instrum. 96 (2025)

TT 85: Superconductivity: Yu-Shiba-Rusinov and Andreev Physics

Time: Thursday 15:00–17:15 Location: CHE/0089

TT 85.1 Thu 15:00 CHE/0089

Tip-gated quantum phase transition via valence change in a single Yu-Shiba-Rusinov impurity — •Xingsen Chen[1], Junyi Zhang[2], and Hao Zheng[1] — [1]Tsung-Dao Lee Institute, Shanghai Jiao Tong University, Shanghai, China — [2]Johns Hopkins University, Baltimore, USA

We report the real-space visualization of a quantum phase transition driven by a valence change in a single magnetic impurity coupled to a superconductor. Using a scanning tunneling microscope on a proximitized $Bi_2Te_3/NbSe_2$ substrate, we employ tip-induced band bending to precisely gate the energy level of a single Fe-based impurity cluster across the Fermi energy.

This tuning induces the formation of Yu-Shiba-Rusinov states inside the superconducting gap. Their evolution and zero-energy crossing signal a quantum phase transition. By correlating the YSR state transition with a concurrent high-energy valence transition, we identify the mechanism as a single-electron valence change of the Fe impurity (Fe^{2+}/Fe^{3+}), rather than conventional Kondo screening. Theoretical modelling using a multi-orbital Anderson impurity model confirms that the transition is governed by resonant hybridization and charge fluctuations at the mixed-valence point.

Our work establishes tip-gating as a powerful method for in-situ control of atomic-scale quantum phases and reveals a distinct mechanism for quantum phase transitions in superconducting hybrids.

TT 85.2 Thu 15:15 CHE/0089

Rare-earth spin chains on superconducting Nb(110) surface — •Yu Wang[1], Artem Odobesko[1], and Matthias Bode[1,2] — [1]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — [2]Wilhelm Conrad Röntgen-Center for Complex Material Systems (RCCM), Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Coupled Yu-Shiba-Rusinov (YSR) states in 1D magnetic chains can yield topologically protected edge modes. While well explored for $3d$ transition metals, studies on $4f$-shell rare-earth metals (REMs) remain scarce. Owing to their localized and shielded $4f$ orbitals, REMs such as Ce, Eu, Gd, Tb, and La provide a promising platform for weakly hybridized magnetic chains on superconductors.

We present a comparative study of YSR excitations in REM adatoms and chains on Nb(110). Building on previous Gd results [1-2], we extend the analysis to Tb and other REM chains along [1$\bar{1}$0] and [001]. Spectra reveal orientation-dependent edge behavior: [1$\bar{1}$0] chains host trivial end states, whereas [001] chains show zero-bias features consistent with non-trivial edge modes. The results highlight the impact of $4f$ magnetism on YSR band formation and topological superconductivity.

[1] Y. Wang *et al.*, arXiv:2506.19514 (2025)
[2] Y. Wang *et al.*, arXiv:2311.09742 (2023)

TT 85.3 Thu 15:30 CHE/0089

Yu-Shiba-Rusinov spectroscopy of triangular molecular trimer on superconducting surface — •Vladislav Pokorný[1], Martin Žonda[2], and Chao Li[3,4] — [1]FZU - Institute of Physics, Czech Academy of Sciences, Na Slovance 2, 182 00 Prague 8, Czech Republic — [2]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, 121 16 Prague 2, Czech Republic — [3]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [4]Institute of Atom Manufacturing, Nanjing University, Suzhou 215163, China

We present a study of a molecular trimer constructed from tetrabromotetraazapyrene molecules deposited on a superconducting Pb(111) surface in a triangular geometry. Scanning tunneling spectroscopy reveals a pair of split Yu-Shiba-Rusinov (YSR) states within the superconducting gap as a result of the spinful nature of the molecules [1]. The system is described using a superconducting three-impurity Anderson model with a single superconducting bath. The model is solved using the numerical renormalization group technique, which provides a quantitative description of the experimental result, revealing the doublet nature of the ground state as a result of the intersite capacitive coupling and explains the behavior of the YSR states. We also briefly discuss the possible source of the peak splitting.

[1] C. Li et al., arXiv:2508.05575 (2025).

TT 85.4 Thu 15:45 CHE/0089

Stochastic resonance realized with a superconducting magnetic impurity state — •Philipp Maier[1], Björn Kubala[1,2], Joachim Ankerhold[1], and Ciprian Padurariu[1] — [1]Institute for Complex Quantum Systems and IQST, Ulm University — [2]German Aerospace Center (DLR), Ulm

The phenomenon of stochastic resonance (SR) was originally studied in the context of climatic changes and has since been observed in a variety of classical and quantum systems. Here, we theoretically investigate the emergence of SR in superconducting junctions to infer the rates of quantum electronic tunneling processes [1, 2].

We focus on a system where one electrode hosts a Yu-Shiba-Rusinov (YSR) state – a discrete bound state within the superconducting gap induced by the magnetic exchange interaction between a magnetic impurity and its superconducting host.

Applying the framework of full counting statistics (FCS), we demonstrate that SR manifests as a reduction of the Fano factor and a resonance of the tunneling current. Crucially, the frequency of this resonance reveals information about the rate of microscopic electronic processes, such as the process responsible for quasiparticle-occupation parity breaking.

[1] M. Hänze et al., Sci. Adv. 7 (2021)
[2] T. Wagner et al., Nat. Phys. 15 (2019)

TT 85.5 Thu 16:00 CHE/0089

Analytical and ab-initio characterization of YSR-state binding energies under magnetic-moment misalignment — •Ilias Klepetsanis[1,2] and Samir Lounis[3] — [1]Forschungszentrum Jülich & JARA, Germany — [2]University of Duisburg-Essen and CENIDE, Germany — [3]Martin-Luther University Halle-Wittenberg, Institut für Physik and Halle-Berlin-Regensburg Cluster of Excellence CCE Halle, Germany

Complex spin textures interfaced with superconducting surfaces give rise to a rich variety of phenomena, ranging from the emergence of intricate in-gap states –such as Yu-Shiba-Rusinov (YSR) states– to the realization of topological superconductivity hosting Majorana modes. At the core of these effects lie competing and intertwined interactions involving Cooper pairing, spin-spin coupling, and spin-orbit-driven mechanisms. In this work, we systematically and analytically identify how the binding energies of YSR states in atomic nanostructures depend on the orientation of their magnetic moments. We distinguish between different underlying mechanisms, including those that are independent of spin-orbit coupling (SOC) and those that arise from SOC-driven magnetic misalignment. Results obtained using an Anderson-impurity model coupled to the Bogoliubov-de Gennes (BdG) formalism are compared with both DFT-BdG calculations for Fe nanostructures on a superconducting $BiAg_2$ surface and available scanning tunnelling microscopy measurements.

– We acknowledge funding by the DFG (LO 1659/11-1; Cluster of Excellence Center for Chiral Electronics -EXC3112/1 -533767171).

15 min. break

TT 85.6 Thu 16:30 CHE/0089

Emergence of new zero modes bound to vortices in extended topological Josephson junctions — •Adrian Reich[1], Kiryl Piasotski[1,2], and Alexander Shnirman[1,2] — [1]Institute for Theoretical Condensed Matter Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany

We theoretically study planar Josephson junctions formed on the surface of a three-dimensional topological insulator (Fu-Kane proposal) and examine the experimentally relevant parameter regimes in which the effective velocity of the emergent one-dimensional Majorana modes approaches zero. We show that the frequently employed Fu-Kane effective theory breaks down in this case. As parameters like the chemical potential or the width of the junction are tuned, instances of vanishing effective velocity mark the emergence of additional "Dirac cones" at zero energy and finite momentum. If the junction is subjected to an external magnetic field, Josephson vortices may then bind a number of zero modes in addition to the topological Majorana mode. The additional zero modes are "symmetry-protected" and can be lifted by a broken mirror symmetry (which is to be expected in realistic scenarios) as well as by an in-plane magnetization (or Zeeman field). We note that the ensuing presence of additional low-energy Andreev states can significantly contribute to measured quantities like the Josephson current or microwave absorption spectra.

TT 85.7 Thu 16:45 CHE/0089

Local Observation of Andreev Billiards in an In-Plane Magnetic Field — •Jens Brede, Adrian Greichgauer, and Yoichi Ando — University of Cologne

Quasiparticles in a normal metal can be confined by a surrounding superconductor through Andreev reflection at the N/S interface. For subgap energies, electrons are retroreflected as holes that retrace their paths, forming closed semiclassical trajectories. When their accumulated phase reaches 2π, these trajectories create Andreev bound states (ABS), observed as subgap features in the local density of states (LDOS). We probe these ABS using STM at 400 mK in the two-dimensional electron gas of the Cu(111) surface state, confined to quasi-rectangular islands by superconducting Nb. We observe a hard superconducting gap and, with increasing in-plane magnetic field, nearly periodic LDOS gap closings. The period scales roughly linearly with the island dimension perpendicular to the field direction. A simple model that incorporates the vector potential into the semiclassical trajectories qualitatively reproduces the experimental behavior.

TT 85.8 Thu 17:00 CHE/0089

Assessing effective models of double quantum dot Andreev molecules — •Kacper Wrześniewski[1], Peter Zalom[2], Tomasz Tomáš Novotný[3], and Ireneusz Weymann[1] — [1]Institute of Spintronics and Quantum Information, Faculty of Physics and Astronomy, Adam Mickiewicz University in Poznań, Poland — [2]Institute of Physics, Czech Academy of Sciences, Praha, Czech Republic — [3]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Praha, Czech Republic

We investigate the phase diagram of a parallel double-quantum-dot Andreev molecule, in which the two quantum dots are coupled to a common superconducting lead. Using the numerical renormalization group (NRG) method, we analyze the evolution of the ground state across a broad parameter space, including level detuning, superconducting gap size, lead couplings, and interdot hopping. The resulting phase diagrams exhibit singlet, doublet, and a relatively uncommon triplet ground state, the latter serving as a clear signature of strong lead-mediated interactions between the quantum dots.

To evaluate the reliability of simplified theoretical descriptions, we benchmark the applicability of several effective models, including the atomic limit and zero-bandwidth approximations. Our results reveal notable limitations of these approaches: with the exception of the extended zero-bandwidth approximation, the effective models fail to reproduce the triplet ground state. These findings provide valuable guidance for interpreting experimental data and for the design of superconducting devices based on quantum dots.

TT 86: Correlated Magnetism – Spin Liquids II

Time: Thursday 15:00–16:45 Location: CHE/0091

TT 86.1 Thu 15:00 CHE/0091

Classical spin liquids from frustrated Ising models in hyperbolic space — •Fabian Köhler[1], Johanna Erdmenger[2], Roderich Moessner[3], and Matthias Vojta[1] — [1]Institut für Theoretische Physik and Würzburg-Dresden Cluster of Excellence ct.qmat, Technische Universität Dresden, 01062 Dresden, Germany — [2]Institute for Theoretical Physics and Astrophysics and Würzburg-Dresden Cluster of Excellence ct.qmat, Julius-Maximilians-Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]Max-Planck-Institut für Physik komplexer Systeme and Würzburg-Dresden Cluster of Excellence ct.qmat, Nöthnitzer Str. 40, 01187 Dresden

Antiferromagnetic Ising models on frustrated lattices can realize classical spin liquids, with highly degenerate ground states and, possibly, fractionalized excita-

tions and emergent gauge fields. Moti- vated by the recent interest in many-body system in negatively curved space, we study hyperbolic frustrated Ising models. Specifically, we consider nearest-neighbor Ising models on tesselations with odd-length loops in two-dimensional hyperbolic space. For finite systems with open boundaries we determine the ground-state degeneracy exactly, and we perform extensive finite-temperature Monte-Carlo simulations to obtain thermodynamic data as well as correlation functions. We show that the shape of the boundary, constituting an extensive part of the system, can be used to control low-energy states: Depending on the boundary, we find ordered or disordered ground states. Our results demonstrate how geometric frustration acts in curved space to produce classical spin liquids.

TT 86.2 Thu 15:15 CHE/0091

Unconventional Spin Dynamics and Supersolid Excitations in the Triangular-Lattice XXZ Model — •Rafael Alvaro Flores Calderon[1], Roderich Moessner[2], and Frank Pollmann[1] — [1]Department of Physics, Technical University of Munich, 85748 Garching, Germany — [2]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Strasse 38, D-01187 Dresden, Germany

Motivated by recent experiments, we investigate the spin-1/2 XXZ model on the triangular lattice with strong Ising anisotropy, combining large-scale numerical simulations and analytical methods to uncover unconventional spin dynamics at $T = 0$. First, we compute the dynamical spin structure factor using density matrix renormalization group (DMRG) simulations and find excellent agreement with inelastic neutron scattering data on the layered compound $K_2Co(SeO_3)_2$. The low-energy spectrum reveals a roton-like minimum at the M point, absent in linear spin-wave theory, accompanied by peak intensity and a broad continuum above it. Near the Γ point, we observe an approximately linear dispersion with vanishing spectral weight. Second, we compare multiple analytical frameworks that reproduce the observed features. Remarkably, a variational supersolid QDM wavefunction and the DMRG ground state exhibit nearly identical structure factors with pronounced transverse photon-like excitations. Together, our comprehensive theoretical and numerical analysis elucidates the microscopic origin of supersolid excitations in the XXZ triangular lattice model and their proximity to a spin liquid phase observed experimentally.

TT 86.3 Thu 15:30 CHE/0091

Magnetization-driven spinon Landau levels and ordering instabilities in a Dirac spin liquid — Wen Wang[1], •Urban F.P. Seifert[2], Oleg A. Starykh[3], and Leon Balents[1] — [1]Kavli Institute for Theoretical Physics, University of California, Santa Barbara, California 93106-4030, USA — [2]Institute for Theoretical Physics, University of Cologne, Zülpicher Str. 77a, 50937 Cologne, Germany — [3]Department of Physics and Astronomy, University of Utah, Salt Lake City, UT 84112, USA

A particularly fascinating example of a quantum spin liquid is the U(1) Dirac spin liquid (DSL), which at low energies is described by emergent quantum electrodynamics (QED3), a strongly coupled conformal field theory. Motivated by recent numerical evidence for its realization in triangular lattice J1-J2 Heisenberg antiferromagnets as well as the identification of several candidate materials, we revisit the problem of the U(1) DSL in a Zeeman magnetic field. Equipped with recent numerical and field-theoretical insights into the field-induced behaviour of the QED3 low-energy theory, we analyze a microscopic (lattice) model using Gutzwiller-projected wavefunctions. We analyze how the applied field may induce an instability towards in-plane antiferromagnetic ordering, and discuss observables that may be unique to such a field-induced state. In experiments, these may allow one to infer the presence of an underlying DSL at zero field.

TT 86.4 Thu 15:45 CHE/0091

Monopole condensation in U(1) Dirac spin liquids: AFM and VBS orders — •João C. Inácio[1] and Fakher Assaad[1,2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Am Hubland, 97074 Würzburg, Germany

Quantum spin liquids are states of matter where quantum fluctuations prohibit magnetic order down to zero temperature. Such states cannot be described by conventional mean-field theories. In U(1) Dirac spin liquids (DSL), the low-energy degrees of freedom are emergent gauge fields coupled to fractionalised spinon excitations. Spinons behave like Dirac fermions coupled to a compact U(1) gauge field, giving rise to QED_3. Within this framework instanton excitations of the gauge fields, i.e. monopoles, are central to understand the spin liquid state. Monopoles carry antiferromagnetic (AFM) or valence bond solid (VBS) charge leading to a Dirac mass upon their condensation, creating a large competition between different magnetic orders. We study a U(1) lattice gauge theory coupled to phonons by the means of exact fermionic quantum Monte Carlo simulations in order to understand this competition. By doing a scan over the spinon-phonon coupling (g) and the gauge field fluctuations (J) we are able to create a phase diagram where AFM, VBS and DSL phases coexist.

TT 86.5 Thu 16:00 CHE/0091

Exactly solvable spin liquids in Kitaev bilayers and moiré superlattices — •Ivan Dutta[1,2], Anamitra Mukherjee[1,2], Onur Erten[3], and Kush Saha[1,2] — [1]National Institute of Science Education and Research, Jatni, 752050, India — [2]Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai 400094, India — [3]Department of Physics, Arizona State University, Tempe, Arizona 85287, USA

Building on the recent advancements on moiré superlattices, we propose an exactly solvable model with Kitaev-type interactions on a bilayer honeycomb lattice for both AA stacking and moiré superlattices. Employing Monte Carlo simulations and variational analysis, we uncover a rich variety of phases where the intra and interlayer Z2 fluxes (visons) are arranged in a periodic fashion in the ground state, tuned by interlayer coupling and out-of-plane external magnetic field. We further extend our model to moiré superlattices at various commensurate twist angles around two distinct twist centers represented by C3z and C6z of the honeycomb lattice. Our simulations reveal generalized patterns of plaquette values correlated with the AA or AB stacking regions across the moiré unit cell. In addition, depending on the twist angle, twist center and interlayer coupling, moiré superlattices exhibit a variety of gapped and gapless spin liquid phases and can also host corner and edge modes. Our results highlight the rich physics in bilayer and twisted bilayer models of exactly solvable quantum spin liquids.

TT 86.6 Thu 16:15 CHE/0091

N-state Potts ices as generalizations of classical and quantum spin ice — •Mark Potts[1], Roderich Moessner[1], and Siddharth Parameswaran[2] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Rudolf Peierls Centre for Theoretical Physics, Oxford, UK

Classical and quantum spin ice models are amongst the most popular settings for the study of spin liquid physics. N-state Potts ice models have been constructed that generalize spin ice, hosting multiple emergent U(1) gauge fields and excitations charged under non-trivial combinations of these fields. We present a general treatment of classical N-state Potts ices relating their properties to the su(N) Lie algebras, and demonstrate how the properties of charged excitations in the classical model can be related to this symmetry group. We also introduce quantum generalizations of the Potts Ice models, and demonstrate how charge flavour changing interactions unique to $N > 2$ models dominate their low energy phase diagram. We further show how symmetries inherited from the su(N) algebra can lead to the frustration of flux vacuum states.

TT 86.7 Thu 16:30 CHE/0091

Phases and dynamics of the quadrupolar Kitaev model — •Partha Sarker and Urban Friedrich Peter Seifert — Institute for Theoretical Physics, University of Cologne, Zülpicher Straße 77, D-50937, Köln, Deutschland

The study of multipolar exchange interactions for local spin moments ($S > \frac{1}{2}$) has rapidly expanded in recent years. A crucial inquiry in this research landscape is whether the concept of quantum spin liquid can be generalized to multipolar liquids where multipolar moments fractionalize, giving rise to novel emergent phenomena. Recently, a model involving frustrated quadrupolar interactions between local $S = 1$ moments has been numerically shown to host a deconfined phase with $\mathbb{Z}_2$ topological order. We investigate various phases and dynamics of this model using a combination of mean-field and perturbative methods.

We first analytically demonstrate the existence of an extensively large set of ground states by probing the bare Hamiltonian with trivial deformations within the framework of generalized spin wave theory. The extensive degeneracy can be explained by the explicit construction of mean field ground states. These mean field ground states map to emergent electrostatics and can be divided into topological sectors in periodic boundary condition. Although perturbative analysis for anisotropic exchange coupling does not exhibit any evidence of deconfined excitations or topological ground state degeneracy, using parton analysis we can show that near the isotropic point the system hosts fractionalized gauge excitations. Finally, using parton mean field theory, we analyze the spectrum and various correlation functions.

TT 87: Many-body Quantum Dynamics II (joint session DY/TT)

Time: Thursday 15:00–16:30 Location: HÜL/S186

TT 87.1 Thu 15:00 HÜL/S186

general framework for understanding and modeling irreversibility: relaxator Liouville dynamics — •Martin Janssen and Janos Hajdu — Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

Irreversibility is explained as an emergent phenomenon brought about by a separation between two characteristic time scales: the time t_s up to which relevant degrees of freedom of a system are tracked is extremely much shorter than the spectral resolution time t_e necessary to resolve the spectrum of all degrees of freedom involved. A relaxator that breaks reversibility condenses in the Liouville operator of the relevant degrees of freedom. The irrelevant degrees of freedom act as an environment. The relaxator Liouville equation is a most general equation of motion in a many body quantum system and contains memory effects and initial correlations of all degrees of freedom, generalizing the well known semi-group dynamics. Stationary states turn out to be generically unique and independent of the initial conditions and exceptions are due to degeneracies. Equilibrium states lie in the relaxator's kernel yielding a stationary Pauli master equation and a non negative entropy production rate is identified. Kinetic equations for one-particle densities are constructed as special cases and Kubo's linear response theory is generalized to relaxator Liouville dynamics. In weak coupling between system and environment the relaxator can be factorized in environmental correlations and bilinear system operators.

TT 87.2 Thu 15:15 HÜL/S186

Ground-State Exploration Driven by Thermal and Quantum Fluctuations — •Yoshiaki Horiike[1] and Yuki Kawaguchi[1,2] — [1]Department of Applied Physics, Nagoya University, Nagoya, Japan — [2]Research Center for Crystalline Materials Engineering, Nagoya University, Nagoya, Japan

Simulated annealing provides a heuristic solution to combinatorial optimization problems. The cost function of a problem is mapped onto the energy function of a physical many-body system, and, by using thermal or quantum fluctuations, the system explores the state space to find the ground state, which may correspond to the optimal solution of the problem. Studies have highlighted both the similarities and differences between thermal and quantum fluctuations. Nevertheless, fundamental understanding of thermal and quantum annealing remains incomplete, making it unclear how quantum annealing outperforms thermal annealing. Here, we investigate the many-body dynamics of thermal and quantum annealing by examining all possible interaction networks of $\pm J$ Ising spin systems up to seven spins. Our comprehensive investigation reveals that differences between thermal and quantum annealing become prominent for particular interaction networks, indicating that the structure of the energy landscape distinguishes the two dynamics. We identify the microscopic origin of these differences through probability fluxes in state space, finding that the two dynamics are broadly similar but that quantum tunnelling produces qualitative differences. (arXiv:2511.16457)

TT 87.3 Thu 15:30 HÜL/S186

Symmetry re-breaking in an effective theory of quantum coarsening — •Federico Balducci[1], Anushya Chandran[2], and Roderich Moessner[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden — [2]Boston University, Boston, MA

We present a simple theory accounting for two central observations in a recent experiment on quantum coarsening and collective dynamics on a programmable quantum simulator [T. Manovitz et al., Nature 638, 86 (2025)]: an apparent speeding up of the coarsening process as the phase transition is approached; and persistent oscillations of the order parameter after quenches within the ordered phase. Our theory, based on the Hamiltonian structure of the equations of motion in the classical limit of the quantum model, finds a speeding up already deep within the ordered phase, with subsequent slowing down as the domain wall tension vanishes upon approaching the critical line. Further, the oscillations are captured within a mean-field treatment of the order parameter field. For quenches within the ordered phase, small spatially-varying fluctuations in the initial mean-field lead to a remarkable long-time effect, wherein the system dynamically destroys its long-range order and has to coarsen to re-establish it. We term this phenomenon symmetry re-breaking, as the resulting late-time magnetization can have a sign opposite to the initial magnetization.

TT 87.4 Thu 15:45 HÜL/S186

Pairing-induced phase transition in the non-reciprocal Kitaev chain — •Pietro Brighi and Andreas Nunnenkamp — Faculty of physics, University of Vienna, Boltzmanngasse 5, 1090, Vienna, Austria

Investigating the robustness of non-reciprocity in the presence of competing interactions is central to understanding non-reciprocal quantum matter. In this work, we use reservoir engineering to induce non-reciprocal hopping and pairing in the fermionic Kitaev chain, and reveal the emergence of a pairing-induced phase transition. The two phases appear in the spectrum of the non-Hermitian Kitaev Hamiltonian describing the dynamics of correlations, separated by an exceptional point. In the non-reciprocal phase, dynamics are characterized by directionality and slow relaxation, and the steady state supports non-reciprocal density and spatial correlations. At strong pairing, we uncover an unexpected density wave phase, featuring short relaxation times, a modulation in particle occupation and strikingly different correlation spreading depending on pairing non-reciprocity. Our work highlights the non-trivial breakdown of non-reciprocity due to superconducting pairing and invites experimental investigation of non-reciprocal fermionic systems.

TT 87.5 Thu 16:00 HÜL/S186

Harnessing spin qubit decoherence to probe strongly interacting quantum systems — Marcin Płodzień[1], •Sambunath Das[2], Maciej Lewenstein[1,3], Christina Psaroudaki[4], and Katarzyna Roszak[2] — [1]Institut de Ciencies Fotoniques, The Barcelona Institute of Science and Technology, 08860 Castelldefels (Barcelona), Spain — [2]Institute of Physics of the Czech Academy of Sciences, Na Slovance 1999/2, 182 00 Prague, Czech Republic — [3]Passeig Lluis Companys 23, 08010 Barcelona, Spain — [4]Laboratoire de Physique de l' École Normale Supérieure, Université PSL, CNRS, Sorbonne Université, Université de Paris, 75005 Paris, France

Using a mobile qubit as a probe to study the properties of a larger quantum system is a novel technique that leverages the quantum nature of the probe, the system under study, and the interaction between them [1-3]. By analyzing qubit decoherence, one accesses to properties that are difficult to measure classically. We apply this method to the anisotropic Heisenberg XXZ spin-1/2 chain, an archetypal example of strongly correlated system, and show that qubit dynamics encode key system parameters, including quantum phase transitions and perturbation propagation velocity [4]. This demonstrates the effectiveness of small quantum probes for exploring large quantum systems.

References: 1. F. Casola, T. van der Sar et al, Nat. Rev. Mat. 3, 17088 (2018). 2. J. F. Rodriguez-Nieva, K. Agarwal et al. Phys. Rev. B 98, 195433 (2018). 3. S. Chatterjee, J. F. Rodriguez-Nieva et al, Phy. Rev. B 99, 104425 (2019). 4. M Płodzień, S. Das et al, Phy. Rev. B 111, L161115 (2025).

TT 87.6 Thu 16:15 HÜL/S186

Enhancing efficiency of local-information time evolution — •Moksh Bhateja[1], Jonas Rigo[2], and Markus Schmitt[2,3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Universität Regensburg, Regensburg, Germany — [3]PGI-8: Forschungszentrum Jülich, Jülich, Germany

The time evolution of an initially unentangled system under the von Neumann equation generally leads to rapid entanglement growth. This poses challenges for numerical tractability. The Information Lattice framework addresses this by systematically discarding accumulated non-local information (i.e., entanglement) to maintain computational feasibility. Within the local-information time evolution (LITE) approach, we propose Rényi-2 entropy as a measure of information, eliminating the need for matrix decomposition. When combined with additional approximations, this approach significantly enhances the efficiency and scalability of simulations in terms of both system size and duration of time evolution. We demonstrate the accuracy of this method by computing high-quality diffusion coefficients and local observables for a large non-integrable system.

TT 88: Spin Transport and Orbitronics, Spin-Hall Effects II (joint session MA/TT)

Time: Thursday 15:00–17:00 Location: POT/0361

TT 88.1 Thu 15:00 POT/0361

Spin-pumping and induced magnetic polarization in permalloy/platinum heterostructures — •Verena Ney[1], Kilian Lenz[2], Fabrice Wilhelm[3], René Hübner[2], Fabian Ganss[2], Andrei Rogalev[3], Jürgen Lindner[2], and Andreas Ney[1] — [1]Johannes Kepler Universität Linz, Österreich — [2]Helmholtz Zentrum Dresden-Rossendorf, Deutschland — [3]ESRF, Grenoble, Frankreich

Spin pumping is the transfer of angular momentum across interfaces into a non-ferromagnetic material driven by the precessing magnetization of an adjacent ferromagnet. Using ferromagnetic resonance (FMR) the presence of spin pumping can be evidenced by an increase of the Gilbert damping parameter α [1]. Here we study platinum-permalloy (Pt/Py) heterostructures using temperature-dependent broadband FMR. A clear increase of α is seen in a temperature range

from 10 to 300 K when Pt and Py are in direct contact. The temperature dependence of the spin-pumping contribution can be derived by comparing with an Al-sandwiched Py reference film from [2]. Surprisingly, upon insertion of a thin Al spacer layer between Pt and Py the increase in α is suppressed. X-ray magnetic circular dichroism at the Pt L_3-edge reveals a clear magnetic polarization in Pt/Py whereas it is absent when a spacer layer of only 2 nm of Al is inserted. The induced polarization of Pt can thus be associated with spin pumping, while non-polarized Pt in proximity to Py shows an almost identical $\alpha(T)$ behavior as the Py reference sample in [2].

[1] Y. Tserkovnyak Phys. Rev. Lett. **88**, 117601 (2002)
[2] V. Ney et al. Phys. Rev. Materials **7**, 124403 (2023)

TT 88.2 Thu 15:15 POT/0361

Single and double spin Hall anomalous Hall and Hanle effects in Pt/YIG and Ta/YIG bilayers — •Akashdeep Akashdeep, Duc Minh Tran, Mathias Kläui, Gerhard Jakob, and Timo Kuschel — Johannes Gutenberg University Mainz, Germany

Anomalous Hall effect data of heavy metal / magnetic insulator bilayers, such as $Pt/Y_3Fe_5O_{12}$ (YIG), are commonly explained by magnetoresistance effects that are quadratically depending on the spin Hall angle (SHA) [1-4]. This is because they usually consist of two spin Hall processes as for example valid for spin Hall magnetoresistance [1,2]. In addition, S. Zhang et al. predicted theoretically a single spin Hall process combined with interfacial spin-dependent scattering which results in a linear SHA dependence [5] not reported experimentally so far.

In this contribution, we present anomalous Hall effect results for Pt/YIG and Ta/YIG with opposite sign in SHA of Pt and Ta. Thus, we can probe even and odd SHA dependencies. For thin Pt and Ta thicknesses, we observe results that are even in the SHA which is consistent with experimental literature. However, we found an odd SHA dependence for thicker heavy metal layers which is only partially mentioned in theory. We will present the separation of the effects and discuss the impact of the SHA on the individual effect contributions.

[1] H. Nakayama et al., Phys. Rev. Lett. 110, 206601 (2013)
[2] S. Meyer et al., Appl. Phys. Lett. 106, 132402 (2015)
[3] S. Vélez et al., Phys. Rev. Lett. 116, 016603 (2016)
[4] J. Li et al., Phys. Rev. B 106, 184420 (2022)
[5] S. S.-L. Zhang, G. Vignale, Phys. Rev. Lett. 116, 136601 (2016)

TT 88.3 Thu 15:30 POT/0361

Current-induced spin and orbital polarization in the ferroelectric Rashba semiconductor GeTe — •Sergio Leiva-Montecinos[1], Libor Vojáček[2], Jing Li[2], Mairbek Chshiev[2], Laurent Vila[2], Ingrid Mertig[1], and Annika Johansson[3] — [1]Martin-Luther-Universität Halle-Wittenberg, Germany — [2]Univ. Grenoble Alpes, CEA, CNRS, Grenoble, France — [3]Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

The Edelstein effect is a promising mechanism for generating spin and orbital polarization from charge currents in systems without inversion symmetry. In ferroelectric materials, such as Germanium Telluride (GeTe), the combination of bulk Rashba splitting and voltage-controlled ferroelectric polarization provides a pathway for electrical control of the sign of the charge-spin conversion [1, 2].

In this work [3], we investigate current-induced spin and orbital magnetization in bulk GeTe using Wannier-based tight-binding models derived from *ab initio* calculations and semiclassical Boltzmann theory. Employing the modern theory of orbital magnetization, we demonstrate that the orbital Edelstein effect surpases its spin counterpart by one order of magnitude. Moreover, the orbital Edelstein effect remains largely unaffected in the absence of spin-orbit coupling, highlighting its distinct physical origin compared to the spin Edelstein effect.

[1] D. Di Sante *et al.*, Adv. Mater. **25**, 509 (2012).
[2] C. Rinaldi *et al.*, Nano Lett. **18**, 2751 (2018).
[3] S. Leiva-Montecinos *et al.*, arXiv:2505.21340 (2025).

TT 88.4 Thu 15:45 POT/0361

Orbital contribution to g-tensor from first-principles modern theory — •Garima Ahuja[1], Mirco Sastges[2,3], Dongwook Go[4], Shobhana Narasimhan[1], Yuriy Mokrousov[2,3], and Stefan Blügel[2,5] — [1]Theoretical Sciences Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru, India — [2]Peter Grünberg Institut, Forschungszentrum Jülich and JARA, Jülich, Germany — [3]Institute of Physics, Johannes Gutenberg University Mainz, Mainz, Germany — [4]Department of Physics, Korea University, Seoul, South Korea — [5]Institute for Theoretical Physics, RWTH Aachen University, Aachen, Germany

The electronic g-factor, which measures how angular momentum couples to magnetic fields, is a key descriptor of magnetic behavior in solids. In crystalline materials, the orbital contribution to the g-factor can significantly modify its value. In this talk, we present a first-principles framework for computing g-factors, based on multiband perturbation theory with the DFT-Wannier approach, to reveal microscopic origins of the orbital contribution, highlighting the roles of local and non-local orbital currents. We resolve both orbital and spin responses, determine the full g-tensor, and show how interband couplings and band geometry shape the g-tensor across the Brillouin zone. g-tensor plays a key role in quantum technologies, where qubit coherence and control depend on accurate knowledge of magnetic response. We present our findings for some interesting bulk and 2D systems, offering a predictive route for engineering magnetic responses in materials relevant to quantum computing, spin-orbitronics, and spectroscopy.

TT 88.5 Thu 16:00 POT/0361

Inherent Electro-Optic Kerr Rotation — •Erlend Syljuåsen[1], Alireza Qaiumzadeh[1], Rembert Duine[2,3], and Arne Brataas[1] — [1]Center for Quantum Spintronics,Trondheim, Norway — [2]Institute for Theoretical Physics, Utrecht University, The Netherlands — [3]Department of Applied Physics, Eindhoven University of Technology, The Netherlands

Static electric-field–induced Kerr rotation of reflected light is used to probe symmetry breaking, electronic properties, and transport phenomena as the spin and orbital Hall effects. In this talk, we uncover a previously overlooked contribution to the electric-field–induced Kerr rotation, arising from the interplay of matter, the static electric field, and the magnetic component of light. This contribution remains nonzero even in isotropic nonmagnetic homogeneous materials, making this effect inherent to any such Kerr measurement. We present analytical expressions for both two-dimensional layers and semi-infinite bulk metals, and find within the relaxation-time approximation signal magnitudes directly relevant for experiments.

TT 88.6 Thu 16:15 POT/0361

Thermally Activated Spin Transport in a Multiferroic $LiCu_2O_2$/Pt Heterostructure — •Mathew James, Ankita Nayak, István Kézsmárki, and Aisha Aqeel — University of Augsburg, 86159 Augsburg, Germany

Multiferroics, in which electric and magnetic orders are coupled, are potential materials for low-power spintronic devices. $LiCu_2O_2$ is a Type II multiferroic material known to exhibit spiral (non-collinear) spin ordering below its antiferromagnetic transition temperature, $T_N \approx 23$ K [1]. In this material, the magnetic Cu^{2+} ions form double chains along the crystallographic b-axis, resulting in a double-leg spin-ladder configuration.

In this study, we use the Spin Seebeck Effect (SSE) as an electric probe to investigate the thermally activated magnetic response of $LiCu_2O_2$ across different magnetic configurations. In the SSE, a temperature gradient across a magnetic insulator generates non-equilibrium magnons that carry a spin current. This spin current is converted into a measurable voltage in a heavy-metal layer deposited on top of the insulator, via the Inverse Spin Hall Effect [2]. Our preliminary results indicate that the SSE voltage is sensitive to the spiral ordering in $LiCu_2O_2$. References: [1]S. Park, et al., Phys. Rev. Lett., 98, 5 (2007). [2]K. Uchida et al., Nature, vol. 455, no. 7214, (2008).

TT 88.7 Thu 16:30 POT/0361

Current-induced orbital dynamics in magnetic oxides — •Mahmoud Zeer[1], Marjana Ležaic[1], Dongwook Go[1,2], Leonid Pourovskii[3], Stefan Blügel[1,4], Mathias Kläui[2], Olena Gomonay[2], and Yuriy Mokrousov[1,2] — [1]Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institute of Physics, Johannes Gutenberg-University Mainz, 55099 Mainz, Germany — [3]CPHT, CNRS, École polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France — [4]Institute of Theoretical Physics, RWTH Aachen University, 52074 Aachen, Germany

Magnetic oxides provide an ideal platform for exploring orbital de- grees of freedom emerging from strong orbital angular momentum and spin-orbit coupling. The resulting unquenched orbital moments en- able rich orbital-transport phenomena, particularly in antiferromag- netic systems. In this work, we investigate current-induced orbital dy- namics in representative transition-metal oxides using first-principles calculations in both bulk and thin-film geometries. We identify siz- able orbital response and highly efficient orbital-to-spin conversion mechanisms, which give rise to substantial torque components on the magnetic sublattices [1]. In addition, we analyze the contributions of dipole, quadrupole, and octupole magnetic moments to the overall orbital response. Our findings establish magnetic oxides as a promis- ing and realistic platform for harnessing orbital degrees of freedom for next-generation spin-orbital technologies. [1] S. Krishnia, C. Schmitt, M. Zeer et al., under review.

TT 88.8 Thu 16:45 POT/0361

Disentangling angular momentum transport in ferromagnet-diamagnet structures via suspended systems — •Fiona Sosa Barth[1,2], Matthias Grammer[1,2], Richard Schlitz[3], Tobias Wimmer[1,2], Janine Gückelhorn[1,2], Luis Flacke[1,2], Sebastian T.B. Goennenwein[3], Rudolf Gross[1,2,4], Hans Huebl[1,2,4], Akashdeep Kamra[5], and Matthias Althammer[1,2] — [1]Walther-Meißner-Institut, BAdW, Garching, Germany — [2]School of Natural Sciences, TUM, Garching, Germany — [3]Department of Physics, University of Konstanz, Konstanz, Germany — [4]Munich Center for Quantum Science and Technology, München, Germany — [5]RPTU Kaiserslautern-Landau, Kaiserslautern, Germany

Spintronics relies on the transfer of angular momentum between electrons and solid state excitations such as magnons and phonons. In our recent work, we

demonstrate angular momentum transfer between two ferromagnetic strips on diamagnetic substrates [1]. A DC current on one of the strips is converted into a non-equilibrium magnon accumulation, which transfers angular momentum to the magnonic system of the second FM strip, detected electrically by the inverse processes. In this work, we investigate how the nature of this angular momentum transport is affected by the substrate. We first examine how SiOx, SiN and SiN/SiOx layers on Si substrates impact the transport response, and then study the effect in freestanding ferromagnetic strips fully decoupled from the substrate. This allows us to separate potential dipolar from phononic contributions to the coupling between the FM strips. [1] R. Schlitz et al., Phys. Rev. Lett. 132, 256701 (2024)

TT 89: Cryotechnique: Refrigeration

Time: Thursday 16:45–17:45 Location: HSZ/0103

TT 89.1 Thu 16:45 HSZ/0103

Twin low frequency stirling type Pulse Tube Cryocoolers driven by a single metal bellows compressor — •Xaver O. Herrmann[1,2], Jack-André Schmidt[1,2], Bernd Schmidt[2], Jens Höhne[3], and André Schirmeisen[1,2] — [1]Instiute of Applied Physics, Justus-Liebig University, Giessen, Germany — [2]TransMIT-Center for Adaptive Cryotechnology and Sensors, Giessen, Germany — [3]Pressure Wave Systems GmbH, Taufkirchen, Germany

GM-Type Pulse Tube Cryocoolers (PTC) offer cooling power at temperatures down to 2.2 K with ^{4}He as a working fluid[1]. With increasing reliability of PTCs, they have become a dependable and cost-effective option for cooling sensitive sensors[2] to temperatures even below typical LHe bath cryostats. In contrast to conventional GM cryocoolers, PTC require only one moving part: the rotary valve. For critical applications with "high demand" for reliable and continuous cooling, GM-type PTC offer service intervals in excess of 3 years. In order to increase the service interval further as well as to reduce losses within the rotary valve, omitting this valve is the most effective option. In this contribution we present our current status of development of a pair of small low frequency Stirling-type PTC, derived from the two stage GM-type PTC SUSY, both driven by one metal bellows compressor.

[1] N. Jiang et al., Cryogenics 44 (2004) 809.
[2] R. Güsten et al., Nature 568 (2019) 357.

TT 89.2 Thu 17:00 HSZ/0103

Adiabatic demagnetization refrigeration to below 100 mK with frustrated Gd^{3+} compounds — •Tim Treu, Marvin Klinger, Felix Kreisberger, Anton Jesche, and Philipp Gegenwart — Experimental Physics VI, Center for Electronic Correlations and Magnetism, University of Augsburg

Adiabatic demagnetization refrigeration (ADR) is becoming increasingly important for achieving temperatures below 1 K as the global supply of helium-3 continues to tighten. Although ADR in this temperature range has long relied on paramagnetic hydrated salts, recent work shows that frustrated rare-earth oxides provide greater entropy densities and practical benefits, particularly their stability against heating and vacuum exposure [1]. In this study, we present the structural, magnetic, and thermodynamic characteristics of frustrated Gd^{3+} compounds. We evaluate their excellent ADR performance to below 100 mK and compare the results with existing literature. Also, we demonstrate on these compounds how the ADR measurement itself can be used to gain information about the heat capacity, phase transitions, phase boundaries and magnetic interactions below ^{3}He temperatures.

The work was supported by the Deutsche Forschungsgemeinschaft (DFG, German Research 298 Foundation), Grants No. 514162746 (GE 1640/11-1) and No. TRR 360-492547816.

[1] T. Treu et al., J. Phys. Condens. Matter 37, 013001 (2025).

TT 89.3 Thu 17:15 HSZ/0103

Cooling of electrons via superconducting tunnel junctions and their arrays exhibiting nodal lines — •Linus Aliani and Viktoriia Kornich — Institute for Theoretical Physics and Astrophysics, University of Würzburg, 97074 Würzburg, Germany

Condensed matter physics demands experimental control over a systems' temperature. This is usually achieved by the use of commercial dilution refrigerators. However cooling to temperatures below mK is still an issue and usually phonons are cooled down instead of electrons. We therefore propose a setup, which cools *electrons via electrons*.

We consider theoretically a small current running from an electron bath through a setup based on superconducting tunneling junction(s). We employ tunneling junctions with a π phase difference in order to host nodal lines. These nodal lines and their surrounding spectrum depend on external parameters. Thus the setups' entropy is adjustable via its' dependence on their nodal lines. The high entropy of the setup forces electrons entering it to increase their entropy, thereby removing heat from the electron bath. We demonstrate the working principle of this approach by first studying the entropy of a simple superconductor-insulator-superconductor (SIS) junction and compare it to the free electron gas at chemical potential. Subsequently we modify the setup in various ways in order to introduce opportunities for fine tuning for possible experimental uses. For this we investigate superconducting tunnel junctions with a ferroelectric insulator and an array of such junctions with ferroelectrics in-between.

TT 89.4 Thu 17:30 HSZ/0103

Optomechanical Cooling without Residual Heating — Surangana Sengupta[1], Björn Kubala[1,2], Joachim Ankerhold[1], and •Ciprian Padurariu[1] — [1]Institute for Complex Quantum Systems and IQST, Ulm University — [2]German Aerospace Center (DLR), Institute of Quantum Technologies, Ulm

Resolved-sideband cooling is a standard technique in cavity optomechanics enabling quantum control of mechanical motion, but its performance is ultimately limited by quantum backaction heating. This fundamental effect imposes a limit on the minimum achievable mechanical phonon number, establishing a finite-temperature floor regardless of the applied cooling strength. We generalize the semi-classical model for optomechanical cooling to describe universal cavity Hamiltonians incorporating both passive and active nonlinearities. As a concrete demonstration, we analyze the simplest circuit optomechanical system that implements a nonlinear drive via a Josephson junction. Our analysis reveals that this active nonlinear drive can eliminate the residual heating backaction, thereby comparing favorably with alternative optomechanical cooling schemes based on passive nonlinearities [1]. By successfully overcoming the finite-temperature floor that limits conventional schemes, our method paves the way for unprecedented quantum control over mechanical systems and establishes the experimental viability of zero-heating optomechanical cooling.

[1] D. Zoepfl et al., Phys. Rev. Lett. 130, 033601 (2023).

TT 90: Quantum Impurities and Kondo Physics

Time: Thursday 17:00–18:30 Location: CHE/0091

TT 90.1 Thu 17:00 CHE/0091

Unveiling local magnetic moments in copper-oxide atomic junctions — •Marcel Strohmeier[1], Samanwita Biswas[2], Wolfgang Belzig[1], Regina Hoffmann-Vogel[2], and Elke Scheer[1] — [1]Department of Physics, University of Konstanz, 78457 Konstanz, Germany — [2]Institute of Physics and Astronomy, University of Potsdam, 14476 Potsdam-Golm, Germany

Incorporating oxygen into metallic atomic-scale junctions modifies the interatomic bonding and may even promote the formation of monoatomic chains [1]. In the specific case of copper oxide, first-principles studies have predicted the emergence of ferromagnetic ground states, attributing certain atomic configurations with spin-filtering capabilities [2]. By means of low-temperature transport measurements, we provide a series of experimental evidence indicating the presence of local magnetism in air-oxidized mechanically controllable copper break junctions. Our investigations on ultimately small contacts range from magneto-transport measurements [3] to the analysis of anomalous shot noise in the presence of strong zero-bias anomalies [4]. The analysis of the latter reveals signatures of spin-polarized currents, a finding that needs to be reconciled with the spectroscopic features being interpreted within a Kondo model [5].

[1] Thijssen et al., New J. Phys. 10, 033005 (2008)
[2] Zheng et al., J. Appl. Phys. 117, 043902 (2015)
[3] Strigl et al., Nat Commun 6, 6172 (2015)
[4] Tewari et al., Nano Lett. 18, 5217 (2018)
[5] Calvo et al., PRB 86, 075447 (2012)

TT 90.2 Thu 17:15 CHE/0091

Kondo impurities coupled to a Chern insulator — •David A. Krüger[1] and Michael Potthoff[1,2] — [1]Department of Physics, University of Hamburg, Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany

We study a system consisting of two spin-$\frac{1}{2}$ impurities that are exchange-coupled to a two-dimensional Qi-Wu-Zhang Chern insulator. The interplay between the truncated Kondo effect, the truncated RKKY interaction, and the mass parameter m gives rise to a complex phase diagram comprising RKKY singlet and triplet phases, the Kondo singlet, and a partially Kondo-screened phase. Furthermore, we examine how the phase diagram depends on the coupling orbitals and the inter-impurity distance.

Using a Lanczos transformation, we map the problem to a one-dimensional chain with the impurities at the first site, which is then solved using an adaptive natural-orbital configuration-interaction technique. We also consider fictitious local magnetic fields Zeeman-coupled to the impurity spins. The field directions form a four-dimensional base manifold $\mathscr{M} \cong \mathbb{S}^2 \times \mathbb{S}^2$. The bundle of ground states over $\mathscr{M}$ can be topologically characterized by a Chern number that differs from the usual k-space Chern number and provides further insight into the limit of classical impurity spins.

TT 90.3 Thu 17:30 CHE/0091

Orbital-Selective Mott transition in a U(1) gauge model of the Kondo lattice: a Quantum Monte Carlo study — •Gaopei Pan and Fakher Assaad — University of Würzburg, 97074 Würzburg, Germany

We investigate a U(1) gauge theory formulation of the dimensional mismatch Kondo model describing a spin chain on a semi-metallic surface. Using sign-problem-free determinant quantum Monte Carlo simulations, we compute the single-particle spectra, optical conductivity, and dynamical spin structure factor of the composite fermions across a wide range of parameters.

Our results reveal a clear evolution from a Kondo-screened heavy-fermion regime to a Kondo-breakdown phase where the composite fermion spectral weight collapses. Most strikingly, the zero-frequency optical conductivity displays a sharp suppression at the breakdown point, accompanied by a redistribution of spectral weight, which cannot be explained by simple band-structure effects. Instead, the data support an interpretation in terms of an orbital-selective Mott transition, where the f-sector becomes localized while the conduction c electrons remain itinerant.

Together, these findings provide unbiased numerical evidence for a gauge-fluctuation-driven Kondo breakdown and demonstrate how composite-fermion and optical conductivity can diagnose orbital-selective Mott transition in strongly correlated metals.

TT 90.4 Thu 17:45 CHE/0091

Kondo effect competing superconductivity in Van Hove systems — •Grzegorz Michałek and Krzysztof P. Wójcik — Institute of Molecular Physics, Polish Academy of Sciences, ul. M. Smoluchowskiego 17, 60-179 Poznań, Poland

Higher-order Van Hove singularities, characterized by a power-law divergence in the electron density of states near the Fermi surface, are known to boost effects of electronic correlations and in general destabilize conventional Fermi-liquid states. We investigate the influence of such singularity on the magnetic impurity in a superconductor. In general, the Kondo effect is known to compete with superconductivity. Due to this competition, the impurity is expected to undergo a transition between the screened phase, where Kondo screening locally overcomes the superconducting pairing, and Yu-Shiba-Rusinov in-gap state formation, where impurity moment remains intact [1]. We use numerical renormalization group calculations to analyze how a singularity in the normal-state density of states influences the Kondo scale. By incorporating modified density of states into the BCS gap equation, we show the evolution of the Kondo quantum critical point with singularity exponent r.

[1] K. Satori, H. Shiba, O. Sakai, Y. Shimizu, *J. Phys. Soc. Jpn.* **61**, 3239 (1992).

TT 90.5 Thu 18:00 CHE/0091

The work distribution function of a qubit and of the Anderson impurity model — •Theodoulos Costi[1], Hoa Nghiem[2], Steven Campbell[3,4], and Andrew Mitchell[3,4] — [1]Peter Günberg Institute, Research Centre Jülich, 52428 Jülich, Germany — [2]Phenikaa Institute for Advanced Study, Phenikaa University, 12116 Hanoi, Vietnam — [3]School of Physics, University College Dublin, Belfield, Dublin 4, Ireland — [4]Centre for Quantum Engineering, Science and Technology, University College Dublin, Ireland

The work distribution function (WDF) of two representative quantum impurity models, the Anderson impurity model (AIM) of strongly correlated electrons, and the Ohmic spin-boson model (SBM) of a qubit coupled to an environment, is investigated within the non-perturbative time dependent numerical renormalization group (TDNRG) approach [1]. For level quenches, the zero temperature WDF, $P(W)$, exhibits a threshold behavior above the minimum work, $W_{\rm min}$, taking the form $P(W) = a|W - W_{\rm min}|^{-(1-\alpha_{\rm OC})}$ where $\alpha_{\rm OC}$ is the Anderson orthogonality exponent. We calculate $\alpha_{\rm OC}$ analytically, finding agreement with that obtained from the TDNRG. The calculations are further validated by verifying the first three moments of the WDF and the Crooks relation. This work demonstrates the ability of the TDNRG approach to capture the quantum thermodynamics of nanoscale quantum impurity systems for strong quenches beyond the linear response regime [1].

[1] H.T.M. Nghiem, T.A. Costi, S. Campbell, A.K. Mitchell, preprint (2025)

TT 90.6 Thu 18:15 CHE/0091

Conventional and singlet-triplet Kondo effect in radical single-molecule junctions — •Elke Scheer[1], Gautam Mitra[1], Jueting Zheng[1,2], Michael Deffner[3], Karen Schaefer[3], Jonathan Z. Low[3], Luis M. Campos[4], Carmen Herrmann[4], and Theo A. Costi[5] — [1]Uni Konstanz, Germny — [2]Xiamen Univ., China — [3]Univ. Hamburg, Germany — [4]Columbia Univ., USA — [5]Research Center Jülich, Germany

The Blatter radical has been suggested as a building block in future molecular spintronic devices due to its expected long-spin lifetime [1]. Whether its radical character is maintained in single-molecule junctions depends on the environment [2]. For about 25% of single-molecule junctions investigated at low-temperature (4.2 K) we observe zero-bias anomalies that can be assigned to the Kondo effect and hence support the radical character. Additionally, a strong negative magnetoresistance is observed in junctions that do not reveal a zero-bias anomaly. By combining distance-dependent and magnetic-field-dependent measurements, quantum-chemical and quantum-transport calculations, we show that both observations can be consistently explained by a singlet-triplet Kondo model. [3,4].

[1] L. Ji et al., Adv. Mater. 32, e1908015 (2020)
[2] J. Z. Low et al., Nano Lett. 19, 2543 (2019)
[3] J. Paaske et al., Nat. Phys. 2, 460 (2006)
[4] G. Mitra et al., Chem 11, 102500 (2025)

TT 91: Superconductivity: Theory II

Time: Thursday 17:30–18:30 Location: HSZ/0101

TT 91.1 Thu 17:30 HSZ/0101

Superconducting length scales and currents from first principles — Mitsuaki Kawamura[1], Takuya Nomoto[2], •Niklas Witt[3], and Ryotaro Arita[4,5] — [1]Yokohama National University, Japan — [2]Tokyo Metropolitan University, Japan — [3]JMU Würzburg, Germany — [4]University of Tokyo, Japan — [5]RIKEN CEMS, Japan

Superconducting length scales, namely the coherence length and the penetration depth, as well as critical currents, are central to the performance of superconductors but remain challenging to obtain from first principle calculations. While density functional theory for superconductors (SCDFT) has been widely used to predict transition temperatures, magnetic and current related superconducting properties are far less explored.

We present a fully ab initio implementation of a recently introduced method [1] within SCDFT, which gives access to superconducting length scales and depairing currents by introducing a finite-momentum pairing constraint. The approach has been integrated into the open-source superconducting-toolkit (SCTK) [2] and applied to representative elemental, alloy, and high-pressure hydride superconductors. The results demonstrate a viable route to predicting magnetic superconducting properties directly from electronic structure calculations.

[1] N. Witt et al., npj Quantum Mater. 9, 100 (2024)
[2] M. Kawamura et al., Phys. Rev. B 101, 134511 (2020)

TT 91.2 Thu 17:45 HSZ/0101

Cavity-control of the Ginzburg-Landau stiffness in superconductors — •Vadim Plastovets and Francesco Piazza — Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

Confining light around solids via cavities enhances the coupling between the electromagnetic fluctuations and the matter. We predict that in superconductors this cavity-enhanced coupling enables the control of the order-parameter stiffness, which governs key length scales such as the coherence length of Cooper pairs and the magnetic penetration depth. We explain this as a renormalization of the Cooper-pair kinetic mass caused by photon-mediated repulsive interac-

tions between the electrons building the pair. This effect is generic for Bardeen-Cooper-Schriffer superconductors and is most pronounced in low-Tc materials. The strength of this effect can be tuned via the length of the cavity and we estimate it to be sizable for cavities in the infrared range.

TT 91.3 Thu 18:00 HSZ/0101

Influence of Cavity-Induced Polariton Formation on Superconductivity — •Paul Bodewei[1], Paul Fadler[1], and Michael A. Sentef[1,2] — [1]Institute for Theoretical Physics, University of Bremen/ Bremen Center for Computational Material Science — [2]Max Planck Institute for the Structure and Dynamics of Matter, CFEL, Hamburg

Cavities have emerged as a powerful tool for manipulating quantum materials, leveraging vacuum fluctuations to alter fundamental material properties. Recent experiments on the organic high-T_c κ-salts report a dramatic suppression of the superfluid density when those are coupled to a cavity [1]. The prevailing hypothesis for this suppression arises from a resonant coupling between the cavity modes and infrared-active molecular phonon modes in the κ-salt. However, the microscopic mechanism by which such cavity-induced phonon/polariton coupling alters superconductivity remains unknown. To gain further understanding on this, we focus on charge-transfer κ-salts with strong electronic correlations, which are well captured by a Hubbard model [2,3]. Building on that, our goal is to understand how the emergence of cavity-mediated phonon polaritons modifies the effective interactions (e.g. spin fluctuations [4] or mediated electron pairing), and thereby to examine how and why the superconducting state is suppressed.

[1] I. Keren, T.A. Webb, S. Zhang et al., arXiv:2505.17378 (2025)
[2] M. Buzzi et al., *Phys. Rev. X*, **10**, 031028 (2020)
[3] H. Menke et al., *Phys.l Rev. Lett.* **133** 136501 (2024)
[4] J. Schmalian, *Phys. Rev. Lett.*, **81**, 4232 (1998)

TT 91.4 Thu 18:15 HSZ/0101

Unraveling Quantum Effects of Flexible Molecules in Superfluid Solvents — •Katharina Leitmann[1], Harald Forbert[1,2], and Dominik Marx[1] — [1]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, 44780 Bochum, GER — [2]Center for Solvation Science ZEMOS, Ruhr-Universität Bochum, 44780 Bochum, GER

Protonated methane (CH_5^+) is a fluxional molecule whose sensitivity to its environment makes it an excellent probe for low-temperature molecular interactions. We investigate CH_5^+ microsolvation in *para*-hydrogen clusters $(pH_2)_n$ at low temperatures using two distinct simulation approaches: Ring Polymer Molecular Dynamics at 15 K to compute IR spectra and a hybrid simulation approach that combines Path Integral Molecular Dynamics for CH_5^+ and bosonic Path Integral Monte Carlo to establish Bose-Einstein statistics of the $(pH_2)_n$ quantum solvation environment, subject to bosonic exchange at 1 K.

All simulations are based on highly accurate High-dimensional Neural Network Potentials and the IR spectra are computed using a Neural Network Dipole Moment Surface, both parameterized using CCSD(T) theory. Our simulations demonstrate stable solvation of CH_5^+ at least up to $n = 12$ pH_2 molecules, which build the first solvation shell. We revealed that the structure of CH_5^+ is not significantly perturbed by the solvation with pH_2. However, we found significant fluctuations in the large amplitude motion of CH_5^+ associated with partial hydrogen scrambling as a function of cluster size n. These dynamic influences are consistently observed in the IR spectra, underscoring the robustness of our findings across different methodologies and temperatures.

TT 92: Transport – Poster

Time: Thursday 18:00–20:00 Location: P4

TT 92.1 Thu 18:00 P4

Development of a scanning NV magnetometer for quantum senisng experiments at room-temperature — •Yue Yu, Ricardo Javier Peña Román, and Aparajita Singha — IFMP, TU Dresden, Dresden, Germany

Nitrogen-Vacancy (NV) center based sensors are widely used because they are versatile, precise, and suitable for exploring a broad range of systems. We have previously designed NV setups capable of operating in ultra high vacuum (UHV) and cryogenic environments, which, however, are only meaningful to use with samples that mandate such extreme measurement conditions. In order to expand our measurement capabilities to room temperature (RT) systems (such as exploration of nanomagnetism in RT-stable 2D materials, antiferromagnetic / ferromagnetic spin textures, stable molecular systems) as well as to enable rapid pre-screening of both samples and NV probes prior to transferring them into the UHV cryogenic setups, we are now setting up a room-temperature-scanning-NV magnetometer. This system integrates atomic force microscopy (AFM) with optical readout of single NV centers and will feature microwave delivery directly on the AFM tip to achieve highly localized and efficient spin control. This setup will also feature piezo-controlled permanent magnets, thus enabling quantitative magnetic-field mapping with nanometer-scale spatial resolution. Together with our UHV low-temperature scanning NV magnetometer and UHV confocal microscopes, it will form a unified platform for a complete workflow across ambient, cryogenic, and UHV environments.

TT 92.2 Thu 18:00 P4

Development of an Ultra High Vacuum and Low Temperature Scanning NV Magnetometer — •Sandip Maity[1], Ricardo Javier Peña Román[2,1], Dinesh Pinto[1,3], Isabel Pfander[1], Klaus Kern[1,3], and Aparajita Singha[2,4] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]IFMP, TU Dresden, Germany — [3]Institut de Physique, École Polytechnique Fédérale de Lausanne, Lausanne — [4]Wurzburg-Dresden Cluster of Excellence (ct.qmat)

The nanoscale spatial resolution and calibration-free quantifiable magnetic field measurement capabilities of nitrogen-vacancy (NV) centers have enabled us to investigate the properties of magnetic spin textures with high magnetic sensitivity through scanning probe microscopy across a wide range of temperatures and pressure. In the poster I will be presenting the development of a scanning probe magnetometer capable of imaging magnetic textures under ultra-high vacuum and low temperature. Moreover, we have integrated commercial NV tips with a home-built tip holder equipped with an AFM amplifier and microwave excitation on the tip (not on the sample). This compact and modular probe holder allows us to have a magnetic image of any sample region without restriction. To exploit the quantifying nature of NV magnetometry using Optically Detected Magnetic Resonance, a coherent microwave (MW) delivery to the probe is mandatory. I will also present different means of delivering MW to the NV probes through different designs of the tip holders in a practical and versatile manner and how effective they are in coherently manipulating the NV spin states.

TT 92.3 Thu 18:00 P4

Advances in building a cryogenic scanning NV magnetometer — •Kilian Srowik[1,2], Lotte Boer[1], Hayden Binger[1], Young-Gwan Choi[1], Ahmet Ünal[1], Luminita Harnagea[2,4], Sabine Wurmehl[2], Bernd Büchner[2,3], and Uri Vool[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Leibniz Institute for Solid State and Materials Research, IFW Dresden, Dresden, Germany — [3]Institute for Solid State and Materials Physics, TU Dresden, Dresden, Germany — [4]Indian Institute of Science Education and Research, Pune, India

In the last decade, the Nitrogen-Vacancy (NV) defect in diamond has emerged as an ideal quantum sensor to probe magnetic stray fields. By using a diamond nanopillar, containing a single NV center, as the tip of an atomic force microscope (AFM), it becomes possible to perform Scanning NV magnetometry (SNVM). This configuration not only enables us to measure with high spatial resolution and sensitivity, it also makes a broad temperature range accessible. While room temperature NV systems are widely used already, cryogenic NV setups still remain sparse. At the MPI CPfS, we are in the final stages of building a cryogenic SNVM setup, capable of measuring at variable temperatures down to 1.8K. This paves the way to study a multitude of interesting phenomena, like magnetic phase transitions and superconductivity. In particular, we want to focus on investigating the magnetic structure of unconventional superconductors, like the recently emerged Weyl semimetal γ-$PtBi_2$, reported to have superconducting surface states with a nodal superconducting gap structure.

TT 92.4 Thu 18:00 P4

On-surface spin characterisation of isolated molecules using room temperature NV magnetometry — •Olga Shevtsova[1,2], Bernhard Putz[3], Ulrich Ziener[3], and Aparajita Singha[1,2] — [1]IFMP, TU Dresden, Germany — [2]Würzburg-Dresden Cluster of Excellence (ct.qmat) — [3]Universität Ulm, Ulm, Germany

Molecular spins have been receiving significant attention as promising candidates for quantum technologies, offering unique advantages in stability, tunability, and scalability. In particular, our work focuses on carbon-based open-shell molecular systems - stable chlorinated trityl radicals that host an unpaired electron spin. Understanding the coherent properties of these molecular spins is a crucial step toward their integration in practical quantum applications. However, probing such properties remains challenging due to limitations in sensitivity, environmental constraints, and the invasiveness of existing techniques.

Nitrogen-Vacancy (NV) centers in diamonds can operate over a wide temperature range and provide non-invasive optical readout, making them versatile and highly suitable tools for deepening existing knowledge. In this study, we leverage NV-center-based quantum sensors to investigate both the coherent properties of molecular spins and the limits of detecting extremely low spin concentrations, potentially down to a single spin. By combining the precision of NV magnetometry with the inherent stability of open-shell systems, our work aims to provide

deeper insight into their viability as stable and controllable components for future quantum technologies.

TT 92.5 Thu 18:00 P4

Probing Vortices in Superconductors with Scanning Quantum Microscope — •Sreehari Jayaram[1], Malik Lenger[1], Lucas Pipim[3], Ruoming Peng[1], Rainer Stoehr[1], Mathias S. Scheurer[3], Jurgen Smet[2], and Joerg Wrachtrup[1,2] — [1]3rd Institute of Physics, University of Stuttgart, Allmandring 13, Stuttgart 70569, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, Stuttgart 70569, Germany — [3]Institute for Theoretical Physics III, University of Stuttgart, Pfaffenwaldring 57, Stuttgart 70569, Germany

Magnetic dynamics at the nanoscale provide crucial insight into the behavior of superconductors. Using single-spin scanning quantum microscopy, we probe vortex dynamics in superconductors. Our measurements reveal a disordered vortex glass phase that melts near the critical temperature. Magnetic noise persists well below **, with a strength that increases at lower temperatures*contrary to expectations. This behavior, detected via spin decoherence, points to an intrinsic origin driven by competition between supercurrent density and thermal fluctuations. Our results establish single-spin microscopy as a powerful platform for investigating fluctuations in 2D superconductors.

TT 92.6 Thu 18:00 P4

Double galvanic access to a microwave cavity for flux-mediated optomechanics with carbon nanotubes SQUIDs — •Julian Sehr, Tim Althuon, Philipp Wiedemann, Sophie Klingel, Philipp Bennett, Tino Cubaynes, and Wolfgang Wernsdorfer — Karlsruher Institut für Technologie (KIT), 76131 Karlsruhe

Carbon nanotubes (CNTs) are attractive as Josephson junction weak links, offering ballistic, one-dimensional transport and the ability to electrostatically tune their carrier density and transmission. By employing two parallel Josephson junctions formed from a single carbon nanotube mechanically transferred onto the circuit after growth, we realised a superconducting quantum interference device (DC-SQUID). The device supports an induced supercurrent of up to 4 nA through a single CNT-based junction. We expect to increase the critical current by changing the superconductor of the electronic circuits from molybdenum-rhenium to niobium. Embedding such a SQUID into a non-linear microwave cavity opens up the possibility to couple the phonon modes of the CNT to cavity photons via flux-mediated optomechanical coupling. This will be realised by making the cavity galvanically accessible from both sides, while the boundaries of the resonator are defined by a filtering stage using an on-chip planar capacitance.

TT 92.7 Thu 18:00 P4

Nonlinear Nanomechanics in Suspended Carbon Nanotubes — •Philipp Bennett, Sophie Klingel, Julian Sehr, Tim Althuon, Tino Cubaynes und Wolfgang Wernsdorfer — Karlsruher Institut für Technologie, Karlsruhe, Germany

Suspended carbon nanotubes (CNTs) serve as a unique platform for the implementation of nanomechanical systems (NEMS), owing to their electrical, mechanical, and quantum properties in a single nanoscale object. Because of their well-defined quantum dot states and mechanical degree of freedom, suspended CNTs are attractive for studying the coupling between electronic transport and nanomechanics and as candidates for mechanical qubits.

Building a two-level phononic system at the quantum level requires a certain degree of nonlinearity. In contrast to other hybrid approaches, we rely on purely intrinsic nonlinearities, which minimizes the additional decoherence arising from external sources. The degree of intrinsic nonlinearity can be quantified via the ratio K/κ, with K being the Kerr nonlinearity and κ the decoherence rate of the resonator. Our group has recently measured the Kerr-constant for a purely mechanical system. The next step is to further reduce the decoherence rate κ. To this end, we follow two complementary strategies: enhancing CNT quality by introducing water during growth, and improving the readout by implementing an MHz-range RLC tank circuit in the dilution cryostat. These improvements are meant to boost the degree of intrinsic nonlinearity in our system, paving the way to various applications, like magnetometers for single-molecule magnets or mechanical qubits.

TT 92.8 Thu 18:00 P4

Transmission resonances for periodically driven local potentials — •Daniel Weber — RPTU University Kaiserslautern-Landau, D-67663 Kaiserslautern, Germany

We model tunneling trough a quantum dot using a locally driven 1D tight-binding Hamiltonian. Using Floquet theory, we produce exact numerical results before we derive an analytic prediction of position and amplitude of transmission resonance in dependence of driving frequency, coupling strength and local energy levels. Starting with a suitable transformation of the Hamiltonian, we use a high frequency approximation to derive a valid analytical approximation for frequencies in the systems energy scales. The results can be used for the design of efficient nano-electronic devices, in photonic waveguides or can be useful for ultra-cold gages in optical lattices.

TT 92.9 Thu 18:00 P4

STM-Break Junction Measurements of Organic Dyes — •Yannic Altmann[1,2], René Matzdorf[1], and Rüdiger Faust[2] — [1]Institute of Physics, University of Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany — [2]Institute of Chemistry, University of Kassel, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

Current research in molecular electronics explores multiple ways to manipulate the conductivity of molecules inside of single-molecule junctions using external stimuli. Examples are magnetic fields [1], external forces [2], as well as electromagnetic radiation [3].

We use a LT-STM to measure the conductance of single oligo(phenylene ethynylene) molecules in STM break junction inspired experiments in two different ways: $I(z)$-spectroscopy as well as $I(t)$-spectroscopy. The goal of the project is to do similar measurements on organic dye molecules to study the effects of molecule excitation with visible light on the molecular conductance.

[1] G. Mitra *et al.*, Nano Letters 22, 5773 (2022)
[2] P. Zhou, *et al.*, Jo. American Chem. Soc. 145, 18800 (2023)
[3] E-D. Fung *et al.*, Nano Letters 17, 1255 (2017)

TT 92.10 Thu 18:00 P4

Vorticity as an Origin-Independent Measure of Electronic Circulation in Crystals — •Aristo Ardyaneira, Leonard Prokisch, Moritz Rübling, and Ferdinand Evers — Institute of Theoretical Physics, University of Regensburg, D-93053 Regensburg, Germany

Orbital angular momentum (OAM) plays a central role in the emerging field of orbitronics, but its definition in real space is problematic because it depends on the choice of origin. Common approaches - such as the atomic-centered approximation or unit-cell integration - either neglect interstitial contributions or are not uniquely defined. We propose vorticity as an alternative, origin-independent measure of the local electronic circulation. Although closely related to the experimentally accessible magnetic field, vorticity has received little attention in solid-state contexts. Using the Mandelung formulation of quantum mechanics, we derive an equation of motion for the electronic vorticity and demonstrate its direct connection to the magnetic field in a crystal. This framework provides a natural and physically transparent description of electronic spinning motion relevant for orbitronic phenomena.

TT 92.11 Thu 18:00 P4

Photogalvanic Effect as a Probe for Distinguishing type-I and type-II Semi-Dirac Systems — •Bristi Ghosh[1], Malay Bandyopadhyay[1], and Snehasish Nandy[2] — [1]Indian Institute of Technology Bhubaneswar, Bhubaneswar, Odisha 752050, India — [2]National Institute of Technology Silchar, Assam, 788010, India

The photogalvanic effect (PGE) generates a direct photocurrent under polarized light in non-centrosymmetric systems, manifesting as the linear photogalvanic effect (LPGE) or circular photogalvanic effect (CPGE) depending on light polarization. Using quantum kinetic theory within the relaxation-time approximation, we theoretically explore the PGE as a probe of quantum geometry in anisotropic type-I and type-II semi-Dirac (SD) systems. The PGE conductivity, comprising injection, shift, resonant, higher-order pole, and anomalous contributions, exhibits a pronounced enhancement in type-II systems compared to type-I. For the CPGE, both anomalous and resonant terms, arising from Fermi surface contributions, decrease with increasing chemical potential in type-I but increase in type-II systems. For the LPGE, the xxx-component of the shift conductivity in type-II SD reverses sign upon tuning the gap tuning parameter δ, while other components remain invariant, similar to type-I behavior. These contrasting CPGE and LPGE responses provide clear optical signatures distinguishing the two SD phases. The predicted effects, potentially realizable in TiO_2/VO_2 heterostructures, establish the PGE as a sensitive probe of quantum geometry and a promising route toward next-generation optoelectronic applications.

TT 92.12 Thu 18:00 P4

Intrinsic Nonlinear Magneto-Electric Hall Effect — •Sunit Das and Amit Agarwal — Department of Physics, Indian Institute of Technology, Kanpur 208016, India

We propose a new mechanism for an intrinsic nonlinear magneto-electric Hall (MEH) response in multilayer van der Waals materials. The predicted Hall conductivity is bilinear in an out-of-plane gate electric field and the magnetic field, independent of scattering time, and can arise even in nonmagnetic systems with weak spin-orbit coupling. This response originates from an emergent layer-orbital quantum geometry whose sign reverses with the gate field, faithfully tracking the underlying layer polarization. Our comprehensive symmetry analysis reveals that a large class of polar and chiral nonmagnetic materials can permit this magnetotransport. Using the gated bilayer as a representative platform, we demonstrate sizable MEH signals. We further show that the same layer-orbital polarizability drives a longitudinal nonlinear response in chiral materials, providing a robust probe of structural chirality. These results reveal an intrinsic nonlinear transport channel that broadens the landscape of magnetoelectric phe-

nomena and establishes layer-orbital quantum geometry as a key tool for novel transport-based material characterization.

TT 92.13 Thu 18:00 P4

QMC study of heat transport in 2D Dirac materials — •Luis Thremer[1], Adrien Reingruber[1], Maksim Ulybyshev[1], and Fakher F. Assaad[1,2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Am Hubland, Würzburg, Germany

Strongly correlated systems can host varying (and often competing) scattering mechanisms, making them an ideal playground for studying their influence on various transport properties. In particular, Dirac systems can undergo a Gross-Neveu phase transition, switching from a semi-metallic to a Mott-insulating phase. Experimental evidence of this transition was long-sought and recently tentatively realised in experiments on twisted WSe_2 tetralayers. We investigate the heat transport and the behaviour of the heat conductivity across the Gross-Neveu phase transition in strongly correlated 2D Dirac materials. In particular, we focus on their dependence on the change in the nature of the low-lying excitations from electrons to antiferromagnetic spin waves, which occurs across the phase transition. For this study, we use unbiased quantum Monte Carlo and Kubo linear response theory to extract the transport coefficients from the Euclidean time correlators. We also investigate the effects of long-range Coulomb interaction on the heat transport. Since long range interaction leads to the appearance of non-local terms in the heat current, long range Coulomb interaction can potentially significantly alter the thermal-transport behaviour.

TT 92.14 Thu 18:00 P4

Curvature, Torsion, and Non-Metricity in the Continuum Theory of Lattice Defects — •Marvin Henke and Nikodem Szpak — Fakultät für Physik, Universität Duisburg- Essen, Duisburg, Germany

The continuum theory of lattice defects provides a tractable mesoscale framework for electron transport, circumventing microscopic complexity. It maps dislocations and disclinations onto curvature and torsion within an effective Riemann-Cartan geometry. The equivalence of the two latter concepts is an ongoing debate in General Relativity. Motivated by two-dimensional systems, like graphene, we investigate the mapping of metric-induced curvature onto torsion while preserving physical aspects of the dynamics. Among them, a crucial problem with the (eigen)time scaling along the trajectories of (quasi)particles appears. Our approach to solve this problem lies in the relaxation on the standard metric compatibility condition, which introduces the non-metricity tensor as an additional geometrical object, thus opening a new opportunity to discuss deep problems of differential geometry in the context of real physical systems.

TT 92.15 Thu 18:00 P4

Magnetotransport measurements of magic angle twisted bilayer graphene — •Monica Kolek Martinez de Azagra, Sirri Batuhan Kalkan, and R. Thomas Weitz — Georg August Universität Göttingen

Magic angle twisted bilayer graphene (MATBG) has in recent years been established as a powerful platform for exploring strongly correlated electron phenomena in two-dimensional materials [1]. The rich phase diagram of two graphene layers stacked on top of each other with a precise twist angle of 1.1° has been widely studied with a special emphasis on investigating the robust superconducting state, whose exact nature and origin have yet to be determined [2,3]. Here, we present our recent progress in the fabrication and electric characterization of high-quality, encapsulated MATBG devices, highlighting key experimental observations.

[1] Bistritzer & MacDonald, PNAS 108, 12233 (2011).
[2] Cao et al., Nature 556, 80 (2018).
[3] Cao et al., Nature 556, 43 (2018).

TT 92.16 Thu 18:00 P4

Competition of FCI and CDW in a Two-Band Model — •Marco Schönleber and Maria Daghofer — Institut für Funktionelle Materie und Quantentechnologien, Stuttgart, Deutschland

Fractional quantum hall physics with vanishing magnetic fields has become an increasingly important research topic in recent years due to new findings in the field of moiré materials. Experimental signatures of these phases are often observed in combination with signatures of charge ordered or other symmetry broken phases. This indicates that band mixing might play an elementary role in the complete description of this phase of matter. For this purpose, an extended Hubbard model on a triangular lattice with $\nu = 2/3$ is considered. This allows the formation of bands of non-trivial topology as well as the formation of commensurate charge density waves. The analysis is carried out by exact diagonalisation and DMRG. By varying band gap and interaction strength the topologically non-trivial FCI competes with the symmetry-broken CDW phase.

TT 92.17 Thu 18:00 P4

Chiral Kondo Lattice Emergence in Moiré Heterostructure — •Benjamin Heinrich and Maria Daghofer — Institute for Functional Matter and Quantum Technologies (FMQ), University of Stuttgart

Moiré systems composed of van der Waals heterostructures provide an experimentally accessible platform to realize a wide range of strongly correlated electron phenomena. Using transition metal dichalcogenide materials, such as an AB-stacked $MoTe_2/WSe_2$ bilayer, gives rise to an effective multi-orbital Hubbard model on the honeycomb lattice, which can be tuned via doping and the introduction of charge transfer energy through external voltages. Including strong Ising spin-orbit coupling leads to chiral Kondo exchange between localized and itinerant electrons in different layers near half-filling [1], To gain a better understanding of experimentally observed phenomena, including magnetic ordering, numerical modeling is performed using exact diagonalization, and finite-size effects are further reduced using the variational cluster approach.

[1] Guerci et al., Sci. Adv. 9, eade7701 (2023)

TT 92.18 Thu 18:00 P4

Simulation of charge density wave effects in the layered van der Waals material $GdTe_3$ — •Shen van Hassel[1], Sergii Grytsiuk[1], and Malte Rösner[1,2] — [1]Radboud University, Nijmegen, Netherlands — [2]Bielefeld University, Bielefeld, Germany

In this study, we use *ab initio* downfolding techniques to demonstrate that the Fermi surface (FS) of the undistorted rare-earth tritelluride $GdTe_3$ can be accurately represented by a minimal tight-binding model derived from the in-plane *p*-orbitals of the Te bilayer. To examine the effect of the charge density wave (CDW) in $GdTe_3$, we expand our Hamiltonian to effectively model electron-phonon interactions by assuming and testing self-energy models within the Nambu-Gor'kov space. We calculate the spectral function, which agrees well with experimental ARPES data. Our results provide a simple and effective model for simulating CDW effects in $GdTe_3$, paving the way for a fully *ab initio* approach applicable to a broader class of materials.

TT 92.19 Thu 18:00 P4

Ultra-Low Temperature Fast QPI on Quantum Materials — •Alexander LaFleur, Rian A.M. Lighthart, Kevin Hauser, Gleb Neplyak, and Fabian D. Natterer — Department of Physics, Univeristy of Zurich, Winterthurerstrasse 190, CH-8057, Switzerland

Scanning tunneling microscopy/spectroscopy (STM/S) is a powerful experimental technique capable of elucidating the hidden nature of many quantum materials and phases. The characterization of unconventional superconductors, topological insulators, heavy-fermion systems, Kagome superconductors, and Weyl semimetals, have been broadly pushed forward by atomic resolution STM/S imaging. Yet, for many candidate quantum materials, current techniques for acquiring STM data, such as energy-dependent local density of state (LDOS) maps, fall short of the energy resolution necessary to show definitive band structure characteristics of these phases. We propose to combine ultra-low temperature STM (330 mK) with Fast Quasi-Particle Interference (Fast QPI) techniques to increase the effective hold time and energy resolutions of LDOS Maps taken on quantum materials. The Fourier transform of Fast QPI, which uses parallel spectroscopy to simultaneously measure LDOS across many channels in frequency space, allows the energy dependent LDOS to be measured in a fraction of the time of conventional dI/dV lock-in techniques. This increase in energy resolution given the time constraints of ultra-low temperature measurements holds the potential to demonstrate new and novel observable phenomena in quantum materials and the elusive states they harbor.

TT 93: Superconductivity – Poster II

Time: Thursday 18:00–20:00 Location: P4

TT 93.1 Thu 18:00 P4

The Search for 1144 Phases under Pressure — •Leonard Essich, Kristin Kliemt, and Cornelius Krellner — nstitute of Physics, Goethe University Frankfurt, Germany

Alternative stacking of 122 Fe-based pnictides has enabled the synthesis of the 1144 phase $AB Fe_4As_4$ (A = alkali, B = alkaline earth). Examples include $CaKFe_4As_4$, where a *half-collapsed* tetragonal phase emerges under pressure, and $EuRbFe_4As_4$ or $EuCsFe_4As_4$, where Eu magnetism coexists with superconductivity [1,2]. Theoretical studies predict the stability of further 1144 Fe-arsenides and an extension to phosphides ($AB(TM)_4P_4$ where TM = Fe, Ru, Co, or Ni). Notably, $CaKRu_4P_4$ has been successfully synthesised [1]. This work investigates the synthesis of other 1144 phases under high-pressure conditions, designed to sup-

port the incorporation of smaller phosphorus atoms on arsenic lattice positions. Multi-anvil presses offer precise pressure and temperature control, large sample sizes, and adaptable setups for crystal growth research. In this contribution, we present the capabilities of a multi-anvil press, the challenges encountered during sample preparation, and outline the pathway to synthesising 1144 phases. A Walker-type module, previously utilized in our laboratory, contains a 6-8 anvil configuration within a steel cylinder [3]. The choice of pressure-transmitting medium and internal configuration is crucial to achieving the desired outcome in these experiments.

[1] B. Q. Song *et al.*, Phys. Rev. Materials **5**, 094802 (2021)
[2] U. S. Kaluarachchi *et al.*, Phys. Rev. B **96**, 140501 (2017)
[3] A. A. Haghighirad *et al.*, Cryst. Growth Des. **8**, 1961 (2008)

TT 93.2 Thu 18:00 P4

MBE Growth and STM/STS Characterization of Monolayer and Bilayer Sb on $NbSe_2$ — •Zihao Ma, Ruijun Xi, and Hao Zheng — Shanghai Jiao Tong Univ, Tsung Dao Lee Inst, Key Lab Artificial Struct & Quantum Control, Sch Phys & Astron, Shanghai 200240, Peoples R China

Two dimensional antimony (Sb) has attracted increasing interest due to its strong spin-orbit coupling, unprecedented level of structural tunability, and potential topological phases. The atomically flat surface, weak interlayer bonding, and superconducting ground state of $NbSe_2$ make it an ideal substrate for epitaxial growth of Sb. Studying Sb/NbSe van der Waals heterostructures enables investigation of growth behavior, electronic reconstruction, and possible interface driven phenomena. Furthermore, the combination may be a new strategy to achieve topological superconductors. By molecular beam epitaxy (MBE), we achieve controlled growth of monolayer (1L) and bilayer (2L) Sb on $NbSe_2$. By STM/STS, we characterize surface morphology, atomic structure, and electronic states.

TT 93.3 Thu 18:00 P4

Superconductivity, CDW, and quasiparticle interaction in 2H-TaS_2 probed by point contacts — •Oksana Kvitnitskaya[1,2], Yurii Naidyuk[2], and Bernd Büchner[1] — [1]Leibniz-Institute for Solid State Research, IFW Dresden, Dresden, Germany — [2]B. Verkin Institute for Low Temperature Physics and Engineering NAS of Ukraine, Kharkiv, Ukraine

Among Ta-based dichalcogenides, metallic 2H-TaS_2 exhibits physical properties that depend on its lattice perfection, vacancies, intercalation, and external pressure, etc. TaS_2 represents a classic example of a material in which charge density wave (CDW) order and superconductivity coexist and compete. Point contacts (PCs) propose a direct method for measuring electron-quasiparticle interaction by Yanson PC spectroscopy and superconducting gap via Andreev reflection. Also the phase transitions that affect electron transport can be detected using PC as a probe. In this report, we demonstrate the first PC study of 2H-TaS_2. Firstly, we observed enhanced Tc in produced PCs, which can reach up to 7 K, instead of 1 K in the bulk, and the critical magnetic field reaches up to 5T at 2K. The nonlinear current-voltage characteristics I(V) of PC also demonstrate features associated with the CDW transition, which is evident in dV/dI as dips symmetrically placed with respect to zero-bias voltage. Still, electron-phonon interaction features are not resolved undoubtedly in PC spectra, instead quadratic dependence of dV/dI(V) points out that the electron-electron interaction can be dominant at low biases. These preliminary results are very intriguing and give impetus to their deeper investigation.

TT 93.4 Thu 18:00 P4

Comprehensive Optimization of Structural Properties, Flux Pinning, and EXAFS-Revealed Local Structure in HgO-Engineered BiPb-2223 Superconductors — •Mustafa Shalaby[1], Ahmed Shalaby[2], Duc Tran[3], An Pham[3], Latif Khan[4], and Messoud Harfouche[4] — [1]NCRRT, Egyptian Atomic Energy Authority, Cairo, Egypt. — [2]Egyptian Russian University. Badr City, Cairo, Egypt — [3]Faculty of Physics, VNU University of Science, Hanoi, Vietnam — [4]SESAME, P.O. Box 7, Allan 19252, Jordan

A systematic investigation of HgO nanoparticle enhancement in $Bi_{1.6}Pb_{0.4}Sr_2Ca_2Cu_3O_{10-\delta}$ (BiPb-2223) HTSC, with strategic incorporation of 1-2 wt% HgO nanoparticles demonstrates an increase in high-T_c Bi-2223 phase fraction from 69% to 78% while effectively suppressing the detrimental Bi-2212 phase. Cu K-edge EXAFS analysis unveils exceptional structural stabilization, with achieved electronic structure with Cu valence states (V_{Cu}) was 3.04, 2.87, and 3.1 for pristine and HgO-doped samples respectively, maintaining the critical Cu^{+2}/Cu^{+3} mixed valence configuration necessary for superconducting behaviour in the CuO_2 planes. HgO works as a structural stabilizer rather than conventional substitutional dopant, evidenced by non-uniform distribution patterns and preserved superconducting frameworks. Critical current densities reach 900 A/m^2 at 10 K with irreversibility fields exceeding 100,000 Oe for the pure sample, while the 2% HgO composition exhibits optimized flux pinning force characteristics with J_c = 600 A/m^2 at 10K.

TT 93.5 Thu 18:00 P4

From surface to bulk: Superconductivity in doped γ-$PtBi_2$ — •Joshy Kochummachen Oommen, Manaswini Sahoo, Luminita Harnagea, Sabine Wurmehl, Anja Wolter-Giraud, and Bernd Büchner — Leibniz Institute for Solid State and Materials Research Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany

Trigonal platinum bismuthide (γ-$PtBi_2$) has recently attracted significant interest due to the observation of superconductivity and its topologically protected surface states. So far, superconductivity has been detected only through surface-sensitive techniques such as ARPES and STM, with no signatures observed in bulk thermodynamic measurements. However, doped polycrystalline samples show bulk superconductivity. In this work, we investigate how chemical doping modifies this behaviour by studying $PtBi_{(2-x)}A_x$ (A = Te, Pd) in single crystals. Introducing the dopants transforms the system from a surface-confined superconductor into a bulk superconductor. DC and AC susceptibility measurements reveal a clear superconducting transition between 2-2.4 K, with the transition temperature T_c strongly dependent on the dopant concentration. The emergence of bulk superconductivity suggests a doping-induced structural change from a non-centrosymmetric to a centrosymmetric phase, offering an intriguing route to tune the interplay between structure and superconductivity in γ-$PtBi_2$. These results highlight the potential of doped γ-$PtBi_2$ as a platform for exploring exotic superconducting states and understanding how topological surface states evolve into bulk superconductivity.

TT 93.6 Thu 18:00 P4

Nanoscale Characterization of Superconducting NbN Thin Films — •Janine Lorenz[1,2,3], Sven Linzen[4], Mario Ziegler[4], Gregor Oelsner[4], Rony Stolz[4], Evgeni Il'ichev[4], Thomas Smart[1], Yorgo Haddad[1], Marc Neis[1], Pavel Bushev[1], Rami Barends[1], F. Stefan Tautz[1,2,3], and Felix Lüpke[1,5] — [1]Peter Grünberg Institut, Forschungszentrum Jülich, Germany — [2]Jülich Aachen Research Alliance (JARA), Germany — [3]Institut für Experimentalphysik IV A, RWTH Aachen, Germany — [4]Leibniz Institute of Photonic Technology, 07702 Jena, Germany — [5]II. Physikalisches Institut, Universität zu Köln, Germany

Due to their high kinetic inductance, niobium nitride (NbN) films have recently gained attention for their application in quantum phase-slip devices. In this study, we use scanning tunnelling microscopy to investigate the spatial variation of the superconducting order parameter of NbN films grown by atomic layer deposition (ALD). Despite the increased likelihood of defect formation associated with the use of organic precursors in ALD, our measurements reveal a remarkably uniform superconducting gap, which surpasses the reported values for sputtered NbN films. We attribute this to the well controlled thickness and small grain size of ALD grown films. For a 5 nm (4 nm) NbN film grown on a silicon (sapphire) substrate, we obtain an average BCS order parameter of 2.02 meV (1.59 meV), with a standard deviation of 0.04 meV (0.05 meV). This result highlights the high homogeneity of the superconducting order parameter in ALD-grown NbN films.

TT 93.7 Thu 18:00 P4

Development of Lenz lenses for NMR of micron-sized superconductors — •P. Swatosch[1,2], H. Kühne[1], F. Bärtl[1,2], and J. Wosnitza[1,2] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL) and Würzburg-Dresden Cluster of Excellence ctd.qmat, HZDR — [2]IFMP, TU Dresden

Nuclear magnetic resonance (NMR) experiments on novel superconductors are often limited in their sensitivity when only submillimeter-sized samples are available, as in this case only a few nuclear spins contribute to the measurement signal, resulting in a low signal-to-noise ratio. One approach to solving this problem is to locally focus the high-frequency magnetic field of the NMR experiment in the sample volume. For this, structured conductor geometries in the form of Lenz lenses can amplify and shape magnetic fields through targeted eddy currents. For this purpose, we have performed comprehensive numerical simulations of the spatial distribution of electromagnetic fields. Based on geometries that have already proven useful in earlier studies [1-3], we have modeled various designs and evaluated them with respect to their field-focusing capabilities and NMR signal. The results provide a basis for the fabrication of optimized Lenz-lens geometries for highly sensitive NMR measurements of small-volume samples.

[1] Meier *et al.*, Sci. Adv. **3**, eaao5242 (2017)
[2] Schoenmaker *et al.*, Rev. Sci. Instrum. **84**, 085120 (2013)
[3] Sprengler *et al.*, PLoS ONE **12**, e0182779 (2017)

TT 93.8 Thu 18:00 P4

physical properties of the superconductor $NiBi_3$ — •Po-Yuan Cheng[1,2], Shan-Fu Chang[1,2], Pang-Shun Kuo[1,2], and Chien-Lung Huang[1,2] — [1]Department of Physics, National Cheng Kung University, Tainan 701, Taiwan — [2]Center for Quantum Frontiers of Research & Technology (QFort), National Cheng Kung University, Tainan 701, Taiwan

We investigate the superconducting properties of the needle-like compound $NiBi_3$ by electrical resistivity and specific-heat measurements down to low temperatures. Both probes reveal a superconducting transition at a critical temper-

ature T_c = 4 K, with an upper critical field H_{c2} = 4 kOe. High-pressure resistivity measurements up to 20 GPa show that T_c decreases linearly with pressure, which is consistent with phonon-mediated superconductivity. The temperature dependence of the electronic specific-heat is well described by a single-gap s-wave model. In conclusion, these experimental results demonstrate that $NiBi_3$ is a conventional BCS superconductor.

TT 93.9 Thu 18:00 P4

Optical Response of Multi-orbital Superconductors: Role of Fermi Surface Topology and Geometry — •Meghdad Yazdani-Hamid[1], Mehdi Biderang[2], and Akbari Alireza[3] — [1]Department of Physics, Bu-Ali Sina University, 65178, 016016 Hamedan, Iran — [2]Department of Physics, University of Toronto, 60 St. George Street, Toronto, Ontario M5S 1A7, Canada — [3]Beijing Institute of Mathematical Sciences and Applications (BIMSA), Huairou District, Beijing 101408, China

Motivated by the sensitivity of Sr_2RuO_4 to Fermi surface reconstructions under strain, we investigate how Fermi surface geometry and Van Hove singularities influence the optical Hall response and polar Kerr effect. Within a three-orbital model, we explore the impact of chemical potential and interlayer hopping on superconducting pairing and response functions. We find that $d_{x^2-y^2}$ and $d_{x^2-y^2} + ig$ symmetries are the leading candidates for the quasi-2D orbital, while a chiral p-wave state in the quasi-1D orbitals is essential for generating an accessible Kerr angle. Increasing interlayer hopping amplifies coherence factors, producing sharp signatures in T_c and optical transport. Inter-orbital charge transfer further enhances these effects by modifying the balance between quasi-1D and quasi-2D contributions. These results provide a framework for interpreting Kerr effect experiments in multi-orbital superconductors.

[1] M. Yazdani-Hamid, M. Biderang, A. Akbari, arXive:2501.14254

TT 93.10 Thu 18:00 P4

Resistance Measurements of $SmFe_{1-x}Co_xAsO$ single crystall — •Assem Adam[1], Nils-Torben Hahn[1], Thomas Teröde[1], Franz-Michel Eckelt[1], Ralph Wagner[1], Christian Hess[1,2], Bernd Büchner[2], Felix Anger[2], and Sabine Wurmehl[2] — [1]Fakultät für Mathematik und Naturwissenschaften, Bergische Universität Wuppertal, Wuppertal, Germany — [2]Leibniz-Institut für Festkörper- und Werkstoffforschung (IFW) Dresden, 01069 Dresden, Germany

Doped SmFeAsO is has been discovered in the early days of Fe-based superconductivity. However, sizeable single crystals of this material have not been available for a long time. Here, we present resistance measurements of Co-doped SmFeAsO as a function of temperature. The data reveal well defined anomalies, presumably related to the structural and magnetic transitions in this compound. The evolution upon doping is discussed.

TT 93.11 Thu 18:00 P4

Pressure-driven evolution of upper critical field and Fermi-surface reconstruction in strong-coupling superconductor Ti_4Ir_2O — •Lifen Shi[1], Bosen Wang[2,3], and Jinguang Cheng[2,3] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China — [3]School of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100190, China

We report on pressure-driven evolution of the superconducting transition temperature (T_c) and upper critical field $B_{c2}(0)$ of strong-coupling superconductor Ti_4Ir_2O that possesses an unusually large $B_{c2}(0)$ at ambient pressure (AP). Our results reveal an extremely low-pressure coefficients of T_c, i.e. dT_c/dP = -0.047 K/GPa for P < 15 GPa and -0.017 K/GPa for 15 < P < 50 GPa, presumably associated with an inherent large bulk modulus of 252 GPa. Interestingly, we find that its Bc2(0) undergoes a smooth crossover at 35.6 GPa from well beyond to less than the Pauli paramagnetic limit BpBCS(0) = 1.84Tc; i.e., the $B_{c2}(0)$ = 18.2 T = 1.7 $B_{pBCS}(0)$ at AP decreases to 5.8 T = 0.88 $B_{pBCS}(0)$ at 50 GPa. The density functional calculations predicted the possible occurrence of pressure-induced Fermi-surface reconstruction for the energy bands near the K point with strong spin-orbit coupling in 31-41 GPa. The present work sheds more light on this intriguing superconductor capable of resisting to large external compression and strong magnetic fields.

TT 93.12 Thu 18:00 P4

Fluxon mass in superconductors probed by circularly polarized terahertz radiation — •Roman Tesař[1], Michal Šindler[1], Pavel Lipavský[2], Christelle Kadlec[1], and Jan Koláček[1] — [1]Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic — [2]Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

We employ an original method for detecting magnetic circular dichroism in YBCO thin films using FIR/THz laser radiation. The observed dichroism is clearly related to Abrikosov vortices (fluxons). Differential transmission of left- and right-handed circular polarization arises in the superconducting state under an applied magnetic field, but vanishes at zero magnetic field and in the normal state. Fluxon dynamics can be understood within a theoretical model that incorporates the fluxon mass, the equation of fluxon motion, and the interaction with circularly polarized light. The electric field drives a supercurrent that deflects fluxons via the Magnus effect perpendicular to the current flow. The resulting cyclotron motion of fluxons affects the supercurrent and thus the transmittance. We measured circular dichroism as a function of magnetic field and temperature at several laser frequencies for two YBCO samples with distinct doping. A good agreement with theoretical predictions allowed us to estimate the effective mass of a fluxon. Nevertheless, the fluxon mass still remains somewhat controversial and not fully resolved. The presented experimental technique is also applicable for the investigation of cyclotron resonance in semiconductors and magnon modes in magnetic materials.

TT 93.13 Thu 18:00 P4

Statistics of the local spectral gap and order parameter in disordered superconducting films — Johannes Dieplinger[1], Animesh Panda[1], •Arpan Das[1], Ferdinand Evers[1], and Matthias Stosiek[2,3] — [1]Institute of Theoretical Physics, University of Regensburg, Universitaetsstrasse 31, 93053 Regensburg, Germany — [2]Department of Applied Physics, Aalto University, Otakaari 24, 02150 Espoo, Finland — [3]Physics Department, Technical University of Munich, James-Frank-Str. 1, 85748 Garching, Germany

The disorder-tuned superconductor-insulator transition has been a widely studied phenomenon that highlights the interplay between superconductivity and disorder. Local fluctuations in superconducting observables are crucial for understanding related effects, such as superconducting islands and the disorder-induced enhancement of the critical temperature. Using a self-consistent Bogoliubov-de Gennes Hamiltonian, we present a study of 2D disordered superconductors, focusing on the statistics of the local spectral gap and the local order parameter. We emphasise the fact that the similarity of three energy scales - the spectral gap E_g, the order parameter Δ, and the critical temperature T_c - is a peculiarity of clean superconductors. For instance, in the presence of disorder, the mean-field T_c can increase, while the mean $\langle\Delta(T=0)\rangle$ might even decrease. Further, we analyse the flow of the distribution functions of the local order parameter and the local spectral gap as disorder changes. At large disorder, the flow of the (mean-field) distribution functions exhibits a percolation-type transition that appears to have gone unnoticed so far.

TT 93.14 Thu 18:00 P4

nematic fluctuations and electronic correlations in heavily hole-doped $Ba_{1-x}K_xFe_2As_2$ probed by Elastoresistance — •Franz Eckelt[1], Xiaochen Hong[1,2], Steffen Sykora[3], Vilmos Kocsis[3], Vadim Grinenko[4], Kunihiro Kihou[5], Chul-Ho Lee[5], Bernd Büchner[3], and Christian Hess[1] — [1]University of Wuppertal, School of Mathematics and Natural Sciences, 42097 Wuppertal, Germany — [2]Department of Applied Physics and Center of Quantum Materials and Devices, Chongqing University, 401331 Chongqing, China — [3]Leibniz-Institute for Solid State and Materials Research, 01069 Dresden, Germany — [4]Tsung-Dao Lee Institute, Shanghai Jiao Tong University, Shanghai 201210, China — [5]National Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki 305-8568, Japan

We measure the elastoresistance of $Ba_{1-x}K_xFe_2As_2$ in the strongly hole-doped regime using longitudinal and transverse configurations. The subsequent symmetry decomposition of the elastoresistance reveals a crossover from dominant nematic fluctuations in the B_{2g} channel at low doping to a correlation-driven A_{1g} contribution that becomes visible for $x > 0.7$. Complementary multi-orbital model calculations reproduce this doping evolution and indicate that strengthened electronic correlations in the d_{xy} orbital govern the observed A_{1g} response in the heavily hole-doped regime.

TT 93.15 Thu 18:00 P4

Atomic-scale visualization of the superconducting order parameter in the misfit compound $(SnS)_{1.17}NbS_2$ — Dongming Zhao[1], •Shamarita Deb[1,2], Dmytro S. Inosov[2], Claudia Felser[1], Sushmita Chandra[1], and Jian-Feng Ge[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Technical University of Dresden, 01062 Dresden, Germany

Misfit compounds are naturally stacked heterostructures, composed of layers with distinct sublattices. Owing to the incommensurate structural modulations and interlayer coupling, they can exhibit exotic phenomena such as Ising superconductivity and charge density waves. Here, we investigate the high-quality misfit superconductor $(SnS)_{1.17}NbS_2$, a non-centrosymmetric superconductor composed of alternating Sn_2 and NbS_2 layers. Utilising scanning tunnelling microscopy, we obtained atomic-resolution images that clearly resolve, for the first time, both the square lattice on the SnS layer and the hexagonal lattice on the NbS_2 layer. Scanning tunnelling spectroscopy measurements further reveal well-defined superconducting gaps on both layers. Our ongoing experiments aim to visualise its superconducting order parameter with atomic resolution and to explore possible unconventional pairing mechanisms enabled by the intrinsic structural modulations.

TT 93.16 Thu 18:00 P4

Transport properties of superconducting misfit layered compound — •Tarushi Agarwal, Chandan Patra, Poulami Manna, Shashank Srivastava, Priya Mishra, Suhani Sharma, and Ravi Prakash Singh — Indian Institute of Science Education & Research Bhopal

Misfit layered compounds, naturally occurring bulk heterostructures, present a compelling alternative to artificially engineered ones, offering a unique platform for exploring correlated phases and quantum phenomena. This study investigates the magnetotransport and superconducting properties of the misfit compound $(PbS)_{1.13}TaS_2$, comprising alternating PbS and 1H-TaS_2 layers. It exhibits distinctive transport properties, including a prominent planar Hall effect and a fourfold oscillatory anisotropic magnetoresistance. Moreover, it shows multigap 2D superconductivity with a high in-plane upper critical field, exceeding the Pauli limit. The coexistence of multigap superconductivity and anomalous transport within the same material firmly positions misfit compounds as an ideal platform for realizing quantum effects in the two-dimensional limit of bulk crystals. This opens the door to the development of quantum devices with less complexity and enhanced tunability.

TT 93.17 Thu 18:00 P4

High pressure magnetic measurements in Cr- and U- based superconductors — •Meghan Moody[1], Ran Tao[1], Mads Hansen[1], Callum Stevens[2], Zheyu Wu[1], Theodore Weinberger[1], Andrej Cabala[3], Michal Vališka[3], Vladimir Sechovský[3], Andrew Huxley[2], Alexander Eaton[1], and Malte Grosche[1] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]School of Physics and Astronomy, University of Edinburgh, UK — [3]Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic

Mapping the high pressure phase diagram of unconventional superconductors can provide new insights into the nature of their superconducting and magnetic states. We present recent high pressure magnetic susceptibility and SQUID magnetisation measurements in d- and f-electron superconductors, focusing on the Cr-based Kagomé system $CsCr_3Sb_5$ and the field-resilient U-based superconductor UTe_2. In the former, antiferromagnetic order is suppressed under pressure, giving way to a superconducting dome that peaks around 7 K at 4 GPa. In the latter, the superconducting transition line bifurcates at a moderate pressure of about 0.3 GPa, above which two transitions are observed in susceptibility and heat capacity measurements.

TT 93.18 Thu 18:00 P4

Granularity-induced higher harmonics in the Little-Parks effect of Kagome superconductors — •Artem Kokovin[1], Daniel Schultz[1], and Jörg Schmalian[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany — [2]Institut für Quantenmaterialien und Technologien, Karlsruher Institut für Technologie, 76131 Karlsruhe, Germany

We develop a theoretical framework for the emergence of higher-order harmonics in the Little-Parks oscillations observed in Kagome superconductors. Motivated by recent experiments suggesting that certain Kagome compounds exhibit pronounced granularity, an effect that appears to be enhanced by the onset of charge-density-wave order, we construct a two-stage model capturing the interplay of microscopic and mesoscopic physics. On the microscopic level, we derive the effective Josephson coupling of a granular structure, including higher-harmonic contributions to the coupling. On the mesoscopic level, we analyze the magnetic-field dependence of the superconducting free energy in the presence of these Josephson couplings, demonstrating how disorder and granularity convert these Josephson interactions into higher-order Little-Parks oscillations. Our central result is that such higher harmonics naturally arise when the underlying pairing state in Kagome materials is unconventional, providing a clear diagnostic for identifying nontrivial superconducting order in this family of systems.

TT 93.19 Thu 18:00 P4

Superconductivity in Mott Altermagnets — •Robin Schleicher and Maria Daghofer — Institute for Functional Matter and Quantum Technologies, University of Stuttgart

Earlier studies on the Hubbard model have shown that the ground state of two holes in a small cluster lattice shows d-wave symmetry. While pairing by holes doped into half-filled Hubbard models has been intensively investigated, we extend such an analysis to the case of doped strong-coupling altermagnets. In this new approach, we investigate differences to strong-coupling antiferromagnets as well as to weak-coupling superconductivity in altermagnets. To do so, we use exact diagonalization techniques for a checkerboard model. In our case, nodes in d-wave altermagnetism do not coincide with gap nodes expected from the Hubbard model. We discuss the extend of d-wave superconductivity and its competition with other pairing symmetries. We find altermagnetism to suppress pairing compared to antiferromangetism. We also discuss applications to inverted Lieb lattices relevant to Mott-altermagnet materials.

TT 94: Correlated Magnetism – Low-Dimensional Systems

Time: Friday 9:30–12:00 Location: HSZ/0101

TT 94.1 Fri 9:30 HSZ/0101

The zoo of states in the 2 dimensional Hubbard model — •Robin Scholle[1], Pietro Bonetti[1,2], Demetrio Vilardi[1], and Walter Metzner[1] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart — [2]Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

We use real-space Hartree-Fock theory to construct a magnetic phase diagram of the two-dimensional Hubbard model as a function of temperature and doping. We are able to detect various spin- and charge order patterns including Néel, stripe and spiral order without biasing the system towards one of them. For an intermediate interaction strength we predominatly find Néel order close to half-filling, stripe order for low temperatures or large doping, and an intermediate region of spiral order. We then combine the approach with the functional renormalization group method and are able to access the superconducting regime. I will give a short summary of the method followed by a presentation of our current results and an outlook for possible further applications.

TT 94.2 Fri 9:45 HSZ/0101

Kondo-driven magnetic instability in Van Hove metals with sparse impurities — •Krzysztof Wójcik[1], Johann Kroha[2,3], and Peter Wahl[3,2] — [1]Institute of Molecular Physics, Polish Academy of Sciences, 60-179 Poznań, Poland — [2]Physikalisches Institut, Universität Bonn, Germany — [3]SUPA, School of Physics and Astronomy, University of St Andrews, United Kingdom

We analyze a metal exhibiting a higher-order Van Hove singularity at the Fermi level and hosting sparse randomly distributed magnetic impurities. We show that a sharp resonance in the impurity local spectral density, characteristic of typical Kondo systems, is absent in the Van Hove-Kondo case. Despite the Kondo singlet ground state, the impurities contribute to total entropy and magnetization by affecting the available excited states, and below a critical temperature for any finite density of impurities these contributions dominate over those of the clean host, leading to hitherto unrecognized instabilities. An especially intriguing instability occurs in the case of a particle-hole asymmetric singularity, such as the one recently observed in $Sr_3Ru_2O_7$ [1]. In such case, despite complete Kondo screening of the impurities, the host becomes magnetically unstable due to their presence, which leads to a ferromagnetic ground state. We comment on relation to the surface magnetism observed in $Sr_3Ru_2O_7$.

[1] C. A. Marques *et al.*, *Sci. Adv.* **8**, eabo7757 (2022).

TT 94.3 Fri 10:00 HSZ/0101

Crystal structure, electronic structure and magnetism in the binary compounds Cr_3S_4 and Cr_3Se_4 — •Helge Rosner[1], Seojin Kim[1], Yurii Prots[1], Vincent Morando[2], Oksana Zaharko[2], Jörg Sichelschmidt[1], Marcus Schmidt[1], and Michael Baenitz[1] — [1]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany — [2]Laboratory for Neutron Scattering and Imaging, 5232 Villigen PSI, Switzerland

Cr_3X_4 (X = S, Se) crystallises in a monoclinic lattice, structurally closely related to the rhombohedral chalcogenite delafossite-like systems $AgCrX_2$. In contrast to these intrinsically semiconducting materials with a nonmagnetic monovalent cation site, in Cr_3X_4 the distorted triangular CrX_2 layers are separated by a formally trivalent and magnetic ion. In consequence, the interlayer distance is strongly reduced, making the system more three dimensional, and thus strongly increasing the magnetic ordering temperature. Here, we present a joint experimental and theoretical study of the binary material Cr_3X_4, including thermodynamic measurements, high resolution XRD, neutron scattering and density functional band structure calculations. Our data consistently demonstrate that the metallic systems undergo an antiferromagnetic ordering up to 160 K which is strongly coupled to the crystal lattice. The band structure calculations show that the conduction bands originate from strongly hybridised Cr-X states with sizeable spin-orbit interaction. In a detailed comparison, we will highlight similarities and differences between Cr_3X_4 and the chalcogenite delafossites, including samples with mixed occupation on the X site.

TT 94.4 Fri 10:15 HSZ/0101

Magnetic vector phases induced by spin-nematicity in high magnetic fields for two anisotropic quasi-1D chain compounds — •Stefan-Ludwig Drechsler[1], Lorenz Wolfram[1], Rössler Ulrich[1], Kuzian Roman[2], Klingeler Rüdiger[3], Skourskii Yurii[4], Zoghlin Eli[5], Wolter-Giraud Anja[1], Büchner Bernd[1], and Nishimoto Satoshi[1,6] — [1]IFW-Dresden, Germany —

[2]DIPC, San Sebastian, Spain — [3]Heidelberg University, Germ. — [4]HLD-EMFL, Dresden, Germ. — [5]Oak-Ridge, USA — [6]TU-Dresden

We report and analyze pulsed high-field data near quasi saturation and low-T thermodynamic ones for Li_2CuO_2 up to 60 T and reanalyze the organic ladder compound verdazyl β-2,3,5 (V) measured at stationary fields below 12 T [1] exhibiting both cusps in the magnetic susceptibilities χ at low-T pointing to field induced magnetic vector phases due to the presence of spin nematicity according to a scenario proposed in [2] making visible the otherwise difficult to detect tensorial nematic order parameter. The symmetric and/or antisymm. spin symmetry as well as a subtile interplay of ferromagnetic (FM) and anti-FM couplings are essential for the appearance of 2-magnon bound states supported by the XYZ magnetism observed for Li_2CuO_2 and the low-symmetry crystalline structure for V, resp. For the former we report specific heat data at ambient field pointing possibly to the onset of a Bose condensation below 1 K of 3-magnon bound states as suggested in [3].

[1] H. Yamaguchi *et al.*, J. Phys. Soc. Jpn. **87**, 043701 (2018).
[2] A. Smerald *et al.*, Phys. Rev. B **91**, 174402 (2015).
[3] C. Agrapidis *et al.*, Phys. Rev. Res. **7**, 043051 (2025).

TT 94.5 Fri 10:30 HSZ/0101

Spins in Rotation: Probing anisotropy in $YbAlO_3$ — •Lipsa Behera[1,2], Javier Landaeta[2], Konstantin Semeniuk[2], and Elena Hassinger[3] — [1]Dresden University of Technology, Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids — [3]Karlsruhe Institute of Technology

$YbAlO_3$ is an example of a quasi-one-dimensional S=1/2 spin-chain system with weak Ising-like interchain coupling. It has an interesting phase diagram for H//a with an anti-ferromagnetic order below 0.9 K, a field induced longitudinal spin-density wave phase, and a transverse anti-ferromagnetic state. It enters the field polarized state at 1.15 K. Here we present magnetic AC susceptibility measurements performed under rotation at 25 mK to study how sample misalignment influences the phase diagram and critical fields. We find that rotating towards the c-axis leaves the overall phases unchanged, with only the critical fields shifting to higher values. Rotation towards the b-axis, on the other hand produces some interesting results. A splitting of the susceptibility maxima (corresponding to the transition to the fully polarized state) is observed. This suggests the presence of two independent sublattices. Some critical fields move to lower values indicating more stability in the transverse direction. These results hold the potential to highlight intriguing quasi-1D physics.

15 min. break

TT 94.6 Fri 11:00 HSZ/0101

Magnetic characterization of the spin-ladder magnet $Bi_2CuO_3(SO_4)$ — •Rodolfo A. Rangel Hernandez[1], Alexander A. Tsirlin[1], Victoria Ginga[1], Kirill Povarov[2], and Sergey Zvyagin[2] — [1]University of Leipzig, Leipzig, Germany — [2]Helmholtz-Zentrum, Dresden-Rossendorf, Dresden, Germany

We present the first comprehensive magnetic characterization of $Bi_2CuO_3(SO_4)$, a spin-ladder magnet with ferromagnetic rungs and antiferromagnetic legs. Heat-capacity, susceptibility and magnetization measurements reveal characteristic signatures of a gapped low-dimensional quantum magnet. Ab initio DFT+U calculations, together with a Wannier-function analysis and quantum Monte Carlo (QMC) simulations, are used to describe the magnetism of the ladder. By fitting the experimental susceptibility with QMC, we estimate a spin-gap of $\Delta \approx$ 20 K and the leading exchange couplings to be $J' \approx$ -208 K (rung) and $J \approx 243$ K (leg). Additionally, electron spin resonance confirms an extrinsic nature of the susceptibility upturn at low temperatures. Our result establishes $Bi_2CuO_3(SO_4)$ as a new realization of a spin-ladder with ferro- and antiferromagnetic interactions and provide reliable microscopic parameters for future research.

TT 94.7 Fri 11:15 HSZ/0101

Symmetry-Protected Topological Phase Diagrams of Dimerized Heisenberg Ladders — Tim Obrock and •Anas Abdelwahab — Leibniz Universität Hannover, Institute für Theoretische Physik, Hannover, Germany

We present symmetry-protected topological phase diagrams of unfrustrated dimerized spin-$\frac{1}{2}$ ladders with perpendicular ($J_\perp$) and diagonal (J_d) rung couplings, studied as a function of dimerization (δ) and inter-wire coupling strength. For two perpendicularly coupled wires, our results reproduce the established picture from previous studies: antiferromagnetic rungs yield a trivial spin-0 phase, while ferromagnetic rungs drive the system into the Haldane symmetry-protected topological phase at small $|\delta|$, with critical lines converging to the dimerized spin-1 chain limit for $J_\perp \ll -1$.

For three perpendicularly coupled wires, earlier work has shown that antiferromagnetic rungs drive a transition from trivial ($\delta > 0$) to Haldane ($\delta < 0$). Under ferromagnetic rungs, the system approaches the dimerized spin-$\frac{3}{2}$ chain limit for $J_\perp \ll -1$, exhibiting a sequence of trivial*Haldane*trivial*Haldane phases as δ evolves from 1 to -1.

Extending beyond these previous studies, we analyze the case of two and three diagonally coupled wires. For two wires, antiferromagnetic rungs produce a Haldane region bounded by $|\delta| \approx J_d/2$, containing the exact spin-1 chain limit at $J_d = 1$ and $\delta = 0$, while ferromagnetic rungs keep the system trivial. For three diagonally coupled wires, our results reveal a phase diagram with trivial and topological phases but without an apparent spin-chain limit.

TT 94.8 Fri 11:30 HSZ/0101

Self-consistent mean-field theory and continuous unitary transformations for ordered quantum antiferromagnets with long-range interactions — •Maximilian Bayer[1], Dag-Björn Hering[2], Vanessa Sulaiman[2], Götz Uhrig[2], and Kai Schmidt[1] — [1]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Condensed Matter Theory, Technische Universität, Dortmund, Germany

We investigate the antiferromagnetic Heisenberg model on a square lattice in the presence of algebraically decaying long-range interaction. The model is first studied using a fully self-consistent mean-field treatment going beyond linear spin-wave theory. We discuss the challenges and solutions to obtain numerical results of these long-range interacting systems using functional self-consistency equations familiar to the superconducting gap equation and a parametrisation using Epstein-zeta functions to capture the long-range behaviour without truncation in the system size. In a next step we go beyond the mean-field level and apply continuous similarity transformations (CST) in momentum space. The associated flow equations are truncated in the scaling dimension to capture consistently quantum fluctuations in the ordered phase in the same manner as for the case of nearest-neighbor interactions [1]. Our aim is to understand the one-magnon dispersion at low and high energies including the fate of the characteristic roton minimum.

[1] M. Powalski, G.S. Uhrig, K.P. Schmidt, PRL 115, 207202 (2015)

TT 94.9 Fri 11:45 HSZ/0101

Electric-field-driven flat band in a distorted generalized sawtooth chain — •Vadim Ohanyan[1,2], Lusik Amiraghyan[1,3], Michael Sekania[4,5], and Marcus Kollar[6] — [1]Laboratory of Theoretical Physics, Yerevan State University, 1 Alex Manoogian, 0025 Yerevan, Armenia — [2]CANDLE, Synchrotron Research Institute, 31 Acharyan Str., 0040 Yerevan, Armenia — [3]Institute of Applied Problems of Physics, 25 Hr. Nersisyan St, Yerevan 0014, Armenia — [4]Rechenzentrum, University of Augsburg, 86135 Augsburg, Germany — [5]Andronikashvili Institute of Physics, Javakhishvili Tbilisi State University, Tamarashvili str. 6, 0177 Tbilisi, Georgia — [6]Theoretical Physics III, Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

We investigate flat magnon bands in a sawtooth chain where symmetric exchange, DM interaction, and axial anisotropy differ on each side of the triangular plaquette. When the DM terms arises from the Katsura-Nagaosa-Balatsky (KNB) magnetoelectric mechanism, the corresponding DM coefficients become functions of the electric field and the lattice geometry. This dependence is governed by two bond angles, which become inequivalent under a distortion of the triangular plaquette. We derive the conditions under which an electric field, aligned along the lattice bonds, drives the one-magnon spectrum into a flat-band regime. The distortion angle dependence of the saturation field is examined as well. We construct a mapping from flat-band solution obtained for a general DM interaction into those arising from its KNB-induced form.

TT 95: Fe-based Superconductors

Time: Friday 9:30–11:45 Location: HSZ/0103

TT 95.1 Fri 9:30 HSZ/0103

Saddle-point-nesting driven formation of charge order and superconducting vortex splitting on heavily hole-doped iron-arsenide superconductors — •Chi Ming Yim — Tsung-Dao Lee Institute & School of Physics and Astronomy, Shanghai Jiao Tong University, Shanghai, China

The study of iron-arsenide superconductor $Ba_{1-x}K_xFe_2As_2$ (BKFA) has resparked considerable interest following the recent discoveries in this material of superconductivity with broken time-reversal symmetry [1], superconducting vortices with fractional flux quantum [2], and quartic states [3]. Most studies focus on its bulk properties, with much less attention paid to its surface(s). This talk reports on our recent STM/S findings on the surfaces of BKFA in its heavily-hole doped regime: On the As- surface of BKFA (x=0.77), we observe of a density wave order with a 2x2 spatial periodicity, with clear-cut evidence(s) confirming its charge origin. Our calculation results indicate that its formation is

saddle-point nesting driven. [4]. On the K- surface of multiband superconductor KFe_2As_2 studied under an external magnetic field, we observe splitting of vortices with integer flux quantum into those with appreciably reduced conductance, demonstrating the possibility of vortex core fractionalization in a multiband superconductor [5].

[1] Grinenko et al., Nat. Phys. 17, 1254 (2021)
[2] Iguchi et al., Science 380, 1244 (2023)
[3] Shipulin et al., Nat. Commun. 14, 6734 (2023)
[4] Hu et al., Nat. Commun. 18, 253 (2025)
[5] Zheng et al., Arxiv 2407.18610 (2024)

TT 95.2 Fri 9:45 HSZ/0103

Measuring Nematic Fluctuations in FeSe under Hydrostatic and Chemical Pressure — •Adrian Merritt[1], Amir Haghighirad[2], Dmitry Reznik[3], Ayman Said[4], Ahmet Alatas[4], Alexei Bosak[5], Michaela Souliou[2,5], and Frank Weber[2] — [1]Karlsruher Institut für Technologie - PHI, 76049 Karlsruhe, Germany — [2]Karlsruher Institut für Technologie - IQMT, 76344 Eggenstein-Leopoldshafen, Germany — [3]University of Colorado, 80309, Boulder, Colorado, USA — [4]Advanced Photon Source, Argonne National Laboratory, 60439, Illinois, USA — [5]European Synchrotron Radiation Facility (ESRF), 38043 Grenoble, France

Nematic correlations in iron-based superconductors have been widely studied through phonon softening measured by INS and IXS. Softening of the transverse acoustic phonons near the tetragonal-orthorhombic transition reflects growing nematic fluctuations, which also appear near the superconducting transition, highlighting the competition between nematicity and superconductivity. Our earlier IXS work on FeSe and Co-doped Ba122 showed similar behavior with and without magnetism and across the superconducting transition, suggesting that nematicity may hinder superconductivity.

Our most recent FeSe studies examine the effects of pressure, using both hydrostatic pressure and isoelectronic chemical pressure via S substitution. Both methods introduce magnetic phases and modify the structural transition order, opening a rich, otherwise inaccessible phase diagram. We present these results and compare how nematic fluctuations evolve across the different pressure-induced phases of FeSe.

TT 95.3 Fri 10:00 HSZ/0103

Magnetic-field-induced Sarma state in atomically thin superconducting FeSe films — •Wantong Huang[1,2], Yuguo Yin[1], Haicheng Lin[1], Wei Chen[1], Yaowu Liu[1], Lichen Ji[1], Zichun Zhang[1], Xinyu Zhou[1], Xusheng Wang[1], Yong Xu[1], Lianyi He[1], Xi Chen[1], Qi-Kun Xue[1], and Shuai-Hua Ji[1] — [1]State Key Laboratory of Low-Dimensional Quantum Physics, Department of Physics, Tsinghua University, Beijing 100084, China — [2]Physikalisches Institut (PHI), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Many-body ground states of imbalanced Fermi gas have long been studied both theoretically and experimentally due to their fundamental significance in condensed matter physics, cold atom physics and nuclear physics. Among the predicted exotic phases, the Sarma state, a gapless spin-polarized superfluid, has remained experimentally elusive. Here, we report direct evidence for the Sarma state in atomically thin FeSe films using a dilution-refrigerator scanning tunneling microscope under high magnetic fields. In the bilayer and trilayer FeSe films, we observe the hallmark signature of the Sarma state: the inner Zeeman splitting coherence peaks cross the Fermi level under high in-plane magnetic fields. The angle dependent critical field exhibits a two-fold symmetry arisng from the anisotropic in-plane g-factor. Moreover, our two-band model shows that the magnetic field induced Sarma phase emerges via a first-order transition at zero temperature, which evolves into a smooth crossover at finite temperature. These findings pave the way to explore the unusual physical properties and potential applications of the spin-polarized Sarma superfluid state.

TT 95.4 Fri 10:15 HSZ/0103

Coupling of Vortex Bound States as a Probe of Majorana Physics in Iron-Based Superconductors — •Raigo Nagashima[1], Iksu Jang[1], and Jörg Schmalian[1,2] — [1]Institute for Theoretical Condensed Matter Physics, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany

Motivated by the widespread observation of zero or near-zero vortex bound states on the surfaces of $FeSe_{1-x}Te_x$ and related iron-based superconductors, we investigate how these states evolve and interact as the magnetic-field-induced vortex density increases. Such coupling effects provide a powerful diagnostic of the underlying nature of the bound states. We compare the behavior expected for conventional Caroli-de Gennes-Matricon (CdGM) vortex states with that arising from Majorana zero modes in two-dimensional topological superconductors. To this end, we analyze the multi-vortex problem in the Fu-Kane model and compute the resulting hybridized bound-state wave functions. Our results reveal striking and qualitative differences between the coupling patterns of CdGM states and those of Majorana modes, demonstrating that the field-induced evolution of vortex bound states offers a clear and experimentally accessible fingerprint for identifying Majorana physics in iron-based superconductors.

TT 95.5 Fri 10:30 HSZ/0103

Intertwined superconductivity and orbital selectivity in a three-orbital Hubbard model for the iron pnictides — Vito Marino[1,2], Alberto Scazzola[2], Federico Becca[3], Massimo Capone[1], and •Luca F. Tocchio[2] — [1]International School for Advanced Studies (SISSA), Trieste, Italy — [2]Politecnico di Torino, Italy — [3]University of Trieste, Italy

We study a three-orbital Hubbard-Kanamori model relevant for iron-based superconductors, using variational wave functions which explicitly include spatial correlations and electron pairing. We span the nonmagnetic sector from filling $n = 4$, which is representative of undoped iron-based superconductors, to $n = 3$, where a Mott insulating state with each orbital at half filling is found. In the strong-coupling regime, we observe spontaneous differentiation in the occupation of the d_{xz} and d_{yz} orbitals, leading to an orbital-selective state with nematic character that becomes stronger with increasing density. One of these orbitals remains half-filled for all densities, while the other hosts (together with the d_{xy} orbital) the excess electron density. Most importantly, in this regime, long-range pairing correlations appear in the orbital with the largest occupation. Our results highlight a strong link between orbital-selective correlations, nematicity, and superconductivity, which requires the presence of a significant Hund's coupling. The interplay with magnetism is also discussed.

[1] V. Marino, A. Scazzola, F. Becca, M. Capone, and L.F. Tocchio, PRL 134, 196502 (2025).

15 min. break

TT 95.6 Fri 11:00 HSZ/0103

Predicting isostructural collapses in the $ThCr_2Si_2$ structure type - fast and efficient — •Adrian Valadkhani[1], Paul Canfield[2], and Roser Valentí[1] — [1]Goethe Universität ITP, Frankfurt am Main, Germany — [2]Ames National Laboratory, Ames, USA

Isostructural collapse transitions in tetragonal $ThCr_2Si_2$(122) compounds strongly affect magnetism, topology, and superconductivity, yet most studies treat materials on a case-by-case basis, making the overall approach computationally inefficient. Here, we present a general, efficient framework to predict isostructural collapses across the 122 family - readily extensible to other structure types. We classify collapsibility from the ambient-pressure unit cell using a linear, supervised classifier. In addition, an ambient-pressure calibration of the density-functional-theory-based calculations anchored to the experimental structure determines both the form of collapse and the critical pressure, if it exists. We validate the method against literature data and recent work on $SrCo2P_2$, and we show how the same calibration subsequently enables efficient exploration of the pressure-dependent electronic structure. Because the procedure requires minimal experimental input and fast, efficient and standard computations, it is directly transferable to other structure families where isostructural transitions or distortions occur. This establishes a practical route for screening and designing materials with collapse-tunable functionalities.

We acknowledge support by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) for funding through TRR 288 - 422213477 (project A05)

TT 95.7 Fri 11:15 HSZ/0103

Inelastic neutron scattering study of magnetic fluctuations in iron germanides YFe_2Ge_2 and $LuFe_2Ge_2$ — •Ran Tao[1], Jiasheng Chen[1], Stephen Hodgson[1], Philipp Niklowitz[2], Malte Grosche[1], Travis Williams[3], David Voneshen[3], Devashibhai Adroja[3], Paul Steffens[4], Alexandre Ivanov[4], and Andrea Piovano[4] — [1]Cavendish Laboratory, University of Cambridge, UK — [2]Department of Physics, Royal Holloway, University of London, UK — [3]ISIS Neutron and Muon Source, Rutherford Appleton Laboratory, UK — [4]Insitut Laue-Langevin, Grenoble, France

The iron-based superconductor YFe_2Ge_2 ($T_c \simeq 1.8$ K) exhibits strong electronic correlations [1,2], and a prior neutron scattering study has demonstrated enhanced magnetic fluctuations [3]. The isoelectronic and isostructural sister compound $LuFe_2Ge_2$ orders antiferromagnetically with $Q_F = (0, 0, 1)$ below $T_N \simeq 6.5$ K, and in clean crystals shows a resistive superconducting transition below 1 K.

Our inelastic neutron scattering experiments in YFe_2Ge_2 indicate that the dynamic response near Q_F deviates from the commonly assumed overdamped oscillator form and could instead best be fitted with an underdamped form. A similar response is also seen in the sister compound $LuFe_2Ge_2$ in the paramagnetic phase. The similarities between the two materials suggest that resonant spin fluctuations may be a more general feature in iron germanides.

[1] J. Chen et al., Phys. Rev. Lett. **125,** 237002 (2020).
[2] J. Baglo et al., Phys. Rev. Lett. **129,** 046402 (2022).
[3] H. Wo et al., Phys. Rev. Lett. **122,** 217003 (2019).

TT 95.8 Fri 11:30 HSZ/0103

Local-moment magnetism in Mn-based pnictides — •Matteo Crispino[1], Niklas Witt[1], Tommaso Gorni[2], Giorgio Sangiovanni[1], and Luca de' Medici[2] — [1]Institut für Theoretische Physik und Astrophysik and Würzburg-

Dresden Cluster of Excellence ct.qmat, Universität Würzburg, 97074 Würzburg, Germany — [2]LPEM, ESPCI Paris, PSL Research University, CNRS, Sorbonne Université, 75005 Paris, France

We report a comprehensive study of electronic-correlation effects in Manganese-based antiferromagnetic pnictides $BaMn_2Pn_2$ (Pn=P,As,Sb,Bi). Our density functional theory plus slave-spin mean-field simulations indicate that all the compounds lie on the strong-coupling side of an itinerant-to-localized moment crossover, corresponding to the critical interaction strength for the Mott transition in the high-temperature paramagnetic phase. We also show that the experimental Néel temperature of each compound scales with the distance from this crossover.

TT 96: 2D Materials: Stacking and heterostructures (joint session O/HL/TT)

Time: Friday 9:30–12:30 Location: HSZ/0401

TT 96.1 Fri 9:30 HSZ/0401

A new fabrication method for metal intercalated epitaxial graphene devices — •Marc Bothe[1], Stefan Wundrack[1,2], Marcelo Jaime[1], Klaus Pierz[1], Frank Hohls[1], Rainer Stosch[1], Hans Werner Schumacher[1], Andrey Bakin[2], and Teresa Tschirner[1] — [1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany — [2]Institut für Halbleitertechnik, TU Braunschweig, Hans-Sommer-Str. 66, 38106 Braunschweig, Germany

Epitaxial graphene grown on silicon carbide is a promising platform to achieve metal intercalation. It enables the creation of two-dimensional metal layers that are encapsulated and protected by graphene. However, the use of metal intercalated graphene samples for lithographic device fabrication presents two critical challenges. First, solvents used in the lithography process lead to the deintercalation of the metal atoms. Second, the presence of lattice defects in the graphene - necessary for the intercalation process - compromises the structural and electronic integrity of the device. We present a novel fabrication method that solves these problems. In our approach, the graphene devices are first pre-structured using lithography and subsequently intercalated. This is made possible by a spatial separation on the sample between the device structures and the intercalation origin and by intercalation channels that can guide the intercalation front reliably to the devices. We demonstrate this method on gallium intercalated epitaxial graphene Hall bars that exhibit superconducting behaviour.

TT 96.2 Fri 9:45 HSZ/0401

Anisotropic Strain Observation in Naturally Occurring Buckling on Twisted Bilayer Graphene: A Nano-Raman Study — •Gustavo Soares[1], Rafael R. Barreto[1], Rafael Nadas[1], Kenji Watanabe[2], Takashi Taniguchi[2], Leonardo C. Campos[1], Luiz G. Cancado[1], and Angelo Malachias[1] — [1]Physics Department, Federal University of Minas Gerais, Belo Horizonte, Minas Gerais, 31270-901, Brazil — [2]National Institute for Materials Science, Tsukuba, Ibaraki, 3050047, Japan

This work investigates naturally occurring buckling and its relation with anisotropic strain relaxation in twisted bilayer graphene (tBG). In the tBG system a twist angle is imposed to influence graphene structural and electronic properties. Such condition directly implies in the occurrence of biaxial in-plane strain, with usual observation of buckled/wrinkled localized regions where the tBG morphology is no longer planar. Using tip-enhanced Raman spectroscopy, we conducted high-resolution mapping to analyze variations in Raman bands associated with twist angle variation and strain effects. Our findings reveal that localized strain gradients, modulated by twist angle variations, induce deterministic buckling in graphene layers, evidencing distinct uniaxial and biaxial strain regions. Finite element modeling further supports these observations, showing that buckling can store elastic energy sufficient to overcome usual tBG-substrate adhesion forces.

TT 96.3 Fri 10:00 HSZ/0401

Kirkendall Voids in Monolayer $Mo_xTa_yS_2$ Alloys on Au(111) — Kai Mehlich[1], Thais Chagas[1], Francis H. Davies[2,3], Alessia Bardazzi[1], Catherine Grover[1], Arkady V. Krasheninnikov[3], and •Carsten Busse[1] — [1]Department Physik, Universität Siegen, Walter-Flex-Straße 3, 57072 Siegen, Germany — [2]Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [3]Department of Physics and Astronomy, University of Exeter, Stocker Road, Exeter, EX4 4QL United Kingdom

During the growth of monolayer MoS_2-TaS_2 heterostructures, we observe the Kirkendall effect: Diffusing vacancies agglomerate in MoS_2, forming what are commonly termed Kirkendall voids - here manifesting as holes in the 2D layer. This phenomenon has not been previously reported in systems with reduced dimensionality.

We prepare the lateral heterostructures by reactive molecular beam epitaxy on chemically inert and weakly interacting Au(111). First, compact MoS_2 cores are grown. In a second step, TaS_2 is added in a sulfur-rich environment at elevated temperatures which promotes diffusion at the interface. The resulting heterostructures exhibit characteristic 2D Kirkendall holes surrounded by a $Mo_xTa_yS_2$ alloy region. These findings reveal defect-mediated processes in low-dimensional systems and open new avenues for designing 2D lateral heterostructures with intricate morphologies.

TT 96.4 Fri 10:15 HSZ/0401

Designing 2D Non-van der Waals Heterostructures — •Anastasiia Nihei[1,2], Tom Barnowsky[1,2], and Rico Friedrich[1,2] — [1]TU Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf

Heterostructure interfaces created by stacking two-dimensional (2D) materials offer a pathway to realizing advanced electronic and magnetic functionalities at the nanoscale. In this work, we present a high-throughput screening of non-van der Waals (non-vdW) 2D heterostructures; including sandwich-like stacking. Non-van der Waals 2D materials can be obtained by both top-down exfoliation as well as bottom-up growth approaches of non-layered bulk crystals [1]. Our approach uses the AFLOW-Hetbuilder - a newly developed tool for stacking 2D systems based on the coincidence lattice algorithm [2-4].

We investigate interfacial binding effects across a wide range of heterobilayers [5] and sandwich-like systems, analyzing their structural, electronic, and magnetic characteristics such as hybrid interface bands and robust magnetic coupling. Furthermore, we compare the binding energetics of non-vdW and conventional vdW heterostructures. The tunable interfacial properties of non-vdW 2D heterostructures provide a versatile platform for advanced functionalities with potential applications in electronics, spintronics, and the energy sector [5].

[1] R. Friedrich *et al.*, Nano Lett. **22**, 989, (2022).
[2] D.S. Koda *et al.*, J. Phys. Chem. C **120**, 10895, (2016).
[3] https://zenodo.org/record/4721346 .
[4] S. Divilov *et al.*, High Entropy Alloys Mater. **3**, 178 (2025).
[5] A. Nihei, *et al.*, arXiv DOI: 10.48550/arXiv.2503.12209 (2025).

TT 96.5 Fri 10:30 HSZ/0401

Second-Order Nonlinear Imaging for Probing 2D van der Waals Structures — •Tao Yang[1], Ben John[1], Kyoung P. Lee[2], Nasim Mirzajani[1], Martin Wolf[1], Xiaoqin Li[2], Martin Thaemer[1], Alexandar Paarmann[1], Niclas S. Mueller[3], and Alexander P. Fellows[1] — [1]Fritz Haber Institute, Berlin, Germany — [2]University of Texas at Austin, Austin, USA — [3]Freie Universitaet Berlin, Berlin, Germany

Twisted and stacked multi-layer architectures offer new opportunities for tailoring the electronic and optical properties of two-dimensional (2D) van der Waals materials. Reliable determination of crystal structure, stacking sequence, and twist angle is therefore crucial. Second-order nonlinear optical microscopy, including second-harmonic and sum-frequency generation (SHG and SFG, respectively), provides high sensitivity to crystal symmetry and orientation in non-centrosymmetric lattices. Recently, we employed heterodyne-detected vibrational SFG microscopy to probe the local structure of hexagonal Boron Nitride (hBN) monolayers with sub-micron resolution. By employing our developed azimuthal-scanning approach, we fully resolved the crystallographic structure and edge termination in monolayer flakes. Here, we extend these measurements to multi-layer hBN structures, using the same azimuthal-scanning approach in a newly developed SHG microscope to gain insight into their different stacking configurations. Our results highlight second-order nonlinear microscopy as a powerful tool for quantitative structural analysis in 2D materials and for future studies of moiré and twisted heterostructures.

TT 96.6 Fri 10:45 HSZ/0401

Moiré-Driven Electronic Modulations in Weakly Coupled h-BN/Graphite — •Fábio J. R. Costa[1,2,7], Daniel Arribas[2], Thiago G. L. Brito[2], Tin S. Cheng[3], Jonathan Bradford[3], Amelia Thompson[3], Alex Saywell[3], Christopher J. Mellor[3], Peter H. Beton[3], Sergey V. Novikov[3], Juliette Plo[4], Bernard Gil[4], Guillaume Cassabois[4,5], Luiz F. Zagonel[1], Klaus Kuhnke[2], Klaus Kern[2,6], and Anna Rosławska[2] — [1]University of Campinas, Brazil — [2]Max-Planck-Institut für Festkörperforschung, Germany — [3]University of Nottingham, UK — [4]Laboratoire Charles Coulomb, France — [5]Institut Universitaire de France, France — [6]EPFL, Lausanne, Switzerland — [7]Current address: Université de Strasbourg, CNRS, IPCMS, Strasbourg, France

Van der Waals materials and their heterostructures offer exciting opportunities for next-generation nanophotonic and electronic technologies. Their electronic and optical properties can be modulated by moiré superlattices that emerge when mismatched layers are stacked together. Hexagonal boron nitride (h-BN) is a key platform in this context, yet the influence of moiré patterns on weakly interacting h-BN interfaces remains underexplored. Here[1], we use scanning tunneling mi-

croscopy to resolve large moiré superlattices in h-BN/graphite and uncover pronounced nanoscale modulations of the electronic landscape, despite their weak interlayer interactions. These findings position moiré engineering in h-BN as a powerful tool to tailor local functionalities in van der Waals heterostructures. Ref.: 1. Fábio J. R. Costa *et al.* ACS Nano 2025 19 (40), 35528-35538

TT 96.7 Fri 11:00 HSZ/0401

μ-ARPES study on the fine electronic structure of misfit layer compound (PbSe)1.16(TiSe2)2 — •Haruki Muramatsu[1], Natsuki Mitsuishi[2,3], Teppei Ueno[4], Kenichi Ozawa[5], Kaya Kobayashi[4,6], and Kyoko Ishizaka[1,2] — [1]Dept. of Appl. Phys. & QPEC, Univ. of Tokyo — [2]CEMS, RIKEN — [3]Grad. Sch. Sci., Nagoya Univ. — [4]Dept. of Physics, Okayama Univ. — [5]KEK-PF — [6]RIES, Hokkaido Univ.

Misfit layered compounds have been attracting significant attention due to their lattice mismatches and resultant two-dimensional electronic structures reminiscent of van der Waals heterostructures. One such compound, (PbSe)1.16(TiSe2)2, consists of alternating stacking of PbSe monolayers (NaCl-type, four-fold symmetry) and TiSe2 bilayers (CdI2-type, three-fold symmetry). To elucidate its electronic structure, we performed μ-ARPES measurements by carefully distinguishing the cleavage surface terminations. In the presentation, we will discuss the novel electronic states reflecting the natural incommensurate heterostructure as well as charge density wave in the buried TiSe2 bilayer.

TT 96.8 Fri 11:15 HSZ/0401

Twisted $NbSe_2$ heterostructures — •Alexander Bäder[1,2], Clara Pfister[3,4], Tobias Wichmann[1,5], Laura Pätzold[3,4], Tim O. Wehling[3,4], and Felix Lüpke[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich — [2]II. Physikalisches Institut, Universität zu Köln — [3]I. Institute of Theoretical Physics, U Hamburg — [4]The Hamburg Centre for Ultrafast Imaging — [5]Institut für Experimentalphysik IV A, RWTH Aachen

We fabricated monolayers (MLs) of the van der Waals material $NbSe_2$ that are rotated with respect to the underlying bulk $NbSe_2$ using our developed ultra-high vacuum (UHV) stacking technique. These heterostructures were characterized through the use of scanning tunneling microscopy and spectroscopy at a base temperature of 1.4 K. The MLs realize a variety of twist angles relative to the underlying bulk lattice, with the lowest observed twist angle being 10°. The MLs display the coexistence of charge density waves (CDW) and moiré effects: In the absence of strain, the MLs develop a 3×3 CDW, however the application of strain through interfacial disorder results in a 2×2 CDW state, supported by theoretical calculations. Compared to isolated MLs the superconducting order parameter is enhanced due to the proximity effect from the underlying bulk.

TT 96.9 Fri 11:30 HSZ/0401

band structure and charge density wave in a natural van der Waals heterostructure 4Hb-TaSe2 — •Fumihiko Kimura[1], Tomoki Maeda[2], Natsuki Mitsuishi[3,4], Kazuki Okada[2], Takuya Nomoto[5], Kenichi Ozawa[6], Masahiro Naritsuka[3], Tetsuo Hanaguri[3], Shunsuke Kitou[7], Yuiga Nakamura[8], Taka-hisa Arima[3,7], Takao Sasagawa[2], and Kyoko Ishizaka[1,3] — [1]Quantum-Phase Electronics Center & Department of Applied Physics, The University of Tokyo — [2]Laboratory for Materials and Structures, Science Tokyo — [3]RIKEN CEMS — [4]Graduate School of Science, Nagoya University — [5]Department of Physics, Tokyo Metropolitan University — [6]Institute of Materials Structure Science, High energy Accelerator Research Organization (KEK) — [7]Department of Advanced Materials Science, The University of Tokyo — [8]Japan Synchrotron Radiation Research Institute (JASRI), SPring-8

4Hb-TaSe2 is a natural van der Waals heterostructure charge density wave (CDW) material consisting of alternative stacking of monolayer 1T-TaSe2 (Mott insulator with Star-of-David CDW) and monolayer 2H-TaSe2 (superconductor with 3 by 3 CDW). Although transport measurements have suggested the existence of multiple CDWs, the details of the CDW and electronic structures remain unclear. In this study, we directly observed the electronic structure of 4Hb-TaSe2 by micro-focused angle-resolved photoemission spectroscopy with careful selection of the surface terminations. We discuss the temperature dependent electronic structure with comparison to the CDW structures obtained by scanning tunneling microscopy and X-ray diffraction.

TT 96.10 Fri 11:45 HSZ/0401

Coexisting charge density waves in twisted NbSe2 bilayers — •Christopher Tat Shun Cheung[1], Zachary A. H. Goodwin[2], Yixuan Han[3], Jiong Lu[3], Arash A. Mostofi[1], and Johannes Lischner[1] — [1]Departments of Physics and Materials and the Thomas Young Center for Theory and Simulation of Materials, Imperial College London, London SW7 2AZ, U.K. — [2]Institute for Functional Intelligent Materials, National University of Singapore, Singapore 117544, Singapore — [3]Department of Materials, University of Oxford, Parks Road, Oxford OX1 3PH, United Kingdom

Twisted bilayers of semiconducting transition metal dichalcogenide (TMD) monolayers have been studied extensively. In contrast, twisted bilayers composed of metallic monolayers, such as NbSe2, remain less understood.

Monolayer NbSe2 can host different types of charge density waves (CDWs), in which the Nb atoms move away from their high-symmetry positions. In twisted bilayer NbSe2, identifying CDWs in relaxed structures is challenging because atomic relaxations occur both because of CDW formation and also because of the moiré pattern.

We have carried out large-scale first-principles calculations using density functional theory to study the moiré relaxations and CDWs in twisted bilayer NbSe2. We have developed methods for revealing the CDWs, and for locally classifying the type of CDW. We find that different types of CDWs coexist in the moiré unit cell due to the interactions with strain induced by moiré relaxations [1].

[1] Cheung et al, Nano Lett. 2024, 24, 12088-12094.

TT 96.11 Fri 12:00 HSZ/0401

MicroARPES studies of contact doping of monolayer transition metal dichalcogenides by RuCl3 — •Thomas Nielsen[1], Edvard Solbrekken[1], Alfred J. H. Jones[1], Zhihao Zhiang[1], Chakradar Sahoo[1], Kenji Watanabe[2], Takashi Taniguchi[2], Jill A. Miwa[1], Søren Ulstrup[1], Christian Overby[1], and Christian V-B. Fokdal[1] — [1]Aarhus University, Denmark — [2]National Institute for Materials Science, Japan

Placing van der Waals materials into contact with α-$RuCl_3$ has recently emerged as a method of modulating their electronic structures. The proximity to α-$RuCl_3$ has been observed to produce strong hole doping in the van der Waals material, and this has been established as a method to create better electrical contacts in transistor devices based on monolayer transition metal dichalcogenides (TMDs). Here, we use the microARPES endstation at the ASTRID2 synchrotron light source at Aarhus University in Denmark to study the valence bands and core levels of semiconducting monolayer TMDs in proximity to α-$RuCl_3$. We observe a large valence-band shift of 0.7 – 0.8eV indicating strong hole doping. α-$RuCl_3$ is highly sensitive to the temperatures and chemicals typically used in the dry-transfer fabrication procedures of van der Waals heterostructures. How the degradation of α-$RuCl_3$ affects the proximity-induced doping of the TMD is discussed based on the ARPES measurements.

TT 96.12 Fri 12:15 HSZ/0401

STEM Investigation of Entropy Forbidden Ordering in CVD Grown WSe_2-$MoSe_2$ Alloys — •Max Bergmann[1], Matvei Kislitsyn[1], Julian Picker[2], Jürgen Belz[1], Robin Günkel[1], Badrosadat Ojaghi Dogahe[1], Shamail Ahmed[1], Andrey Turchanin[2], and Kerstin Volz[1] — [1]mar.quest | Marburg Center for Quantum Materials and Sustainable Technologies, Philipps-Universität Marburg, 35032 Marburg, Germany — [2]Faculty of Chemistry and Earth Sciences, Friedrich-Schiller-Universität, 07743 Jena, Germany

2D transition metal dichalcogenides have gained significant interest due to their optoelectronic properties, which can be tailored by structural variation. However, controllable production, namely growth, of such tailored structures still remains a key challenge towards large-scale production. In this study, we show lateral heterostructures of 2D $MoSe_2$ and WSe_2, grown on a SiO_2 TEM grid by chemical vapor deposition, that at the interface show a highly ordered structure of W and Mo atoms at the TMD positions, as observed by scanning transmission electron microscopy. This is in contrast to *ab initio* calculations, which ascribe unordered alloys as the preferred configuration, since entropy is the main driving force compared to formation enthalpy. We link this unexpected phenomenon to the initial nucleation of the material on a clean $MoSe_2$ crystal edge, present before the alloy growth, together with special precursor chemistry. Furthermore, we show *ab initio* results in conjunction with the special quasirandom structure method on the bandstructure and optical properties of this structure.

TT 97: Superconducting Diodes and Ratchets

Time: Friday 9:30–12:00 Location: CHE/0089

TT 97.1 Fri 9:30 CHE/0089

Josephson Diode Effect of All-Metallic Lateral Junctions with Interfacial Rashba Spin-Orbit Coupling — •Maximilian Mangold[1,2], Lorenz Bauriedl[3], Johanna Berger[3], Chang Yu-Cheng[4], Thomas N.G. Meier[1,2], Matthias Kronseder[3], Pertti Hakonen[5], Christian H. Back[1,2], Christoph Strunk[3], and Dhavala Suri[1,6] — [1]School of Natural Sciences, Technical University of Munich, Garching, Germany — [2]Center for Quantum Engineering (ZQE), Technical University of Munich, Garching, Germany — [3]Department of Physics, University of Regensburg, Regensburg, Germany — [4]Pico Group, QTF Centre of Excellence, Department of Applied Physics, Aalto University, Aalto, Finland — [5]Low Temperature Laboratory, Department of Applied Physics, Aalto University, Espoo, Finland — [6]Centre for Nanoscience and Engineering, Indian Institute of Science, Bengaluru, India

The Josephson diode effect (JDE) is investigated in diffusive Josephson junctions incorporating only metallic materials. We find a magneto-chiral anisotropy in the JDE for devices with Fe/Pt and Cu/Pt weak links between Nb leads. The observed symmetry corresponds to Rashba spin-orbit coupling (SOC). In a simple Cu junction without a structural inversion asymmetry, the diode efficiency is finite, but field-angle independent. Our results suggest the generality of Rashba SOC for the JDE beyond the realm of high-mobility systems. Additionally, we observe an inverted hysteresis in the Fraunhofer patterns of all samples and explain it based on the critical state model of strongly pinned vortices without relying on SOC.

TT 97.2 Fri 9:45 CHE/0089

Giant anomalous Josephson effect as a probe of spin texture in topological insulators — Niklas Hüttner[1], Andreas Costa[1], Leandro Tosi[2], Michael Barth[1], Wolfgang Himmler[1], Dmitriy A. Kozlov[1], Leonid Golub[1], Klaus Richter[1], Jaroslav Fabian[1], Dieter Weiss[1], Christoph Strunk[1], and •Nicola Paradiso[1] — [1]University of Regensburg, Germany — [2]Grupo de Circuitos Cuánticos, Bariloche, Argentina

Topological-insulator surface states are chiral 2D electron systems with spin-momentum locking. Josephson junctions based on such states show nonreciprocal supercurrent features if time reversal symmetry is broken. For example, they show a finite phase at zero current, i.e., an anomalous Josepshon effect. I will present φ_0 measurements on junctions with HgTe nanowires as weak link. We detect an exceptionally large anomalous phase shift in the current-phase relation. We attribute this giant φ_0-shift to the single Fermi-surface contour of HgTe surface states, a key distinction from Rashba systems with two counteracting Fermi contours. By rotating the in-plane magnetic field, we probe the spin texture in momentum space. Interestingly, we find that the spin deviates by 19 degrees from the orientation perpendicular to the momentum. Our findings demonstrate that the anomalous Josephson effect provides a powerful and sensitive probe of the spin texture in chiral two-dimensional systems.

TT 97.3 Fri 10:00 CHE/0089

Josephson diode effect in superconducting hybrids with altermagnets — •Janus F. Niebuhr, Danilo Nikolić, and Matthias Eschrig — Institut für Physik, Universität Greifswald, Felix-Hausdorff-Straße 6, 17489 Greifswald

We present a systematic theoretical study of a ballistic Josephson junction consisting of a d-wave altermagnet (AM) placed between two conventional superconducting leads (S). The study is done by making use of the quasiclassical Green's function method considering two regimes of (i) a weakly and (ii) a strongly spin polarized altermagnet. The former regime in the limit of highly transmissive S/AM interfaces allows for an analytic treatment. The resulting Josephson current-phase relation (CPR) exhibits $0-\pi$ transitions. These significantly depend on the altermagnet's crystal orientation relative to the junction's axis by the display of a dominant second harmonic close to the transition. In the regime of strong spin polarization, the altermagnet is coupled to the superconductors via two spin-dependent interfaces, necessary for the creation of equal-spin triplets, which now entirely mediate the current. For a non-coplanar magnetization profile, a quantum-geometric phase emerges. This phase is coupled to spin and enters the Josephson CPR similarly to the phase difference. Consequently, depending on the altermagnetic crystal orientation, the CPR displays an anomalous Josephson effect, as well as a Josephson diode effect. Finally, we perform a harmonic analysis of the CPR discussing the effects in terms of the number of coherently transferred Cooper pairs across the altermagnet.

TT 97.4 Fri 10:15 CHE/0089

Field-Free Superconducting Diode and Topological FFLO States in Altermagnetic Shiba Chains — •Dibyendu Samanta and Sudeep Kumar Ghosh — Indian Institute of Technology, Kanpur 208016, India

The superconducting diode effect (SDE), characterized by a directional asymmetry in the critical supercurrents, typically requires external magnetic fields to break time-reversal symmetry-posing challenges for device integration. Here, we demonstrate a field-free realization of the SDE in a helical Shiba chain proximitized by a d-wave altermagnet. Using a self-consistent Bogoliubov-de Gennes approach, we uncover a topological Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) superconducting state hosting tunable Majorana zero modes at the chain ends. This state, stabilized by the interplay between the exchange coupling of magnetic adatoms and the induced altermagnetic spin splitting, can be tuned by an applied supercurrent. Crucially, the same FFLO phase supports strong nonreciprocal supercurrents, achieving diode efficiencies exceeding 45% without applied magnetic fields. The d-wave altermagnet simultaneously breaks time-reversal and inversion symmetries via momentum-dependent spin splitting, enabling both topological superconductivity and the field-free SDE in a junction-free setting. Our findings establish Shiba chain-altermagnet heterostructures as a scalable platform for supercurrent-tunable topological superconductivity and intrinsic, field-free superconducting diodes for dissipationless quantum technologies.

TT 97.5 Fri 10:30 CHE/0089

Current pulse manipulation of the superconducting diode effect in FeSe — •Roemer Hinlopen[1], Linus Holeschovsky[1], Rebecca Nicholls[2], Nigel Hussey[2,3], Carsten Putzke[1], and Philip Moll[1] — [1]Max Planck Institute for Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]University of Bristol, HH Wills Laboratory, Tyndall Avenue, BS8 1TL Bristol, UK — [3]High Field Magnet Laboratory (HFML-FELIX) and Institute for Molecules and Materials, Radboud University, Nijmegen 6525ED, Netherlands

The superconducting diode effect (SDE) has seen a surge in popularity in recent years for its potential technological applications. However, switching the sign of the SDE usually relies on reversing the polarity of the applied magnetic field on specifically designed device architectures which break the necessary symmetries. In this talk, we present a new means of control for the intrinsic SDE through microsecond current pulsing. We use focused ion beam (FIB) machining to create single crystalline devices of the strongly correlated nematic superconductor FeSe. We observe a clear intrinsic diode effect with effiency up to 30 %, which remains observable to a record applied magnetic field of 12 T. Our central result is that by sending intense microsecond current pulses through the device, we can deterministically manipulate the sign and strength of this SDE. This finding opens a new channel to control the SDE in devices and potentially realise a zero-field switchable device in the future.

15 min. break

TT 97.6 Fri 11:00 CHE/0089

Nonreciprocal Magnon Fluxonics — •Oleksandr Dobrovolskiy — Cryogenic Quantum Electronics, EMG and LENA, Technische Universität Braunschweig, Braunschweig, Germany

Fluxon dynamics controls the magneto-resistive response of superconductors (S) and becomes nonreciprocal under symmetry break [1]. Magnons - the quanta of spin waves in magnetic materials - are attracting increasing attention as information carriers [2]. In my talk, I will introduce magnon fluxonics as a subdomain of superconducting spintronics. I will discuss nonreciprocal spin-wave dynamics in dipole-coupled superconductor/ferromagnet heterostructures, focusing on two effects. (i) Within the "ratchet window", the application of an AC current to S enables magnon bandgap tuning during one half-wave, while the bandgap frequencies remain constant during the other. This effect arises from the Doppler shift and the nonlinear spin-wave dispersion. (ii) At higher velocities, on the order of a few km/s, the moving vortex lattice excites magnons unidirectionally along the direction of vortex motion. This regime occurs when the wavevector (momentum) and frequency (energy) of the magnons match those of the fluxons, thereby fulfilling the Cherenkov resonance condition [3]. These results demonstrate how the well-studied superconducting diode or ratchet effects can enrich other research areas and enable new functionalities of nonreciprocal steering and unidirectional generation of spin waves.

[1] Kochan & Strunk, Nat. Electr. 8 (2025) 380.
[2] Chumak et al., IEEE Trans. Magnet. 58 (2022) 0800172.
[3] Dobrovolskiy et al., Nat. Nanotechnol. (2025).
https://doi.org/10.1038/s41565-025-02024-w.

TT 97.7 Fri 11:15 CHE/0089

Spin-wave-induced giant ratchet effect in superconductor-ferromagnet heterostructures — •Anton Pokusinskyi and Oleksandr Dobrovolskiy — Cryogenic Quantum Electronics, EMG and LENA, Technische Universität Braunschweig, Germany

Superconducting vortex ratchets enable directed motion of magnetic flux quanta under zero time-average forces and thus act as rectifiers in superconducting circuits. Recent diode realizations exploiting asymmetric edge barriers in superconducting NbN and V/EuS microstructures have achieved ratchet efficiencies of 35-50% [1-3]. However, their tunability remains limited by fixed geome-

tries or magnetic-field reversal, constraining scalability and dynamic control. Here, we theoretically predict a tunable giant ratchet effect in superconductor-ferromagnet heterostructures, arising from the coupling between moving fluxons and spin waves—collective precessions of spins in the ferromagnetic layer. Our modeling, based on time-dependent Ginzburg-Landau simulations under the experimental conditions of [4], demonstrates that spin-wave excitation enables dynamic control of vortex motion, offering a pathway toward reconfigurable superconducting ratchets and fluxonic devices.

[1] Ingla-Aynes et al., Nat. Electron. 8 (2025) 411
[2] Castellani et al., Nat. Electron. 8 (2025) 417
[3] Porrati et al., Small Methods e01430 (2025)
[4] Dobrovolskiy et al., Nat. Nanotechnol. (2025). https://doi.org/10.1038/s41565-025-02024-w.

TT 97.8 Fri 11:30 CHE/0089

Tunable Nonreciprocity in 3D Superconductor Nanoarchitectures — •Igor Bogush and Oleksandr Dobrovolskiy — Cryogenic Quantum Electronics, EMG and LENA, Technische Universität Braunschweig, Germany

Nonreciprocity lies at the heart of superconducting diodes and ratchets, key elements for designing low-dissipative computing devices [1]. However, achieving precise control over the directionality and strength of nonreciprocity is challenging, as it requires local tuning of superconductor properties or applied stimuli. Here, we show that the geometry of curved thin superconductor membranes introduces a new degree of freedom, enabling vortex-motion synchronization [2] and nonreciprocity tunable via the magnetic field direction. In such membranes, only the component of the magnetic field normal to the surface exerts a driving Lorentz force on vortices, while the tangential component is less relevant. Using a conformal approach for time-dependent Ginzburg-Landau simulations [3], we predict that in cap-shaped superconductor membranes, the magnetic field induces effective pinning whose location can be controlled by adjusting the field direction. Even without a pinning potential, this controllable symmetry breaking induces nonreciprocal vortex dynamics and vortex ratchet behavior. These results highlight the geometry in thin curved membranes as a parameter that enhances the tunability of superconducting phenomena in rectifiers and other fluxonic devices.

[1] Plourde, IEEE Trans. Appl. Supercond. 19 (2009) 3698
[2] Bogush et al., Phys. Rev. B 111 (2025) 214510
[3] Bogush et al., Comp. Phys. Comm. 315 (2025) 109736

TT 97.9 Fri 11:45 CHE/0089

Steering of Vortex Jets in Anisotropic Pinning Fields — •Ekaterina Pribytova[1] and Oleksandr Dobrovolskiy[2] — [1]Brno University of Technology, Czechia — [2]Technische Universität Braunschweig, Germany

Understanding how Abrikosov vortices penetrate and move in superconductor films is crucial for fluxonics, which treats vortices as quantized information bits. So far, vortex steering was achieved for their global dynamics across the entire superconductor constriction. Here, we take a different approach of local vortex dynamics [1]: vortices are injected via an edge defect (notch) and guided through a washboard pinning potential (WPP). The resulting arrangement of vortices is a diverging jet rather than a periodic lattice. Numerical modeling via the time-dependent Ginzburg-Landau equation [2] reveals that vortex jets can be focused, deflected, and directed toward given points along the edge opposite to the notch. The underlying vortex steering mechanism is based on the competing vortex-vortex, vortex-current, and vortex-pinning interactions [1]. In return, beyond their potential for fluxonic logic gates, steered vortex jets offer a tool for probing these interactions. Specifically, the vortex jet's opening angle estimates the magnetic penetration depth, while its deflection from the current-normal direction reveals the WPP strength. These results demonstrate the predictive power of TDGL modeling for nanoengineered fluxonic circuits and complement the analytical and experimental results.

[1] Bezuglyj et al., Phys. Rev. B 105 (2022) 214507.
[2] Bishop-Van Horn, Comput. Phys. Commun. 291 (2023) 108799.

TT 98: Altermagnets

Time: Friday 9:30–11:45 Location: CHE/0091

TT 98.1 Fri 9:30 CHE/0091

Low-energy magnons in the altermagnet α-MnTe — •Kirill Povarov[1], J. Wosnitza[1,2], Sahana Rössler[3], Marcus Schmidt[4], Alexander Tsirlin[3], and Sergei Zvyagin[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL) and Würzburg-Dresden Cluster of Excellence ct.qmat, HZDR, Dresden — [2]Institut für Festkörper- und Materialphysik, TU Dresden — [3]Felix Bloch Institute for Solid State Physics, University of Leipzig — [4]Max Planck Institute for Chemical Physics of Solids, Dresden

We report high-field electron spin resonance studies of the altermagnetic material α-MnTe in magnetic fields applied parallel to the triangular Mn^{2+} layers. We observe a single antiferromagnetic resonance (AFMR) mode, displaying isotropic behavior with $g \simeq 2.01$; very close to the free-electron value. At low temperatures the AFMR mode is remarkably sharp, but exhibits a noticeable broadening upon warming indicating the effect of magnon-magnon interactions. Based on this behavior, we estimate the strength of these interactions.

This work was supported by the DFG through the Würzburg-Dresden Cluster of Excellence on Complexity and Topology in Quantum Matter - *ct.qmat* (EXC 2147, project No. 390858490), as well as by HLD at HZDR, member of the European Magnetic Field Laboratory (EMFL).

TT 98.2 Fri 9:45 CHE/0091

Tuning the heavy fermion altermagnet candidate Ce_4Sb_3 by hydrostatic pressure — •Julian Kaiser[1], Bin Shen[1], Franziska Walther[2], Kristin Kliemt[2], Cornelius Krellner[2], Anton Jesche[1], and Philipp Gegenwart[1] — [1]EP VI, EKM, University of Augsburg, Germany — [2]Physikalisches Institut, Goethe-Universität Frankfurt, Frankfurt am Main, Germany

Altermagnets have recently attracted significant attention because they have features of both ferromagnets and antiferromagnets in a novel symmetry framework, giving rise to unconventional electronic and spin-transport phenomena previously believed to be absent in traditional collinear antiferromagnets. The heavy-fermion compound Ce_4Sb_3 has been proposed as an altermagnetic candidate with nontrivial band topology [1], making it an ideal platform for investigating the interplay among magnetism, band topology, and the Kondo effect. To probe this interplay, we performed magnetization measurements under hydrostatic pressure and established a preliminary pressure-temperature phase diagram. Our results reveal that the magnetic order in Ce_4Sb_3 is highly sensitive to pressure and can be gradually suppressed. These findings identify Ce_4Sb_3 as a tunable altermagnetic candidate in which the balance between the Kondo effect and the RKKY interaction, and thus the magnetic order, can be effectively controlled by pressure.

[1] X. He and S. Zhang, Phys. Rev. B **112**, 075138 (2025)

TT 98.3 Fri 10:00 CHE/0091

Effect of pressure on the electronic properties of the Kagome flat band metal $CsCr_3Sb_5$ — •Maria Chatzieleftheriou[1,2], Jonas B. Profe[1], Ying Li[3], and Roser Valentí[1] — [1]Institute for Theoretical Physics, Goethe University Frankfurt, Max-von-Laue-Straße 1, 60438 Frankfurt a.M., Germany — [2]CNRS, CPHT, Ecole polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France — [3]MOE Key Laboratory for Nonequilibrium Synthesis and Modulation of Condensed Matter, School of Physics, Xi'an Jiaotong University, Xi'an 710049, China

$CsCr_3Sb_5$ is a novel type of strongly correlated Kagome superconductor. The material shows non-Fermi liquid like behavior at high temperatures, indicating strong correlations and has an intertwined charge and spin density wave ordering below T 54K. Under external pressure, this order is suppressed and a superconducting phase emerges. This phase diagram in combination with a Kagome flat band near the Fermi-level and potential altermagnetic orders has led to a plethora of theoretical and experimental studies. In this work, we perform a systematic analysis of the changes of the electronic properties induced by pressure. To this end we employ DFT+DMFT calculations revealing a complex interplay of the position of the flat bands and the strength of correlations. Our results support the predominant interpretation that pressure effectively reduces the strength of correlations by stronger hybridization between the orbitals. This finding strongly suggests that the superconducting order is emerging due to short range fluctuations present in the system once the ordered state is suppressed sufficiently.

TT 98.4 Fri 10:15 CHE/0091

Alterelectrics: The Electric Counterpart of Altermagnets — •Viktor Könye[1], Amber Visser[1], Oleg Janson[2], Jeroen van den Brink[2], Corentin Coulais[1], and Jasper van Wezel[1] — [1]University of Amsterdam — [2]IFW Dresden

Altermagnets are a new class of materials that mix features of both ferromagnets and antiferromagnets. They have spin-split bands like ferromagnets but still show no net magnetization. Their underlying symmetries also lead to unusual effects, such as a strong piezomagnetic effect and hyperbolic wave dispersion. This raises an important question: which of these behaviors actually come from magnetism, and which are simply a result of symmetry? In this work, we separate these two aspects by proposing a non-magnetic analogue of an altermagnet, built from polarized chains. These "alterelectrics" show anisotropic piezoelectricity and surface states with hyperbolic wave dispersion, demonstrated through a simple model. Instead of spin-split bands, the electronic states localize on opposite surfaces, producing strongly anisotropic, surface-dependent transport.

TT 98.5 Fri 10:30 CHE/0091

Crossed surface flat bands in three-dimensional superconducting altermagnets — Yuri Fukaya[1], Bo Lu[2], Keiji Yada[3], Yukio Tanaka[3], and •Jorge Cayao[4] — [1]Faculty of Environmental Life, Natural Science and Technology, Okayama University, 700-8530 Okayama, Japan — [2]Department of Physics, Tianjin University, 300354 Tianjin, China — [3]Department of Applied Physics, Nagoya University, 464-8603 Nagoya, Japan — [4]Department of Physics and Astronomy, Uppsala University, Box 516, S-751 20 Uppsala, Sweden

Superconducting altermagnets have proven to be a promising ground for emergent phenomena but their study has involved two dimensional systems. Here, we investigate three-dimensional d- and g-wave altermagnets with chiral d-wave superconductivity and show the formation of crossed surface flat bands due to the underlying symmetries. We find that these crossed flat bands appear at zero energy in the surface along z due to the superconducting nodal lines in the xy-plane, while the number of corners is determined by the crystal symmetry of altermagnets. We also show that the superconducting nodal lines give rise to Bogoliubov-Fermi surfaces, which then affect the appearance of zero-energy arcs in the surface along x. Moreover, we demonstrate that the crossed surface flat bands, surface arcs, and Bogoliubov-Fermi surfaces give rise to distinct signals in charge conductance, hence offering a solid way for their detection and paving the way for realizing higher dimensional topological phases using altermagnets.

15 min. break

TT 98.6 Fri 11:00 CHE/0091

Strongly disordered superconductor-altermagnet heterostructures — •Christian Wiedemann[1], Danilo Nikolić[2], Matthias Eschrig[2], and Wolfgang Belzig[1] — [1]Universität Konstanz, Konstanz, Germany — [2]Universität Greifswald, Greifswald, Germany

Similarly to ferromagnets and antiferromagnets previously [1,2], proximity systems involving superconductors (S) and a recently found class of d-wave magnetic materials known as altermagnets (AM) [3] represent promising platforms for both understanding and applications in superconducting spintronics [4]. Introducing nonmagnetic impurities to systems where superconductivity and altermagnetism coexist can reduce the effect of the altermagnetic exchange field on the critical temperature of the superconductor [5]. We investigate the interplay between the anisotropic altermagnetic influence and the isotropization caused by impurity scattering and its effect on superconductivity in an S/AM bilayer. In particular, we compute the order parameter and the free energy using the quasiclassical Green's function formalism to find stable superconducting states with a special focus on the regime of high impurity concentrations and strong altermagnetic exchange fields.

[1] A. I. Buzidn, Rev. Mod. Phys. **77**, 935 (2005)
[2] M. Eschrig, Rep. Prog. Phys. **78**, 104501 (2015)
[3] L. Šmejkal *et al*, Phys. Rev. X **12**, 040501 (2022)
[4] S. Chourasia *et al*, Phys. Rev. B **111**, 224503 (2025)
[5] M.M. Vasiakin & A.S. Mel'nikov, PRB, **111**, L100502 (2025)

TT 98.7 Fri 11:15 CHE/0091

Nonlinear Sigma Model of an Insulating Altermagnet — •Parasar Thulasiram[1,2], Chris Hooley[3], and Roderich Moessner[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [3]Centre for Fluid and Complex Systems, Coventry University, Coventry, United Kingdom

We applied the Haldane map to derive an O(3) x O(3) nonlinear sigma model of an insulating altermagnet from a transition-metal-dichalcogenide-inspired 3D spin model. The model displays nonrelativistic spin splitting of the magnon bands and anisotropic couplings. We studied the energetics of its preferred topological defects (skyrmions and hopfions), their viability in being generated, as well as the model's behaviour under lightly frustrated couplings. We performed a renormalization analysis of the model and studied its (in)stabilities.

TT 98.8 Fri 11:30 CHE/0091

Projectively implemented altermagnetism in an exactly solvable quantum spin liquid — •Avedis Neehus[1,2], Achim Rosch[3], Johannes Knolle[1,2,4], and Urban Seifert[3] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany — [3]Blackett Laboratory, Imperial College London, London SW7 2AZ, United Kingdom — [4]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany

Altermagnets are a new class of symmetry-compensated magnets with large spin splittings. Here, we show that the notion of altermagnetism extends beyond the realm of Landau-type order: we study exactly solvable $\mathbb{Z}_2$ quantum spin(-orbital) liquids (QSL), which simultaneously support magnetic long-range order as well as fractionalization and $\mathbb{Z}_2$ topological order. Our symmetry analysis reveals that in this model three distinct types of "fractionalized altermagnets (AM^*)" may emerge, which can be distinguished by their residual symmetries. Importantly, the fractionalized excitations of these states carry an emergent $\mathbb{Z}_2$ gauge charge, which implies that they transform *projectively* under symmetry operations. Consequently, we show that "altermagnetic spin splittings" are now encoded in a momentum-dependent particle-hole asymmetry of the fermionic parton bands. We discuss consequences for experimental observables such as dynamical spin structure factors and (nonlinear) thermal and spin transport.

TT 99: Quantum Chaos and Coherent Dynamics (joint session DY/TT)

Time: Friday 9:30–12:45 Location: HÜL/S186

TT 99.1 Fri 9:30 HÜL/S186

Time reversal invariance breaking in quantum chaotic scattering — •Ahmed Aldabag, Nils Gluth, and Thomas Guhr — Universität Duisburg Essen

A. Aldabag, N. Gluth and T. Guhr, Universität Duisburg-Essen

Scattering theory is a key tool for the investigation of quantum systems. Often, the systems are stochastic or in a broad sense chaotic. Using Random Matrix Theory, our group recently derived the distributions of off-diagonal scattering matrix elements and cross sections with the Supersymmetry Method. We did that for the three Dyson classes which are distinguished by the presence or absence of time-reversal invariance in the system. In some important physics situations, time-reversal invariance is weakly broken. We succeeded in analytically calculating the corresponding effects on the universal behavior of the mentioned distributions. Our results provide new tools to analyze time-reversal invariance breaking in data from scattering experiments.

TT 99.2 Fri 9:45 HÜL/S186

Normalization of resonance states in chaotic scattering systems — •Florian Lorenz, Jan Möseritz-Schmidt, and Roland Ketzmerick — TU Dresden, Institut für Theoretische Physik, Dresden, Germany

The normalization of resonance states in scattering systems poses a challenge due to their divergent asymptotic behavior. As a consequence, they cannot be normalized by the usual norm, but instead, by the overlap between left and right resonance states. For dielectric cavities, we demonstrate that this left-right overlap can be computed efficiently using a boundary integral, avoiding divergent integrands. This result provides a practical numerical tool for resonance state normalization. For example, this allows for exact time evolution of wave packets based on resonance states.

TT 99.3 Fri 10:00 HÜL/S186

How exceptional points conduct mode dynamics in optical microcavities — Tom Simon Rodemund[1], Chang-Hwan Yi[2], Jung-Wan Ryu[2], Síle Nic Chormaic[3], and •Martina Hentschel[1] — [1]Institut für Physik, TU Chemnitz, Germany — [2]PCS, IBS, Daejeon, Korea — [3]OIST, Okinawa, Japan

Optical microcavities confine light through total internal reflection, making them inherently open, non-Hermitian systems. Their resonances have a real and an imaginary part, both of which depend on external parameters such as the resonator geometry or the refractive index. When scanning the parameter space, resonances can coincide and when they do so in their real and imaginary part, they form an exceptional point. We illustrate their occurrence and consequences in mesoscopic optics in two examples. First, we consider two coupled two-dimensional microcavities over coupling distances of several resonance wavelengths. Their mode dynamics is determined by a chain of exceptional points that exhibit a periodicity of approximately the wavelength [1]. The second example is a three-dimensional truncated cone. We investigate the interaction between the two mode polarizations, TE and TM, and find that the mode character changes smoothly, with TE and TM coinciding at exceptional points [2]. We confirm this behavior in phase space by generalizing the concept of Husimi functions to three dimensions. [1] C.-H. Yi, J.-W. Ryu, T.S. Rodemund, and M. Hentschel, Phys. Rev. A 112, L031501 (2025). [2] T.S. Rodemund, S. Li, S. Nic Chormaic, and M. Hentschel, Phys. Rev. A 112, 033528 (2025).

TT 99.4 Fri 10:15 HÜL/S186

Describing the spectral behavior around higher-order exceptional points with "periodic orbits" — •Daniel Grom[1], Julius Kullig[1], Malte Röntgen[2], and Jan Wiersig[1] — [1]Institut für Physik, Otto-von-Guericke-Universität Magdeburg, 39016 Magdeburg, Germany — [2]Laboratoire d'Acoustique de l'Université du Mans, 72085 Le Mans, France

Coupled optical microrings can deliver a simple and robust scheme to generate higher-order exceptional points (EPs), where multiple eigen-values and -modes coalesce. A feature of an EP of order n, is the high sensitivity of the eigenvalues to small perturbations. Two types of perturbations can be classified. The generic behavior, where the eigenvalue response is proportional to the nth root and the non-generic type with a different eigenvalue response.

We present a graph theoretical perspective on the spectral characterization of perturbed higher-order EPs. It turns out that specific "periodic orbits" within the graph picture of the non-chaotic system govern the eigenvalue behavior.

TT 99.5 Fri 10:30 HÜL/S186

Dynamic origin of quantum chaos signatures in the zeros of the Riemann zeta function by means of periodic orbit theory — •Andreas Hötzinger, Sebastian Hörhold, Juan Diego Urbina, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, Germany

In the 90's, Berry and Keating [1] provided a qualitative, semiclassical analogy to the counting function of the nontrivial Riemann zeros, i.e. the zeros of the famous zeta function (ZF) $\zeta(s)$. Similar to Gutzwiller's trace formula they obtain a result in which the primes play the role of periodic orbits and argue that the so-called Riemann dynamics, underlying the primes, should be chaotic. It is speculated that this system is the classical limit of a Hermitian quantum Hamiltonian which has eigenvalues coinciding with the nontrivial zeros of $\zeta(1/2+\mathrm{i}t_n)$.

Recently, a promising candidate for such a Hamiltonian has been proposed [2], which has the potential to advance research toward a proof of the Riemann hypothesis. Based on these results, we use a related and simpler, yet non-Hermitian Hamiltonian and consider its semiclassical regime by employing methods from periodic orbit theory.

In this talk, we present our progress in the study of the classical limit of this operator and its dynamics in a complexified phase space. Through this, we hope to unveil a deeper relation between quantum chaos signatures of number theory encoded in the ZF with classical phase space structures.

[1] M. V. Berry and J. P. Keating, SIAM Review 41.2 pp. 236-266

[2] E. Yakaboylu, arXiv:2408.15135

TT 99.6 Fri 10:45 HÜL/S186

Semiclassical geometry of entanglement — •Maximilian Kieler and Peter Schlagheck — CESAM research unit, University of Liège, B-4000 Liège, Belgium

We propose a semiclassical perspective on entanglement in the form of a geometric Schmidt decomposition of regular states, e.g., states associated with invariant tori. Utilizing WKB quantization techniques and classical geometry, we derive the Schmidt spectrum and the corresponding Schmidt states. This framework allows for the reduction of the complexity in many-body states by decomposing them into lower-dimensional components.

15 min. break

Invited Talk TT 99.7 Fri 11:15 HÜL/S186

Anyon dynamics in driven topologically ordered quantum systems — •Francesco Petiziol — Technische Universität Berlin, Institut für Physik und Astronomie, Hardenbergstr. 36, 10623 Berlin

Quantum systems with topological order exhibit long-range entanglement and host quasiparticle excitations with unconventional quantum statistics – anyons. These features make them of great interest from both fundamental and quantum-technological perspectives. Recent progress in realizing topological order in quantum simulators highlights the importance and the challenge of understanding the behaviour of such systems under non-equilibrium conditions. Focusing on Kitaev's toric code, I will discuss how external driving, either coherent or incoherent, can impact and alter anyon properties. Examples include the emergence of more complex anyon classes from simpler ones, the dynamics of entanglement under driven anyon proliferation, and opportunities for controlled anyon transport.

TT 99.8 Fri 11:45 HÜL/S186

Floquet engineering in lattice systems with a parametrically modulated parabolic potential — •Usman Ali[1], Martin Holthaus[1], and Torsten Meier[2] — [1]Institut für Physik, Carl von Ossietzky Universität, D-26111 Oldenburg, Germany — [2]Department of Physics, Paderborn University, Warburger Strasse 100, D-33098 Paderborn, Germany

We present a route to Floquet engineering in lattice systems that exploits a parabolic potential to generate tunable slowly varying on-site energies. When a selected level spacing in the spectrum of the combined parabolic lattice is brought into near resonance with an external periodic drive, nonlinear resonances emerge in the classical phase space and reorganize quantum eigenstates into families of near-resonant Floquet states. Using a Mathieu-resonance approximation together with numerical Floquet calculations, we construct these states and demonstrate how resonant trap eigenstates transmute into resonance-induced effective ground states [1]. The long-time population and transport dynamics are strongly sensitive to the initial phase of the drive, providing a phase-dependent control knob for engineered tunneling and coherence. We identify parameter regimes accessible to present-day cold-atom experiments and argue that selectively populating these Floquet ground states provides a clean testbed for driven many-body and Floquet-band phenomena, enabling novel lattice dynamics inaccessible in solid-state materials [2]. References: [1] U. Ali, M. Holthaus, and T. Meier, New J. Phys. 26, 123016 (2024) [2] U. Ali, M. Holthaus, and T. Meier, Phys. Rev. Research 5, 043152 (2023)

TT 99.9 Fri 12:00 HÜL/S186

Transport through two Floquet-engineered Impurities in a One-Dimensional System: Coherent Control of Fano Resonances, BICs and Localization — •Vincenzo Bruno[1,2], Ameneh Sheikhan[1], Roberta Citro[2,3], and Corinna Kollath[1] — [1]Physikalisches Institut, Universität Bonn, Nussallee 12, 53115 Bonn, Germany — [2]Dipartimento di Fisica "E.R. Caianiello", Università degli Studi di Salerno and INFN, Via Giovanni Paolo II, 132, I-84084 Fisciano (Sa), Italy — [3]CNR/SPIN, Fisciano (Sa), 84098, Italy

Floquet engineering has attracted considerable attention due to its ability to coherently control quantum states, finding successful applications across a wide range of fields such as quantum materials, ultracold atoms, and cavity systems. We investigate particle transport through a one-dimensional system containing two periodically driven impurities. Such a configuration is highly relevant for experimental realizations ranging from ballistic semiconductor wires and electron optics to ultracold atoms, and exhibits remarkably rich transmission properties. A central feature of this system is the emergence of Fano resonances-phenomena arising from the quantum interference between a continuum scattering path and discrete quasi-bound states. We demonstrate how drive parameters can be tuned to dynamically control these resonances. Furthermore, we reveal the existence of Bound States in the Continuum (BICs) and explore the interplay between Fano interference and cavity modes. This interplay leads to a localization mechanism where the system can be switched from a fully localized state to a regime of perfect transparency.

TT 99.10 Fri 12:15 HÜL/S186

Ruelle-Pollicott signatures of unitary quantum systems — •Scott Daniel Linz, Jiaozi Wang, Merlin Füllgraf, and Jochen Gemmer — Department of Mathematics/Computer Science/Physics, University of Osnabrück, D-49076 Osnabrück, Germany

Phenomenological observations demonstrate that unitary quantum systems thermalize and equilibrate. While many concepts have been introduced to describe the equilibrium of a quantum system, the route to this state remains an area of ongoing research. A proposed step towards a general description of this behaviour is that correlation functions of chaotic quantum systems can be described by a superposition of relatively few damped oscillations, where each is weighted and assigned a complex frequency. These frequencies will be called Ruelle-Pollicott signatures after the well-understood Ruelle-Pollicott resonances that govern the decay of correlations in classical chaotic systems featuring dissipation. Following this framework, a deterministic fitting method is applied to the correlation functions of numerical simulations of closed unitary quantum systems. This examination will focus on how the number of frequencies needed to reproduce correlation functions relates to other signatures of quantum chaos.

TT 99.11 Fri 12:30 HÜL/S186

Refinements of the Eigenstate Thermalization Hypothesis — •Elisa Vallini[1], Laura Foini[2], and Silvia Pappalardi[1] — [1]University of Cologne, Köln, Germany — [2]Université Paris-Saclay, France

Understanding how isolated quantum many-body systems reach thermal equilibrium is a central question in nonequilibrium physics. The Eigenstate Thermalization Hypothesis (ETH) provides a powerful framework by linking thermalization to the statistical properties of matrix elements of physical observables in the energy eigenbasis.

In this talk, I will present our recent work, in which we revisit and clarify in detail the ideas that have led to the formulation of full ETH, a generalization of the ETH ansatz that captures multi-point correlation functions. Specifically, using tools from free probability, we explore the implications of local rotational invariance, a property that emerges from the statistical invariance of observables under random basis transformations induced by small perturbations of the Hamiltonian.

This approach allows us to analytically characterize subleading corrections to matrix-element correlations, thereby refining the ETH ansatz. Finally, I will show numerical results from non-integrable Floquet systems that support our analytical predictions.

Physics Education Division
Fachverband Didaktik der Physik (DD)

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Übersicht über Hauptvorträge, Fachsitzungen und Workshops

Hörsaal HÜL/S386
Seminarräume SCH/A101, SCH/A284, SCH/A285 und SCH/A252
Poster P5 – ZEU/0250

Plenarvortrag der Didaktik

PLV V	Wed	8:30– 9:15	HSZ/AUDI	**Reimagining Physics Education for a Planet in Transformation** — •Giulia Tasquier

Hauptvorträge

DD 2.1	Mon	9:30–10:30	HÜL/S386	**Zukunft gestalten: Physik als Werkzeug zum Verstehen und Gestalten unserer Umwelt** — •Bianca Watzka
DD 11.1	Tue	9:30–10:30	HÜL/S386	**Lernen mit KI, Lernen über KI: Perspektiven für die Naturwissenschaftsdidaktik** — •Arne Bewersdorff

Kerschensteiner-Preisvortrag

DD 35.1	Wed	9:30–10:30	HÜL/S386	**Die Bonner Physikshow – ein Öffentlichkeitsprojekt mit Studierenden** — •Herbi Dreiner

Tutorial des Fachverbands Didaktik der Physik

DD 1.1	Sun	16:00–18:15	BEY/0137	**Rethinking University Teaching: Creating interactive and sustainable learning environments in lectures** — •Susanne Heinicke, Christian Kautz, Peter Riegler, Claudia Schäfle, Silke Stanzel, Micol Alemani

Workshops im Programm des Fachverbands Didaktik der Physik

DD 18.1	Tue	12:00–13:30	SCH/A284	**Workshop: SDGs nicht nur als Feierabendprogramm – politische Verantwortung im Physikstudium thematisieren** — •Annemarie Sich, Barbara Obwaller, Manuel Längle, Jonathan Möller, Stefan Brackertz

Gemeinsames Symposium zu Nachhaltiger Entwicklung

(siehe SYSC für die vollständige Beschreibung des Symposiums.)

SYSC 1.1	Mon	15:00–15:30	HSZ/AUDI	**Open-Endedness and Community-Based Approaches to Sustainability Challenges** — •Hiroki Sayama
SYSC 1.2	Mon	15:30–16:00	HSZ/AUDI	**Education as a Social Tipping Element: Evidence from Climate and Physics Education Research** — •Thomas Schubatzky
SYSC 1.3	Mon	16:00–16:30	HSZ/AUDI	**Mechanistic and Material Perspectives on Enzymatic Hydrolysis of Semicrystalline Polyesters** — •Birte Höcker
SYSC 1.4	Mon	16:45–17:15	HSZ/AUDI	**Decarbonization Options for Industry** — •Uwe Riedel
SYSC 1.5	Mon	17:15–17:45	HSZ/AUDI	**Impacts of Cosmic Dust and Space Debris in the Terrestrial Atmosphere** — •John Plane

Fachsitzungen

DD 1.1–1.1	Sun	16:00–18:15	BEY/0137	**Tutorial des Fachverbands Didaktik der Physik (joint session DD/TUT)**
DD 2.1–2.1	Mon	9:30–10:30	HÜL/S386	**Eröffnung und Hauptvortrag I**
DD 3.1–3.3	Mon	10:45–11:45	SCH/A101	**Quantenphysik I**
DD 4.1–4.3	Mon	10:45–11:45	SCH/A252	**Digitale Medien I**
DD 5.1–5.3	Mon	10:45–11:45	SCH/A284	**Astronomie, Inklusion und Lernforschung**
DD 6.1–6.3	Mon	10:45–11:45	SCH/A285	**Lehrkräfteaus- und -fortbildung I**
DD 7.1–7.3	Mon	12:00–13:00	SCH/A101	**Quantenphysik II**
DD 8.1–8.3	Mon	12:00–13:00	SCH/A252	**Außerschulische Lernorte I**
DD 9.1–9.3	Mon	12:00–13:00	SCH/A284	**Neue Konzepte I**
DD 10.1–10.3	Mon	12:00–13:00	SCH/A285	**Hochschuldidaktik I**
DD 11.1–11.1	Tue	9:30–10:30	HÜL/S386	**Hauptvortrag II**
DD 12.1–12.3	Tue	10:45–11:45	SCH/A101	**Praktika und Experimente**
DD 13.1–13.3	Tue	10:45–11:45	SCH/A252	**Digitale Medien II**
DD 14.1–14.3	Tue	10:45–11:45	SCH/A284	**Bildung für nachhaltige Entwicklung**
DD 15.1–15.3	Tue	10:45–11:45	SCH/A285	**Interesse I**
DD 16.1–16.3	Tue	12:00–13:00	SCH/A101	**Experimente**
DD 17.1–17.3	Tue	12:00–13:00	SCH/A252	**Außerschulische Lernorte II**
DD 18.1–18.1	Tue	12:00–13:30	SCH/A284	**BNE Workshop**
DD 19.1–19.3	Tue	12:00–13:00	SCH/A285	**Hochschuldidaktik II**
DD 20.1–20.4	Tue	14:00–16:00	P5	**Poster – Lehrkräfteaus- und -fortbildung**
DD 21.1–21.2	Tue	14:00–16:00	P5	**Poster – Außerschulische Lernorte**
DD 22.1–22.2	Tue	14:00–16:00	P5	**Poster – Astronomie**
DD 23.1–23.5	Tue	14:00–16:00	P5	**Poster – Bildung für nachhaltige Entwicklung**
DD 24.1–24.4	Tue	14:00–16:00	P5	**Poster – Digitale Medien**
DD 25.1–25.3	Tue	14:00–16:00	P5	**Poster – Experimente und Praktika**
DD 26.1–26.5	Tue	14:00–16:00	P5	**Poster – Hochschuldidaktik**
DD 27.1–27.8	Tue	14:00–16:00	P5	**Poster – Lehr- und Lernforschung**
DD 28.1–28.4	Tue	14:00–16:00	P5	**Poster – Neue Konzepte**
DD 29.1–29.1	Tue	14:00–16:00	P5	**Poster – Nature of Science**
DD 30.1–30.10	Tue	14:00–16:00	P5	**Poster – Quantenphysik**
DD 31.1–31.1	Tue	14:00–16:00	P5	**Poster – Physikdidaktik und Inklusion**
DD 32.1–32.1	Tue	14:00–16:00	P5	**Poster – Sprache und Physikunterricht**
DD 33.1–33.1	Tue	14:00–16:00	P5	**Poster – Sonstiges**
DD 34	Tue	18:00–20:00	SCH/A101	**Mitgliederversammlung**
DD 35.1–35.1	Wed	9:30–10:30	HÜL/S386	**Kerschensteiner-Preisvortrag**
DD 36.1–36.3	Wed	10:45–11:45	SCH/A101	**Quantenphysik III**
DD 37.1–37.2	Wed	10:45–11:25	SCH/A252	**Lehr- und Lernforschung**
DD 38.1–38.3	Wed	10:45–11:45	SCH/A284	**Nature of Science**
DD 39.1–39.3	Wed	10:45–11:45	SCH/A285	**Interesse II**
DD 40.1–40.2	Wed	12:00–12:40	SCH/A101	**Quantenphysik IV**
DD 41.1–41.3	Wed	12:00–13:00	SCH/A252	**Lehrkräfteaus- und -fortbildung II**
DD 42.1–42.3	Wed	12:00–13:00	SCH/A285	**Neue Konzepte II**
DD 43	Wed	13:00–13:30	SCH/A101	**Abschlussplenum**

Mitgliederversammlung des Fachverbands Didaktik der Physik

Dienstag 18:00–20:00 SCH/A101

- Genehmigung der Tagesordnung
- Genehmigung des Protokolls der MV vom 01.04.2025
- Berichte aus den Arbeitsgruppen
- Termine
- Verschiedenes

Sessions

– Invited Talks, Prize Talks, Tutorials, Contributed Talks, and Posters –

DD 1: Tutorial des Fachverbands Didaktik der Physik (joint session DD/TUT)

Physics teaching at universities can be significantly enriched by moving beyond traditional lecture formats and embracing interactive, learner-centered approaches that foster deep and sustainable understanding. Drawing on successful practices from universities in Germany and abroad, this workshop highlights how insights from learning psychology and proven teaching innovations can be translated into effective physics education. It invites participants to explore how evidence-based, interactive methods can transform learning experiences and support lasting learning outcomes in everyday teaching practice.

Time: Sunday 16:00–18:15 Location: BEY/0137

Tutorial DD 1.1 Sun 16:00 BEY/0137

Rethinking University Teaching: Creating interactive and sustainable learning environments in lectures — •Susanne Heinicke[1], Christian Kautz[2], Peter Riegler[3], Claudia Schäfle[4], Silke Stanzel[4], and Micol Alemani[5] — [1]Institute for Physics Education, University of Muenster — [2]Hamburg University of Technology — [3]Ostfalia University of Applied Sciences — [4]Technische Hochschule Rosenheim — [5]University of Potsdam

The workshop bridges current findings from learning psychology with experience and research findings on practical teaching formats to enhance effective learning in university physics education. We will give an overview of key principles from educational psychology concerning how we learn to provide a foundation for understanding learning effectiveness. Participants will explore and critically reflect on evidence-based interactive methods like peer instruction, interactive formats, and problem-based learning that can be transferred to their own teaching. The workshop concludes with a discussion on implementation strategies and evaluation approaches to support sustainable integration into everyday teaching practice.

DD 2: Eröffnung und Hauptvortrag I

Time: Monday 9:30–10:30 Location: HÜL/S386

Invited Talk DD 2.1 Mon 9:30 HÜL/S386

Zukunft gestalten: Physik als Werkzeug zum Verstehen und Gestalten unserer Umwelt — •Bianca Watzka — RWTH Aachen

Zukunftsperspektiven auf Physikunterricht umfassen weit mehr als den Einsatz neuer Technologien: Sie betreffen auch den Umgang mit Daten in einer Zeit, in der Informationsqualität, wissenschaftliche Evidenz und Faktenorientierung herausgefordert werden. Parallel dazu rücken Fragen von Teilhabe und Mitgestaltung in den Vordergrund und bilden die Basis für eine zentrale Aufgabe des Physikunterrichts: Lernende zu befähigen, Daten kritisch zu interpretieren, Modelle von Meinungen zu unterscheiden und sich aktiv an wissenschaftlich fundierten Aushandlungsprozessen zu beteiligen. Partizipation versteht sich dabei auch naturwissenschaftlich: Wer eigene Daten erhebt, analysiert und in Kontexte einordnet, erfährt wissenschaftliche Teilhabe unmittelbar. Der Vortrag zeigt, wie Physikunterricht solche Lerngelegenheiten schaffen kann. Anhand von Umweltprojekten mit Sensor-Schlüsselanhängern wird demonstriert, wie Lernende reale Daten erfassen, visualisieren und physikalisch interpretieren können. Kontexte wie Temperaturunterschiede auf dem Schulhof ermöglichen niedrigschwellige Zugänge zu BNE-relevanten Fragen und fördern Data Literacy im Alltag. Doch die Förderung von Data Literacy ist anspruchsvoll: Lernende können Daten zwar erheben, haben jedoch häufig Schwierigkeiten, sie zu strukturieren, zu interpretieren und aus Darstellungen wie Graphen sinnvolle Schlüsse zu ziehen. Hier setzt die empirische Forschung zur visuellen Informationsverarbeitung an: Eye-Tracking-Studien machen typische Fehlinterpretationen sichtbar und liefern Ansatzpunkte für Lernhilfen.

DD 3: Quantenphysik I

Time: Monday 10:45–11:45 Location: SCH/A101

DD 3.1 Mon 10:45 SCH/A101

Mathematisches Sense-Making in der Quantenphysik: Ergebnisse aus Interviews mit Lehrkräften und Schüler:innen — •Moritz Förster und Gesche Pospiech — TU Dresden, Professur für Didaktik der Physik

Quantenphysikalische Prinzipien zeichnen sich auf besondere Weise durch die ihnen zugrundeliegenden mathematischen Strukturen aus. Vor diesem Hintergrund scheint es plausibel, dass mathematische Beschreibungen präzise Erklärungen quantenphysikalischer Sachverhalte sowie Problemlösefähigkeiten von Lernenden unterstützen können.

In einer explorativen Interviewstudie wurden leitfaden- und materialgestützte Einzelinterviews mit Lehramtsstudierenden, Lehrkräften und Schüler:innen der gymnasialen Oberstufe geführt. Dabei wurden grundlegende Prinzipien der Quantenphysik am Beispiel der Polarisation von Photonen eingeführt und zwei mathematische Repräsentationen (Ket-Notation und Bloch-Kugel) fokussiert. Analysiert wurden kognitive Ressourcen, welche bei der Erklärung von Konzepten der Quantenphysik und Lösung von Anwendungsaufgaben genutzt wurden, sowie Argumentationsstrukturen und mathematisches Sense-Making.

Die Ergebnisse deuten darauf hin, dass mathematische Strukturen das Sense-Making der Lernenden unterstützen können. Es zeigt sich, dass Lernende dann erfolgreich Anwendungsaufgaben lösen, wenn sie die Beschreibung physikalischer Phänomene mit mathematischen Strukturen verknüpfen. Weiterhin zeigen die Ergebnisse, dass nur wenige Lernende auf rein innermathematische Diskussionen und eine formale Handhabung des Formalismus zurückgreifen.

DD 3.2 Mon 11:05 SCH/A101

Quantum physics knowledge construction with peers in the problems with different mathematical nature — •Nilüfer Didiş Körhasan[1] and Gesche Pospiech[2] — [1]Ereğli Faculty of Education, Zonguldak Bülent Ecevit University, 67300, Zonguldak, Türkiye — [2]Faculty of Physics, TU Dresden, 01187, Dresden, Germany

Considering the relationship between mathematics and physics, the technical function of mathematics in physics refers to approaches that are often superficial, while the structural role of mathematics in physics refers to deeper linkages (Pospiech, 2019). In this research, we investigate students' quantum physics knowledge construction with peers in problems with different mathematical nature. In an undergraduate level quantum theory course, 36 quantum physics problems categorized as having a "structural" or "technical" nature were asked in different subjects. In several sessions through the semester, students answered the questions in two rounds, first individually and then with their self-constructed groups. Students also reflected on their experiences with the mathematical issues in quantum physics problems. Results indicate how the mathematical nature of quantum physics problems was dealt with by peers during the knowledge construction with peers. Acknowledgement: This research is supported by Alexander von Humboldt Foundation. Reference: Pospiech, G. (2019). Framework of mathematization in physics from a teaching perspective. In G. Pospiech, M. Michelini, & B. S. Eylon (Eds.), Mathematics in Physics Education (pp.1-36), (E-book), Springer.

DD 3.3 Mon 11:25 SCH/A101

Development of Quantum Physics Self-Efficacy Scale (QPSES) — •Gesche Pospiech[1] and Nilüfer Didiş Körhasan[2] — [1]Faculty of Physics, TU Dresden, 01187, Dresden, Germany — [2]Ereğli Faculty of Education, Zonguldak Bülent Ecevit University, 67300, Zonguldak, Türkiye

Previous pedagogical research on quantum physics revealed that students have difficulty learning quantum physics concepts. So, there are research-based methodologies and materials assisting students in overcoming these challenges. However, considering the social cognitive theory, beliefs affecting individuals' behavior, actions, effort, persistence to complete a task, and resilience in adverse situations, called self-efficacy (Bandura, 1986), might be critical for achieving successful results in quantum physics learning. We developed a domain specific self-efficacy scale in quantum physics and implemented it to under-graduate level physics, physics engineering, and physics teacher education students. In this study, we present the factors and items of the Quantum Physics Self-Efficacy Scale (QPSES) and preliminary results from the analyses. Acknowledgement: The authors thank Alexander von Humboldt Foundation. Reference: Bandura, A. (1986). Social foundations of thought and action: A social cognitive theory. New Jersey: Prentice-Hall.

DD 4: Digitale Medien I

Time: Monday 10:45–11:45 Location: SCH/A252

DD 4.1 Mon 10:45 SCH/A252

Education-related design principles for a virtual laboratory — •Sascha Grusche, Onur Oenes, and Christina Schindler — Department of Applied Sciences and Mechatronics, Lothstraße 34, 80335 Munich, Germany

A virtual laboratory is a learning platform where students can practice lab processes remotely. With VLabS (Virtual laboratory for semiconductor technology), we address a diverse audience to foster STEM-related interests and skills in line with industry needs. The educational design of VLabS is based on three principles: The principle of sequence aims at guiding students from everyday experience to laboratory experiments. The principle of modularity enables flexible combination of rooms and equipment. The principle of tendency leverages the habit of reading from left to right. For each principle, we show examples from VLabS, including a gallery opposite each lab room.

DD 4.2 Mon 11:05 SCH/A252

PUMA : Optiklabor - die interaktive WebAR-Simulation in der Praxis — •Stefan Kraus und Thomas Trefzger — Julius-Maximilians-Universität, Würzburg, Deutschland

Das PUMA (Physikunterricht mit Augmentierung) Optiklabor stellt eine webbasierte Augmented Reality Umgebung zur Verfügung, die Schülerinnen und Schülern neue Experimentiergelegenheiten jenseits von Realexperiment und Bildschirmsimulation schafft. Als digitales Schülerexperimentierset verwenden die Jugendlichen auf dem Tisch verteilte Papiermarker. Der Blick *durch* Smartphone oder Tablet-PC ergänzt Geräte wie Laser, Kerzen, Schirme usw., die für den Anfangsunterricht der Optik benötigt werden. Mit diesen Gegenständen kann im dreidimensionalen Raum frei experimentiert werden. Dank des browserbasierten Ansatzes entfällt die Notwendigkeit einer Installation, was einen flexiblen Einsatz ermöglicht.

Zum PUMA : Optiklabor wurde eine Studie mit rund 1000 Teilnehmerinnen und Teilnehmern bayerischer Realschulen und Gymnasien durchgeführt. Das Forschungsinteresse lag dabei primär darauf, zu welchen Gelegenheiten eine solche webbasierte Augmented Reality Simulation von Lehrenden wie auch Lernenden eingesetzt wird und für wie sinnvoll der Einsatz von beiden Gruppen eingeschätzt wird. Darüber hinaus wurden in einem Prä- / Postdesign das Fachwissen sowie affektiv-motivationale Faktoren beobachtet und mit einer Kontrollgruppe verglichen. Im Vortrag werden die Ergebnisse der Studie zusammengefasst.

DD 4.3 Mon 11:25 SCH/A252

Digital gestützte Peer-Interaktion in der Sek. 1: Ein quasi-experimenteller Vergleich zum Thema E-Lehre — •Thomas Sean Weatherby und Thomas Wilhelm — Insitut für Didaktik der Physik, Max-von-Laue-Straße 1, 60438 Frankfurt am Main, Germany

In einer quasi-experimentellen Studie wurde untersucht, ob Lerner-Lerner-Gespräche, die durch eine Tablet-App gezielt strukturiert werden, das konzeptuelle Lernen in der E-Lehre in der Sekundarstufe I verbessern. Über insgesamt 12 Unterrichtsstunden wurden zwei Umsetzungsvarianten verglichen: In Experimentalgruppe 1 (EG1) kamen ausschließlich gedruckte Materialien zum Einsatz, die auf dem Elektronengasmodell basierten; die Experimentalgruppe 2 (EG2) arbeitete in denselben Unterrichtssequenz, ergänzt um kollaborative Aufgaben, die durch eine iPad-App unterstützt wurden.

Es ergab sich kein signifikanter Unterschied zwischen den beiden Bedingungen ($N = 228$, $p = 0.08$); die mittlere Veränderung der Testwerte deutet jedoch auf einen höheren Anstieg bei EG1 hin.

Motivationale Analysen auf Basis von Subskalen des Intrinsic Motivation Inventory zeigen für EG2 eine geringere wahrgenommene Kompetenz ($N = 218$, $p = 0.008$) sowie ein reduziertes Interesse daran, über naturwissenschaftliche Inhalte zu reden ($N = 209$, $p = 0.009$).

Im Vortrag werden diese Befunde im Vergleich zu einschlägigen Studien interpretiert und Unterschiede in Thema, Methode und Schulkontext diskutiert, die für die Wirksamkeit (digital geskripteter) Peer-Gespräche bedeutsam sein dürften. Daraus werden Evidenzlücken abgeleitet, die in künftiger Forschung adressiert werden können.

DD 5: Astronomie, Inklusion und Lernforschung

Time: Monday 10:45–11:45 Location: SCH/A284

DD 5.1 Mon 10:45 SCH/A284

Ein taktiler Himmelsglobus für die inklusive astronomische Bildung — •Ekhardt Preuss — Chemnitz

Die Wirksamkeit des inklusiven Unterrichts in der gymnasialen Oberstufe im Fach Astronomie mit blinden und sehenden Lernenden kann durch spezielle Unterrichtsmittel erhöht werden.

Ein Beispiel ist der am Dr.-Wilhelm-André-Gymnasium Chemnitz entwickelte taktile Himmelsglobus.

Der Globus enthält auf seiner von außen und und von innen tastbaren Oberfläche aus verschiedenen Materialien gefertigte, haptisch unterscheidbare und gleichzeitig farblich gekennzeichnete Elemente sowie eine Beschriftung in Punktschrift.

So wird das gemeinsame Lernen von Sehenden und Blinden sowie die Einflussnahme der Lehrperson bei der Orientierung am Sternenhimmel und der Arbeit mit astronomischen Koordinatensystemem ermöglicht.

Die Lagerung der Globenkugel und die tastbare Modellierung des Ortshorizonts machen den Globus zu einem taktilen Planetarium.

DD 5.2 Mon 11:05 SCH/A284

Discoveries about the physics of space flight and time travel — •Hans-Otto Carmesin — Gymn. Athenaeum, Harsefelder Str. 40, 21680 Stade — Studienseminar Stade, Bahnhofstr. 5, 21682 Stade — Universität Bremen, Fachbereich 1, Pf 330440, 28334 Bremen

At the GPS, we realize the importance of synchronized clocks for navigation. Hereby, relativistic time dilation is essential: The context Laser-Ranging leads to the kinematic time dilation. The gravitative time dilation is discovered at the context free fall tower. The twin paradox is stimulating: One twin remains at Earth, the other travels through space. If the adequate coordinate system (ACS), that describes nature adequately, could be chosen freely, each of the twins could say that he is aging slower. Thus, we need the ACS. For it, already Foucault*s pendulum determined the angular frequency of the ACS: 360° per day relative to Earth. Also in Newton*s mechanics, the ACS is determined: It is the inertial system, as Newton*s laws hold in this coordinate system. An empirical solution of the twin paradox is derived from measurements of the D1-mission in Earth*s orbit. The traveling twin ages slower. An institutional partial solution has been proposed by the International Astronomical Union (IAU): In space flight near Earth, a geocentric coordinate system is recommended. As a consequence, the present * day relativity theory is incomplete, as it does not provide an ACS, instead, it proclaims that all coordinate systems should be equivalent for the description of nature. I derive a complete solution that provides an ACS for each point in the universe. I report about experiences from teaching.

DD 5.3 Mon 11:25 SCH/A284

Wo sind die Knotenpunkte? Transfer zwischen elektrischer Schaltung und Schaltbild — •Ben Osinski und Roger Erb — Goethe-Universität Frankfurt

Der Transfer zwischen abstrakten Schaltbildern und realen Schaltungen stellt insbesondere für Lehramtsstudierende eine zentrale Herausforderung in der Elektrizitätslehre dar, da dies neben fachlichem Wissen auch ein ausgeprägtes to-

pologisches Vorstellungsvermögen erfordert. In einer qualitativ angelegten Untersuchung mit Lehramtsstudierenden der Haupt- und Realschule im Praktikum "Elektrizität und Magnetismus", wurde dieser Transfer im Rahmen eines Versuchs unter Verwendung der Think-Aloud-Methode videografiert. Studierende übten sich dabei sowohl im Aufbau realer Schaltungen anhand vorgegebener Schaltbilder als auch am Skizzieren von Schaltbildern anhand eines gegebenen Aufbaus. Dadurch soll das Wissen und Können der Studierenden nach dem Kompetenzmodell von Blömeke sichtbar gemacht werden, um typische Strategien und Schwierigkeiten zu identifizieren. Ziel ist es, einen Einblick in die kognitiven Prozesse der Studierenden zu gewinnen. Zusätzlich wurden räumliches Denkvermögen, kognitive Belastung und Konzeptverständnis der Studierenden erhoben, um diese als mögliche Prädiktoren für den Transfererfolg zu untersuchen. In diesem Vortrag werden erste Ergebnisse der Videoanalyse präsentiert und mögliche Implikationen für die Hochschullehre diskutiert.

DD 6: Lehrkräfteaus- und -fortbildung I

Time: Monday 10:45–11:45 Location: SCH/A285

DD 6.1 Mon 10:45 SCH/A285

Gründe für die Wahl eines Physik-Lehramtsstudiums — •Lion Cornelius Glatz, Teemu Loh, Pauline Czora, Mark Ullrich, Holger Horz und Roger Erb — Goethe-Universität Frankfurt

Es ist davon auszugehen, dass der bundesweite Lehrkräftemangel vor allem in den naturwissenschaftlichen Fächern als sich verschärfendes Problem bestehen bleiben wird. Um dieser Herausforderung entgegenzuwirken, ist ein besseres Verständnis über die Faktoren notwendig, die für die Wahl und den erfolgreichen Abschluss eines Lehramtsstudiums maßgeblich sind. Um diese Fragestellung zu untersuchen, werden im Rahmen des Projekts "Hessischer Lehrkräftebildungsmonitor" Schüler*innen und Studierende des Lehramts in einem längsschnittlichen Studiendesign empirisch begleitet.

In diesem Beitrag werden qualitative Ergebnisse des ersten Erhebungszeitpunktes vorgestellt, zu dem Schüler*innen des Abschlussjahrgangs unter anderem zu ihrer Berufswahlmotivation, ihren Gründen für oder gegen bestimmte Lehramtstypen und zu ihren Erwartungen an die verschiedenen Phasen der Lehrkräftebildung befragt wurden. Dabei wird ein besonderer Blick auf das Fach Physik und den Vergleich mit anderen Lehramtsfächern geworfen.

DD 6.2 Mon 11:05 SCH/A285

Die DPG-Lehrkräftebefragung — •Andreas Härtel, Andreas Fuchs und Thomas Filk — Physikalisches Institut, Universität Freiburg

Welche Inhalte und Angebote des Physikstudiums erachten Lehrkräfte rückblickend für professionsrelevant? Mit dieser Frage knüpft die während des vergangenen Jahres bundesweit durchgeführte Lehrkräftebefragung an die 2023 veröffentlichte Studie zum Lehramtsstudium in Deutschland an [1], bei welcher Studierende und Fachbereiche zur Qualität des Physiklehramtsstudiums in Deutschland befragt wurden. Ziel der durch die Universität Freiburg und die Deutsche Physikalische Gesellschaft durchgeführten Studie ist es dabei, Hinweise zur Weiterentwicklung des Physik-Lehramtsstudium in Deutschland zu erhalten, auch um dem Lehrkräftemangel entgegen zu wirken. Wir werden den aktuellen Stand der Studie aufzeigen und erste Ergebnisse diskutieren.

[1] A. Woitzik, K. Mecke, G. Düchs. Das Lehramtsstudium Physik in Deutschland. Eine Studie der Deutschen Physikalischen Gesellschaft e.V.. 2023. ISBN 978-3-9818197-7-9. https://www.dpg-physik.de/veroeffentlichungen/publikationen/studien-der-dpg/das-lehramtsstudium-physik-in-deutschland

DD 6.3 Mon 11:25 SCH/A285

Untersuchung der Implementation fachdidaktischer Innovationen auf Basis des Concerns-Based Adoption Models — •Nils Haverkamp, Alexander Pusch und Stefan Heusler — Institut für Didaktik der Physik, Universität Münster

Die Implementation fachdidaktischer Innovationen im Schulkontext gestaltet sich in der Regel schwierig. Dies gilt umso mehr, wenn neuartige experimentelle Materialien genutzt werden, wie es bei den Low-Cost-Experimente zur Wellenoptik aus dem O3Q-Projekt der Fall ist. Um die Implementation sinnvoll zu unterstützen ist es notwendig, den aktuellen Stand und die Schwierigkeiten mit denen Lehrkräfte sich konfrontiert sehen, zu erheben. Dies kann als Basis dienen, um gezielt Unterstützungsangebote zu entwickeln. Ein Rahmenmodell zur Diagnose des aktuellen Stands im Implementationsprozess bietet das Concerns-Based Adoption Model (CBAM). Dazu werden die drei Dimensionen "Innovation Configuration (IC)", "Stage of Concern (SoC)" und "Level of Use(LoU)" in einer Kombination aus Interview und Fragebogen erhoben. Im Vortrag werden erste Ergebnisse einer Studie vorgestellt, in der die drei Dimensionen des CBAM bezogen auf die Implementation der Low-Cost-Experimente zur Wellenoptik erhoben werden.

DD 7: Quantenphysik II

Time: Monday 12:00–13:00 Location: SCH/A101

DD 7.1 Mon 12:00 SCH/A101

Experimente mit Einzelphotonenquellen in der Lehrerbildung — •Kim Kappl[1], Stefan Aehle[2], Simon Koppenhöfer[1], Philipp Scheiger[1] und Ronny Nawrodt[1] — [1]Arbeitsgruppe Physik und ihre Didaktik, 5. Physikalisches Institut, Universität Stuttgart — [2]Arbeitsgruppe Fachdidaktik der Physik und Astronomie, Friedrich-Schiller-Universität Jena

Mit der Einführung der Bildungsstandards der allgemeinen Hochschulreife der Kultusministerkonferenz (2020) hat die Quantenphysik einen deutlich größeren Stellenwert in den gymnasialen Lehrplänen erhalten. Viele der geforderten Inhalte waren jedoch bislang weder Teil der schulischen Vorbildung noch der universitären Ausbildung angehender Lehrkräfte. Um diese Lücke zu schließen, wurde in Kooperation zwischen der Universität Stuttgart und der Friedrich-Schiller-Universität Jena eine Lehrerfortbildung zur modernen Quantenphysik im blended-learning-Stil entwickelt. Im Rahmen dieses Beitrags werden insbesondere Experimente zur Erzeugung einzelner Photonen vorgestellt, die im Präsenzteil der Fortbildung demonstriert werden. Dazu gehört das Quantenoptik-Kit der Firma Thorlabs, sowie ein NV-basiertes Setup zum Nachweis einzelner Photonen. Ergänzend wird diskutiert, wie diese Experimente zur inhaltlichen Klärung und zum Verständnis zentraler quantenphysikalischer Konzepte bei Lehrkräften beitragen können.

DD 7.2 Mon 12:20 SCH/A101

Quantum Edukit: An Experimental Toolkit to Explore Quantum Mechanics — Matteo Stefanini, Oliver Stadler, Berkay Işik, Simon Josephy, Björn Josteinsson, •Nishant Dogra, Andrea Morales, and Gabriel Puebla Hellmann — QZabre AG, Neunbrunnenstrasse 50, 8050 Zurich, Switzerland

With the advancements in quantum technologies, it is essential that the basic understanding of quantum mechanics reaches students, the general public and policy makers in an intuitive way. We have developed Quantum Edukit, an educational kit based on Nitrogen-Vacancy centers to teach quantum mechanics in a hands-on and interactive manner. The kit enables exploration of principles such as level quantization, quantum superposition, light-matter interaction and quantum optical effects in real time. Sample experiments include observation of the Zeeman effect, Rabi oscillations, Ramsay interferometry, and spin echo. Moreover, Quantum Edukit demonstrates how these principles underpin real-world applications including quantum magnetometry, atomic clocks, and qubit manipulation. On an experimental level, students gain hands-on experience in building optical setups, optimizing the performance of quantum systems, and acquiring hand-on skills used in quantum research labs. Quantum Edukit provides a compact and versatile platform to explore quantum systems, and will positively increase students' awareness of quantum mechanics, thereby enhancing their engagement with quantum technologies.

DD 7.3 Mon 12:40 SCH/A101

Quantenbildgebung im Schülerlabor — •Dustin-Philipp Preissler und Holger Cartarius — AG Fachdidaktik der Physik und Astronomie, Friedrich-Schiller-Universität, 07743 Jena

Quantenbildgebung mit undetektiertem Licht oder Ghost Imaging verwenden verschränkte Einzelphotonen und haben neue Anwendungsmöglichkeiten, die mit klassischen Bildgebungsverfahren nicht funktionieren. Wir stellen unseren didaktisch reduzierten Aufbau sowie konzipiertes Begleitmaterial aus unserem Schülerlabor vor, mit dem Schüler/-innen die Detektorbilder mit klassischem Laserlicht im Mach-Zehnder- und Michelson-Interferometer simulieren können und so wichtige Grundgrößen und Eigenschaften von Quantenbildgebung experimentell untersuchen können.

DD 8: Außerschulische Lernorte I

Time: Monday 12:00–13:00 Location: SCH/A252

DD 8.1 Mon 12:00 SCH/A252

Vom Batterielabor zu einer kraftvollen Zukunft: das Forschungscamp Role2Role — •Tessa Horenburger und Anne Geese — Technische Universität Braunschweig, IFdN, Deutschland

Das Forschungscamp Role2Role an der Technischen Universität Braunschweig in Kooperation mit dem Haus der Wissenschaft ist eine interdisziplinäre Initiative zur Förderung der Beteiligung junger Frauen im MINT-Bereich. Sie richtet sich an Oberstufenschülerinnen aus ganz Deutschland und verbindet digitales Mentoring mit praxisorientierten Forschungs-Camps in den Laboren der Batterieforschung. Im Zentrum steht ein nachhaltiges Peer-Mentoring-Modell: Ausgebildete MINT-Studentinnen der TU Braunschweig agieren als Mentorinnen und Rollenvorbilder, begleiten ihre Mentees durch regelmäßige Online-Treffen sowie durch die Experimente im Labor. Sie vermitteln dabei fachliches Wissen, Laborerfahrung und geben authentische Einblicke in wissenschaftliche Arbeitsumgebungen. Diese kontinuierliche Interaktion soll die Selbstwirksamkeit und das Zugehörigkeitsgefühl der Teilnehmerinnen aber auch die der Mentorinnen in männerdominierten Feldern stärken. Das innovative Role-to-Role-Prinzip etabliert eine langfristige Förderungskette, da im besten Fall ein Teil der Mentees zu Mentorinnen aufwächst. Die Umsetzung und Wirkung des Programms werden anhand quantitativer und qualitativer Indikatoren wie der Selbstwirksamkeit, dem Interesse und Veränderungen in der MINT-Identität und der Berufsziele der Teilnehmerinnen evaluiert. Die Ergebnisse der Pilotphase vom Herbst 2025 fließen in die Optimierung der nächsten Kohorte ein, die von Februar bis April 2026 teilnehmen können.

DD 8.2 Mon 12:20 SCH/A252

Labs on Tour - ein Konzept zur niederschwelligen MINT-Interessenförderung mit außercurricularen Nachmittagskursen — •Maria Hinkelmann und Heidrun Heinke — RWTH Aachen University

Seit Jahrzehnten wird daran geforscht, wie sich Interessen von Jugendlichen im MINT-Bereich wirksam fördern lassen. Einen vielversprechenden Ansatz verfolgt das Projekt Labs on Tour, in dem es MINT-Angebote an Schulen bringt, um Jugendlichen in ihrer Freizeit einen niederschwelligen Zugang zu MINT-Themen zu eröffnen. Dafür werden bestehende Angebote der Schülerlabore mobil gemacht und in wöchentlichen Nachmittags-Kursen mit jeweils vier 90-minütigen Einheiten im Rahmen von MINT-AGs an Schulen umgesetzt. Eine AG läuft jeweils über ein Schulhalbjahr und umfasst drei thematisch verschiedene Kurse, sodass die Teilnehmenden Einblicke in unterschiedliche MINT-Bereiche erhalten. Die Durchführung übernehmen studentische Hilfskräfte (SHK) der Schülerlabore, während die Lehrkräfte lediglich Aufgaben vor Ort, wie Werbung, Anmeldung und Aufsicht verantworten. Das Projekt erhält durchweg positive Rückmeldungen - von Schulen, Schülerlaboren, SHK und von Schüler:innen sowie ihren Eltern. Derzeit beteiligen sich zwölf Schulen, und bei einigen AGs wurden Rekordanmeldezahlen erreicht. Im aktuellen Regelbetrieb erreichen die Angebote jährlich rund 210 Schüler:innen - etwa 35 % davon Mädchen - mit insgesamt 18 Stunden intensiver Auseinandersetzung mit unterschiedlichen MINT-Themen. Der Vortrag präsentiert das Konzept von Labs on Tour sowie zentrale Erkenntnisse der ersten drei Projektjahre.

DD 8.3 Mon 12:40 SCH/A252

The Science Pop-Up: Interaktive MINT-Bildung in der Fußgängerzone — •Moritz Kriegel[1], Verena Spatz[2] und Jill Fiedler[2] — [1]Facility for Antiproton and Ion Research (FAIR), Planckstraße 1, 64291 Darmstadt — [2]Technische Universität Darmstadt, Hochschulstraße 12, 64289 Darmstadt

Wissenschaftskommunikation spielt eine zentrale Rolle, um Vertrauen in Forschung zu stärken und Menschen außerhalb formaler Bildungsinstitutionen zu erreichen. Wissenschaftliche Ausstellungen in Form von Pop-Up Stores bieten hierfür ein niedrigschwelliges Format. Der SCIENCE POP-UP des GSI Helmholtzzentrums für Schwerionenforschung bringt seit März 2025 die Forschung an Teilchenbeschleunigeranlagen in die Darmstädter Innenstadt. Das Konzept kombiniert eine interaktive Ausstellung zur Kern- und Teilchenphysik mit Vorträgen, Workshops und einem Schülerlaborversuch in einem zuvor leerstehenden Ladenlokal. Begleitet wurde das Projekt durch eine Prä-Post-Befragung (N=265) zur wahrgenommenen Relevanz von Naturwissenschaften sowie den Einstellungen und der Zugänglichkeit zur naturwissenschaftlichen Forschung. Trotz eines hohen Eingangsinteresses zeigten sich nach dem Besuch signifikante Verbesserungen in nahezu allen Skalen. Besonders deutlich waren die Zuwächse in den Skalen Relevanz und Zugänglichkeit, beide mit Veränderungen mittlerer Effektstärke. Besonders starke Verbesserungen zeigten sich bei Frauen sowie jüngeren Besuchenden. Der Beitrag zeigt, wie Science-Pop-Ups wirksame Orte informellen Lernens sein können, die Interesse fördern und neue Zielgruppen für wissenschaftliche Themen erschließen.

DD 9: Neue Konzepte I

Time: Monday 12:00–13:00 Location: SCH/A284

DD 9.1 Mon 12:00 SCH/A284

Mathematische Auffrischung des Schulstoffs durch Gamification in der Studieneingangsphase — •Caroline Wortmann, Malte Beran Kosan und Ruth Dornhege — TU Dortmund University, Dortmund, Germany

Das Verbundprojekt beVinuS.nrw (TU Dortmund, BU Wuppertal, RWTH Aachen) zielt darauf ab, Studienabbruchquoten in MINT-Studiengängen zu reduzieren, die aufgrund mangelnder schulischer Mathematik-Kompetenzen in der Studieneingangsphase zustande kommen. Obwohl digitale Auffrischungsangebote (OER-basiert, mit Selbsttests und passenden Lernmodulen abgestimmt auf die Veranstaltungen der ersten drei Semester) entwickelt wurden, blieb die Akzeptanz und Nutzungsbereitschaft seitens der Studierenden gering. Daraufhin konzeptionierte die Pilotfakultät Physik der TU Dortmund eine mathematische Alpaka-Wanderung als analoges Gesellschaftsspiel. Dieses beruht auf wissenschaftlich evaluierten Fragen, dient zum Kennenlernen der Studierenden untereinander und stärkt deren Teamzusammenhalt, welcher das gemeinsame Lernen in Kleingruppen während des Studiums unterstützt. Die Gamification-Elemente ermöglichen den Studierenden einen neuen Zugang zum Mathematikstoff der Sekundarstufe I und II. Gleichzeitig reflektieren sie ihre eigenen Kompetenzen und erkennen potentielle Schwachstellen. Erstmals spielten (Medizin)Physik-Studierende das Spiel in der Orientierungswoche im WiSe 2025/26. Der Vortrag beleuchtet die Entstehungsgeschichte sowie erste Zwischenergebnisse der Begleitforschung. Zudem erfolgt ein Ausblick zur Weiterentwicklung des Spiels und zur Zugänglichkeit für andere Fakultäten.

DD 9.2 Mon 12:20 SCH/A284

Der Einfluss narrativer Immersion auf das Verständnis quantenphysikalischer Konzepte in Serious Games — •Caroline Wermann, Karina Avila, Jochen Kuhn und Stefan Küchemann — Lehrstuhl Didaktik der Physik, LMU München

Educational Games werden zunehmend eingesetzt, um akademische Inhalte spielerisch zu vermitteln. Außerhalb fest eingebetteter Lernaktivitäten stehen sie jedoch in direkter Konkurrenz zu anderen Freizeitangeboten, wodurch Aufmerksamkeit und Engagement der Lernenden zu zentralen Lernerfolgsfaktoren werden. Relevante Faktoren wie Narration, um Spielinhalte zu kontextualisieren und Engagement und Aufmerksamkeit zu erhöhen, zeigen jedoch bislang keinen oder einen negativen Effekt auf den Lernzuwachs. Die Ursachen für diesen Zusammenhang sind bislang unklar. Die aktuell laufende Studie mit 250 Teilnehmenden untersucht, wie narrative Immersion das Konzeptverständnis über Quantentechnologien Lernender in einem Educational Game beeinflusst und welche Rolle Presence, situationales Interesse, Selbstwirksamkeit, intrinsische Motivation und cognitive load in diesem Zusammenhang spielen. Dazu werden zwei Versuchsbedingungen verglichen: eine Kontrollbedingung, in der die Spielenden die Level ohne narrativen Kontext absolvieren, und eine Experimentalbedingung, in der zusätzliche Videosequenzen und Texte die übergeordnete Spielgeschichte vermitteln und somit die narrative Immersion erhöhen sollen. Die Analyse erfolgt über ein Strukturgleichungsmodell sowie über den Vergleich beider Versuchsgruppen.

DD 9.3 Mon 12:40 SCH/A284

Physik trifft Kunst: Praxisbeispiele für fächerverbindenden MINKT-Unterricht — •Nathalie Wolke und Susanne Heinicke — Universität Münster

Physik und Kunst erschaffen auf den ersten Blick ganz unterschiedliche Welten im Klassenzimmer, doch laden Sie beide auf ihre Art Lernende dazu ein, Phänomene der Welt zu erforschen, zu gestalten und zu hinterfragen. Der MINKT-Ansatz, eine deutsche Adaption des internationalen STEAM-Ansatzes, greift dieses Potenzial auf und betrachtet die Verbindung von MINT-Fächern und Kunst als Chance, kognitive, kreative und ästhetische Kompetenzen gleichermaßen zu fördern. Besonders in der Kombination von Physik und Kunst lassen sich Lernende auf verschiedenen Ebenen ansprechen: analytisch, haptisch, emotional und gestalterisch. Da in beiden Fächern das Interesse der Lernenden im Verlauf der SEK I zurückgeht und es deutliche Interessensunterschiede zwischen den Geschlechtern gibt, fokussiert das vorliegende Forschungsvorhaben auf dem

Potential des fächerverbindenden Unterrichts für die Interessenförderung. Dafür verankert es die Idee in der schulischen Praxis und stellt die Entwicklung und Erprobung von fächerverbindenden Unterrichtsreihen in den Mittelpunkt. Praxisnah fungieren die Unterrichtsreihen als Curriculum Replacement Units: Sie berücksichtigen die Lehrpläne beider Fächer und könnten Regelunterricht somit ersetzen. Im Zentrum des Vortrags steht neben einer theoretischen Rahmung des MINKT-Konzepts und der Interessenförderung die Vorstellung dieser fächerverbindenden Unterrichtsreihen sowie erster empirischer Rückmeldungen zum Ansatz aus der Praxis.

DD 10: Hochschuldidaktik I

Time: Monday 12:00–13:00 Location: SCH/A285

DD 10.1 Mon 12:00 SCH/A285

Einfluss multi-repräsentationaler Lernaufgaben auf die Anwendung vektoranalytischer Konzepte in der Physik — •Larissa Hahn[1,2], Alexander Voigt[3], Philipp Mertsch[3] und Pascal Klein[1] — [1]Universität Göttingen, Deutschland — [2]Universität Koblenz, Deutschland — [3]RWTH Aachen, Deutschland

Um Vektorfeldkonzepte wie Divergenz oder Rotation in physikalischen Kontexten anzuwenden, ist ein solides Verständnis ihrer mathematischen Grundlagen erforderlich. Empirische Befunde zeigen jedoch wiederkehrende Schwierigkeiten, insbesondere bei der visuellen Interpretation von Richtungsableitungen, die auch in physikalische Anwendungsbereiche wie die Elektrodynamik transferieren. Im Einklang mit lerntheoretischen Ansätzen wurden Lernaufgaben entwickelt, die einen visuellen und interaktiven Zugang zur Vektoranalysis eröffnen. Sie kombinieren multiple Repräsentationen, Zeichenaktivitäten und ein dynamisches Vektorfeld-Visualisierungstool. Die Aufgaben wurden in die begleitenden Übungen einer Vorlesung im zweiten Physikstudiensemester an der RWTH Aachen integriert. Vor sowie nach der Implementation bearbeiteten die Studierenden (N = 49) einen Performanztest mit Aufgaben zur Anwendung der Vektoranalysis in der Fluidmechanik, Elektro- und Magnetostatik. Dieser Beitrag präsentiert Ergebnisse der Wirksamkeitsanalyse der Lernaufgaben hinsichtlich der Anwendung der Vektoranalysis in physikalischen Kontexten und diskutiert verschiedene Lösungsstrategien sowie -ansätze der Studierenden.

DD 10.2 Mon 12:20 SCH/A285

Untersuchung der Wirksamkeit von aktivierenden Arbeitsmaterialien in der Strömungsmechanik für Studierende in den Ingenieurwissenschaften — •Max Vincent Uzulis und Christian Kautz — Technische Universität Hamburg

Studierende in den Ingenieurwissenschaften befassen sich in verschiedenen Grundlagenfächern intensiv mit physikalischen Fachinhalten. Besonders die Fluiddynamik ist ein komplexes Themengebiet, das starke Grundlagen in der Mechanik erfordert und Studierende vor große Herausforderungen stellt. Um dieses Problem zu adressieren, untersuchen wir seit 2023 mit Hilfe regelmäßiger Kurztests zunächst spezifische Verständnisschwierigkeiten der Studierenden in der Strömungsmechanik. Abgeleitet aus den Ergebnissen wurden aktivierende Arbeitsmaterialien erstellt, die in den Jahren 2024 und 2025 das klassische Unterrichtsformat unterstützt haben. In dieser Studie präsentieren wir quantitative und qualitative Daten zur Wirksamkeit der Intervention. Vor- und Nachtest Fragen zu drei Kernkonzepte der Fluiddynamik (Hydrostatischer Druck, Kontinuitätsprinzip, Bernoulli Gleichung) wurden ausgewertet, um Aussagen über auftretende Fehlvorstellungen und deren Behebung im Laufe der Intervention zu treffen. Dabei konnten einerseits Erfolge in Bezug auf die Reduktion von Fehlvorstellungen und verbesserte Testergebnisse nachgewiesen werden, andererseits erwiesen sich gewisse Probleme als hartnäckig. Diese gaben Anlass zu weiteren Änderungen an den Lehrmaterialien für das Sommersemester 2026.

DD 10.3 Mon 12:40 SCH/A285

Effektivität von Whiteboards als Kollaborationstool in der Physik-Hochschullehre: Untersuchungen anhand des ICAP-Modells — •Silke Stanzel, Claudia Schäfle und Christine Lux — TH Rosenheim, Hochschulstraße 1, 83024 Rosenheim

Analoge Whiteboards sind ein zentrales Element der Lehrmethoden der Physics Education Research. In Physiklehrveranstaltungen an der TH Rosenheim bearbeiten Studierende Aufgaben in Zwei- bis Dreiergruppen auf DIN-A2-großen Whiteboards. Diese fungieren als "public thinking space", der das Festhalten und Überarbeiten von Ideen erleichtert, die Kollaboration fördert und der Lehrperson eine schnelle Einschätzung zur gezielten Rückmeldung ermöglicht. Untersucht wird, ob und in welcher Weise Whiteboards konstruktives und interaktives Lernen im Sinne des ICAP-Modells (Chi & Wylie, 2014) unterstützen. Mittels Unterrichtsbeobachtungen werden in Zwei-Minuten-Intervallen die Aktivitäten der Studierenden und der Lehrperson erfasst und den ICAP-Stufen zugeordnet. Zusätzlich wird analysiert, inwiefern die Lehrperson dazu beitragen kann, dass die interaktive Stufe erreicht wird. Die Ergebnisse zeigen, dass das Setting aus Whiteboards, Gruppen von zwei bis drei Personen sowie runden Tischen im SCALE-UP-Raum günstige Bedingungen für konstruktive und interaktive Lernprozesse schafft. Die Studierenden arbeiteten rund 75 % der Zeit in den hohen ICAP-Stufen konstruktiv (C) und interaktiv (I). Zudem deutet sich an, dass Whiteboard-Aufgaben mindestens zehn Minuten dauern sollten, damit Studierende mit höherer Wahrscheinlichkeit die höheren ICAP-Stufen erreichen.

DD 11: Hauptvortrag II

Time: Tuesday 9:30–10:30 Location: HÜL/S386

Invited Talk DD 11.1 Tue 9:30 HÜL/S386

Lernen mit KI, Lernen über KI: Perspektiven für die Naturwissenschaftsdidaktik — •Arne Bewersdorff — University of Georgia, Athens, USA

Künstliche Intelligenz gewinnt im Naturwissenschaftsunterricht sowohl als Lerntechnologie als auch als Lerngegenstand zunehmend an Bedeutung. Dieser Hauptvortrag verbindet beide Perspektiven. Im ersten Teil werden Studien vorgestellt, die den Einsatz KI-basierter Systeme für automatisiertes Assessment und adaptives Feedback beim Experimentieren untersuchen. Darauf aufbauend werden Potenziale multimodaler KI-Systeme diskutiert.

Im zweiten Teil steht die Frage im Zentrum, wie Lernende zu einem reflektierten Umgang mit KI befähigt werden können, als Lerntechnologie, im Alltag und in den Fachwissenschaften. Dazu werden Studien vorgestellt, die KI-Grundwissen (sog. AI Literacy) und verwandte Konstrukte erfassen. Zusammenhänge zwischen AI Literacy und Einstellungen, Nutzung, Interesse sowie Selbstwirksamkeitserwartungen werden berichtet. Ein Fokus liegt auf dem KI-Interesse als möglicher vermittelnder Größe zwischen KI-Nutzung und AI Literacy. Abschließend werden daraus erste Implikationen für Unterricht und Lehrkräftebildung abgeleitet.

DD 12: Praktika und Experimente

Time: Tuesday 10:45–11:45 Location: SCH/A101

DD 12.1 Tue 10:45 SCH/A101

Einflüsse von multimodaler Interaktion auf den Fachwissenserwerb im physikalischen Experiment — •Dane-Vincent Schlünz[1,2], Stephan Dutke[3] und Daniel Laumann[1,2] — [1]Physikalisches Institut, Universität Münster — [2]Institut für Didaktik der Physik, Universität Münster — [3]Institut für Psychologie in Bildung und Erziehung, Universität Münster

Die Gestaltung multimedialer Lernumgebungen unter Einbezug von Experimenten erfordert empirisch geprüfte Designprinzipien (vgl. Cognitive-Affective Theory of Learning with Media) wie u. a. das Modalitätsprinzip. Im klassischen Verständnis wird so der Verteilung von verbal und piktorial präsentierten Informationen auf zwei Modalitäten (Hören, Sehen) eine lernförderliche Wirkung zugewiesen. Lernumgebungen können jedoch zusätzlich Formen inhaltlich relevanter Interaktion bieten, welche neben Hören und Sehen auch somatosensorische Modalitäten Lernender adressieren. Ob das Modalitätsprinzip somit auch in Experimenten gilt, die durch Augmented Reality (AR) erweiterte Gestaltungs- und Handlungsmöglichkeiten aufweisen, wurde bisher kaum

empirisch untersucht. Theoretische Ansätze wie die Embodied Cognition weisen darauf hin, dass somatosensorische Modalitäten im Lernprozess grundsätzlich lernförderlich sein können. Im Rahmen eines AR-erweiterten Experiments zu optischer Polarisation wird in einer Interventionsstudie (visuell vs. visuell-somatosensorisch) untersucht, wie somatosensorische Modalitäten den Fachwissenserwerb beeinflussen. Die Stichprobe umfasst N=107 Studierende der Biowissenschaften, Pharmazie, Landschaftsökologie und Physik.

DD 12.2 Tue 11:05 SCH/A101

Wie bewerten Lernende unterschiedliche Messverfahren hinsichtlich der Validität von Schlussfolgerungen? — •Benz Gregor und Seyfferth Simon — Technische Universität München, München, Deutschland

Die Validität von Schlussfolgerungen zu bewerten, wird heutzutage immer wichtiger (Sharma, 2006) und ist daher ein zentrales Ziel von Physikunterricht (KMK, 2024). Ein Einfluss auf die Validität kann u.a. das verwendete Messverfahren haben. Forschung zeigt, dass Lernende hierbei Schwierigkeiten haben, indem sie z.B. Unsicherheits- und Fehlerquellen nicht systematisch berücksichtigen (Kanari & Millar, 2004). Vor diesem Hintergrund klärt diese Studie, wie Lernende den Einfluss verschiedener Messverfahren auf die Validität von Schlussfolgerungen beurteilen. 45 Sek-2-Lernende haben hierfür vier Messverfahren (Analog-, Digitalthermometer, digitales Messwerterfassungssystem, Wärmebildkamera) zur Ermittlung eines optimalen Zeitpunkts der Milchzugabe zum Kaffee (Kaffee-Milch-Problem) hinsichtlich bester Validität sortiert und deren Reihung begründet. Mittels einer kategorienbildenden Inhaltsanalyse konnten ein pauschaler, drei heuristische, vier messdatenbasierte und drei experimentbasierte Gründe identifiziert werden. Die Ergebnisse verdeutlichen, dass Lernende Schwierigkeiten haben, ihre Bewertungen zur Validität auf Messverfahren zu stützen, und stattdessen auch Datenmuster oder Heuristiken anführen. Implikationen für die Physikausbildung und zukünftige Forschung werden diskutiert.

DD 12.3 Tue 11:25 SCH/A101

Students' reasoning in choosing measurement instruments in an introductory physics laboratory course — •Micol Alemani[1], Karel Kok[2], and Eva Philippaki[3] — [1]University of Potsdam — [2]Humbold University of Berlin — [3]King's College London

Recent research studies on laboratory courses highlight the importance of fostering students' experimental design skill and decision making. However, research on students reasoning about measurement apparatus remains sparse. To extend this line of inquiry, this study examines students' decision-making processes in choosing between simple measurement instruments in a laboratory context. We developed a short, 10 minutes, questionnaire answered by students at the University of Potsdam in a pre-/post-test setting. In the questionnaire students are asked to reason about the choice of simple instruments to measure the length of different objects. For the analysis of students' justifications we have inductively developed a coding manual and used it to characterise students' considerations regarding their choice of measurement instruments. In this talk, the questionnaire, the creation of the coding manual and the analysis of students' instrumental choices as well as the corresponding justifications will be presented and discussed. The results of this study contribute to the ongoing investigation of students' experimental skills and uncover possible misconceptions when working with instrumentation and measurement data.

DD 13: Digitale Medien II

Time: Tuesday 10:45–11:45 Location: SCH/A252

DD 13.1 Tue 10:45 SCH/A252

Kognitive Entlastung und affektiv-motivationale Förderung beim Physiklernen: Ein empirischer Vergleich von KI-Chatbots und gestuften Hilfen — •Eleonore Becker[1], Johannes Wünsche[1], Joaquin Veith[1], Johanna Schrader[2,3] und Philipp Bitzenbauer[1] — [1]Institut für Didaktik der Physik, Universität Leipzig — [2]L3S Forschungszentrum, Leibniz Universität Hannover — [3]CAIMed - Niedersächsisches Zentrum für KI & Kausale Methoden in der Medizin, Hannover

Zur Unterstützung der Aufgabenbearbeitung im Physikunterricht sind Scaffolding-Methoden wie gestufte Hilfen etabliert, in der Erstellung jedoch oft ressourcenintensiv. Diese Studie untersucht das Potenzial von KI-Chatbots als Alternative. In diesem Beitrag präsentieren wir die Ergebnisse einer quasi-experimentellen Feldstudie mit 273 Neuntklässler:innen, die eine Aufgabe zum Thema Auftrieb lösten. Wir untersuchen, wie sich die Unterstützung durch einen prompt-engineerten KI-Chatbot im Vergleich zu klassischen gestuften Hilfen und Lehrbucherklärungen auf die kognitive Belastung sowie das affektiv-motivationale Erleben auswirkt. Während beide Scaffolding-Methoden die kognitive Belastung der Lernenden im Vergleich zu Lehrbucherklärungen signifikant senken, fördert nur der Chatbot zusätzlich signifikant positives affektiv-motivationales Erleben wie situatives Interesse, Selbstwirksamkeitserwartung und Freude. Wir diskutieren, wie die interaktive und soziale Natur von KI-Chatbots über reine kognitive Entlastung hinausgeht und zu diesem positiveren Gesamterleben führt.

DD 13.2 Tue 11:05 SCH/A252

KI-gestützte Lernumgebung für das Physikpraktikum: Entwicklung und empirische Evaluation — •Tilmann Steinmetz[1], Jan-Philipp Burde[1] und Peter Gerjets[2] — [1]Universität Tübingen, Tübingen, Germany — [2]Leibniz-Institut für Wissensmedien, Tübingen, Germany

Studierende kommen häufig ohne ausreichende fachliche Vorbereitung in das physikalische Grundpraktikum. Um diesem Problem zu begegnen, wurde eine KI-gestützte Lernumgebung für einen Versuch zum ohmschen Gesetz entwickelt, mit der sich Studierende auf das Praktikum vorbereiten können. Versuchsanleitung und Systemprompt des KI-Tutors wurden anhand des fachdidaktisch etablierten EPo-Konzepts (Elektrizität mit Potenzial) entwickelt, das typische Verständnisschwierigkeiten beim Thema einfache Stromkreise berücksichtigt. Die digitale Lernumgebung enthält die Versuchsanleitung, den KI-Tutoren sowie die Möglichkeit für automatisiert generierte Verständnisfragen zu einzelnen Versuchsteilen. Die Wirksamkeit der Lernumgebung wurde in einer quasi-experimentellen Treatment-Kontrollgruppen-Studie mit Prä-Post-Design mit ca. 200 Studierenden untersucht. Während sich die Kontrollgruppe lediglich mit der Versuchsanleitung im PDF-Format auf den Versuch vorbereitete, hatte die Experimentalgruppe zusätzlich die Möglichkeit, die KI-gestützte digitale Lernumgebung zu nutzen. Die Ergebnisse zeigen eine erhöhte Lernwirksamkeit zugunsten der Experimentalgruppe. Eine qualitative Analyse der Chatverläufe weist darauf hin, dass der KI-Tutor die zentralen Konzepte des EPo-Konzepts verstärkt.

DD 13.3 Tue 11:25 SCH/A252

Desinformation und Physikunterricht aus der Perspektive von Lehrkräften — •Julia Hädrich und Rita Wodzinski — Didaktik der Physik, Universität Kassel

Soziale Netzwerke und KI-Dienste gewinnen bei der Informationssuche von Jugendlichen zunehmend an Bedeutung: Rund ein Viertel der 12- bis 19-Jährigen nutzt Instagram oder TikTok mehrmals pro Woche als Informations-Tool, etwa vier von zehn greifen dafür auf ChatGPT zurück (Medienpädagogischer Forschungsverbund Südwest, 2025). Diese Entwicklung birgt Herausforderungen, da vielen Jugendlichen die nötigen Kompetenzen fehlen, um Informationen kritisch zu bewerten und Desinformation zu erkennen (vgl. PISA, 2024; ICILS, 2023). Die Förderung solcher Kompetenzen stellt eine Aufgabe der Lehrkräfte dar und setzt spezifische professionelle Handlungskompetenzen im Kontext dieser Medien voraus (Baumert & Kunter, 2011). Ob und in welchem Umfang entsprechende Unterrichtskonzepte von den Lehrpersonen umgesetzt werden, hängt dabei entsprechend der Theory of Planned Behavior (vgl. Fishbein & Ajzen, 2010) unter anderem von der individuellen Einstellung zum Thema Desinformation. Angesichts wissenschaftsfeindlicher Tendenzen ist die Reflexion von Wissenschaft gesellschaftlich besonders relevant. Zusammen mit Themenfeldern, wie der Energie, ergeben sich für das Fach Physik besondere Anknüpfungspunkte, um einen reflektierten Umgang mit Medien zu fördern. In einer Online-Befragung wurden Physiklehrkräfte der Sekundarstufe I zu ihrer Perspektive auf die genannten Inhalte befragt. Der Beitrag stellt den Fragebogens und erste Ergebnisse der Erhebung vor.

DD 14: Bildung für nachhaltige Entwicklung

Time: Tuesday 10:45–11:45 Location: SCH/A284

DD 14.1 Tue 10:45 SCH/A284

Tutorials zum Klimawandel — •Sarah Wildbichler[1], Rainer Wackermann[2], Mieke DeCock[3], Lana Ivanjek[4], Magdalena Micoloi[5], Gesche Pospiech[5] und Thomas Schubatzky[1] — [1]Universität Innsbruck, Innsbruck, Österreich — [2]Ruhr-Universität Bochum, Bochum, Deutschland — [3]KU Leuven, Leuven, Belgien — [4]JKU Linz, Linz, Österreich — [5]TU Dresden, Dresden, Deutschland

Die Stabilisierung unseres Klimas ist eine der wichtigsten Aufgaben der Menschheit im 21. Jahrhundert. Klimabildung hat das Potenzial, zum Gelingen dieser Stabilisierung beizutragen. Vor diesem Hintergrund wurden im Erasmus+ Projekt ENGAGING "Tutorials zum Klimawandel" für den Einsatz in der Sekundarstufe II und in der Lehrkräfteaus- und -fortbildung entwickelt. Im Fokus der Tutorials stehen die qualitative Auseinandersetzung mit den naturwissenschaftlichen Grundlagen des Klimawandels, Conceptual Change Prozesse der Lernenden, sowie Fähigkeiten des Kritischen Denkens. Im Beitrag werden die Tutorials, dahinterliegende fachdidaktische Prinzipien und Erkenntnisse, sowie die Ergebnisse einer Evaluierung mit Lehramtsstudierenden vorgestellt.

DD 14.2 Tue 11:05 SCH/A284

Lernen im BNE Escape Game Lab - ein außerschulischer Lernort zu Klima- und Energiewende — •Fabian Schäfer, Timo Graffe, Johannes Lhotzky und Klaus Wendt — Johannes Gutenberg-Universität, Mainz, Deutschland

Das BNE Escape Game Lab der Johannes Gutenberg-Universität Mainz ist ein außerschulischer Lernort, an dem physikalische Grundlagen des Klimawandels und der Energiewende in einer spielerischen und handlungsorientierten Lernumgebung vermittelt werden. Im Mittelpunkt stehen sogenannte Educational Escape Games - narrative Teamspiele, in denen Schüler:innen physikalische Experimente durchführen, Rätsel lösen und Zusammenhänge zwischen Energie, Strahlung, Klima und menschlichem Handeln entdecken. Das Lab umfasst mehrere thematische Stationen, etwa zu Albedo, Treibhauseffekt, Meeresspiegelanstieg oder Ozeanversauerung, die reale Experimente mit digitalen Elementen kombinieren. Die Teilnehmenden messen, berechnen und reflektieren physikalische Prozesse, um so schrittweise ein gemeinsames Ziel im Spiel zu erreichen. Der Vortrag gibt Einblicke in Aufbau und Konzeption des Labs und zeigt auf, wie Escape Games didaktisch so gestaltet werden können, dass sie ein physikalisches Verständnis fördern.

DD 14.3 Tue 11:25 SCH/A284

Von CO2e zur Flächenrepräsentation - die faszinierenden Widersprüche bei der Modellierung der Treibhaustaler — •Jonathan Grothaus, Franziska Beisler, Anna Herold, Jonas Hofmann und Thomas Trefzger — Uni Würzburg

Die Voraussetzungen eines Lebens in Deutschland machen es für jeden unmöglich, ein Leben innerhalb des 1,5°C Ziel Budgets zu leben. Deshalb ist es wichtig, sich vom CO2-Fußabdruck ab, hin zur Frage struktureller Veränderungen zu wenden: 10 km Zugfahrt in Deutschland und Polen emittieren das 20-fache derselben Entfernung in Skandinavien.

Die Treibhaustaler repräsentieren über proportionale Flächen die Emissionen aller relevanten Verhaltensweisen und setzen sie in Relation zu Klimazielen. Sie machen verschiedene Lebensstile und gesellschaftliche Voraussetzungen vergleichbar, und bereiten didaktisch den Schritt vom Fuß- zum Handabdruck: individuelles Verhalten ist durchaus relevant, strukturelle Veränderungen aber zwingend notwendig.

Der Vortrag stellt die Bewertungsdilemmata und Widersprüchlichkeiten bei der Modellierung dar: Wie berechnen sich die Emissionen von 10 km Elektroautofahrt oder dem Beheizen eines 20 qm Zimmers in einem Mehrfamilienhaus. Der zweite Teil behandelt die fertige und unter Creative Commons Lizenz veröffentlichten Treibhaustaler und die Begleitmaterialien: Sieben Arbeitseinheiten und eine Handreichung bringen die Bewertung von Strommix, Mobilitätsformen und öffentlichen Emissionen in Bildungsprozesse.

DD 15: Interesse I

Time: Tuesday 10:45–11:45 Location: SCH/A285

DD 15.1 Tue 10:45 SCH/A285

Wie Jugendliche ihre Interessen in ihrem Alltag wahrnehmen — •Hermann Lidberg und Roger Erb — IDP, Goethe-Universität Frankfurt am Main

Die positive Korrelation zwischen dem Interesse von Schüler*innen und ihren Lernleistungen konnte in verschiedenen Studien gezeigt werden. Die Förderung von Interesse an naturwissenschaftlichen Themen kann deswegen als zentrales Ziel naturwissenschaftlichen Unterrichts angesehen werden. Krapp beschreibt in seinem Interessenkonzept die wiederholte Auseinandersetzung mit einem Interessengegenstand in Begleitung positiv erlebter emotionaler Zustände als Voraussetzung für die Entwicklung individueller Interessen. Durch groß angelegte Studien (IPN-Interessenstudie, ROSE) ist bekannt, welche physikalischen Themen Jugendliche interessant finden, allerdings gibt es bisher wenige Erkenntnisse darüber, wie dieses Interesse im Alltag konstruiert und ausgelebt wird und welche Aufgabe der Schule dabei zukommt. Im Vortrag sollen Einblicke in die Ergebnisse einer Fragebogenstudie gegeben werden, die untersucht, in welchen Bereichen ihres alltäglichen Lebens (soziales Umfeld, Schule) Jugendliche ihre Interessen wahrnehmen und wie sich diese Wahrnehmung auf ihr Sach- und Fachinteresse an Physik auswirkt. Die Ergebnisse der quantitativen Studie werden mit Ausschnitten aus parallel geführten Interviews illustriert.

DD 15.2 Tue 11:05 SCH/A285

Welche Personenmerkmale prägen das Interesse an Physik? — •Daniel Laumann[1], Julia Welberg[1] und Jan Winkelmann[2] — [1]Universität Münster — [2]PH Schwäbisch Gmünd

Zahlreiche Studien zeigen, dass viele Lernende nur ein geringes Interesse am Fach Physik haben. Nach der Person-Gegenstands-Theorie des Interesses wird dieser Befund wesentlich durch individuelle Eigenschaften der Lernenden geprägt. Wie genau solche Personenmerkmale mit dem Physikinteresse zusammenhängen und dieses determinieren, untersucht fachdidaktische Forschung bisher vor allem im Hinblick auf Gender. Weitere Personenmerkmale wie z. B. die Persönlichkeit von Lernenden, ihre epistemische Neugierde oder Neigungen zu bestimmten Denkweisen werden dagegen seltener und zudem meist isoliert betrachtet. Die vorliegende Studie analysiert, inwiefern ein Spektrum an neun unterschiedlichen Personenmerkmalen mit dem Interesse von Lernenden an Physik zusammenhängt oder dieses ggf. determiniert. Es werden Befunde einer umfangreichen Stichprobe aus Lernenden der Sekundarstufe I präsentiert, die hinsichtlich der Relevanz für physikdidaktische Interessenforschung und -förderung diskutiert werden.

DD 15.3 Tue 11:25 SCH/A285

Schüler*innenperspektiven auf Physik- und Chemie-Anfangsunterricht: Ergebnisse einer offenen Befragung — •Bub Frederik[1], Rabe Thorid[1], Lisa-Marie Christ[2] und Krey Olaf[2] — [1]Martin-Luther-Universität Halle-Wittenberg — [2]Universität Augsburg

Im durch das BMBFSFJ geförderten Forschungsprojekt IdentMINT wird die Identitätsentwicklung von Schüler*innen während des Anfangsunterrichts in einem mixed-methods Längsschnittdesign untersucht. Im Rahmen des Projekts wurden n=688 Schüler*innen in Bayern und Sachsen-Anhalt schriftlich zu ihrer Wahrnehmung des Anfangsunterrichts in Physik und Chemie in einem offenen Antwortformat befragt. Die Schüler*innen haben Auskunft zu wahrgenommenen positiven Aspekten und zu ihren Veränderungs- bzw. Verbesserungswünschen gegeben. Die Antworten wurden kategorisiert und die relative Antworthäufigkeit im Sample bestimmt. Experimente, die Lehrkraft, konkrete Unterrichtsthemen und Verstehensbedingungen wurden dabei als die relevantesten Aspekte aus Schüler*innensicht identifiziert. Neben den Ergebnissen für die Gesamtstichprobe berichten wir signifikante Unterschiede zwischen Subgruppen (u.a. Gender und Extremgruppen im Hinblick auf Interesse) und die längsschnittliche Entwicklung der Einschätzung der Schüler*innen.

DD 16: Experimente

Time: Tuesday 12:00–13:00 Location: SCH/A101

DD 16.1 Tue 12:00 SCH/A101

Pilotierung einer Studie zum Vergleich zweier Versuchsvarianten eines Praktikumsversuches zur Erhaltung von Impuls und Energie — •Saskia Riedel, Frank Stallmach und Jan Bauer — Universität Leipzig, Institut für Didaktik der Physik

Für den Vergleich der Lernwirksamkeit und des wahrgenommenen Cognitive Loads von zwei Varianten eines Lehr-Lern-Szenarios zur Erhaltung von Energie und Impuls bei Stoßexperimenten mit digitaler Messwerterfassung wurde eine Pilotstudie im physikalischen Grundpraktikum für Lehramtsstudierende durchgeführt. Die Studierenden untersuchten die Impuls- und Energieerhaltung beim zentralen elastischen Stoß zweier Rollwagen, indem sie mit den Positionssensoren der Rollwaagen (Variante 1) bzw. über eine Analyse von Videoaufzeichnungen (Variante 2) die Positionen der Stoßpartner als Funktion der Zeit aufnahmen. Anschließend analysierten sie die zeitliche Entwicklung von Impuls und kinetischer Energie für verschiedene Massenverhältnisse während des gesamten Stoßprozesses.

In der Pilotierung wurde der Einfluss dieser beiden Umsetzungsvarianten auf den Lernzuwachs mit einem Pre-Post-Test und der wahrgenommene Cognitive Load der Studierenden mit einer Umfrage untersucht. Im Vortrag werden die beiden Varianten des Praktikumsversuches, das Design der Studie sowie deren Ergebnisse vorgestellt und es wird ein Ausblick zur daran anknüpfenden Hauptstudie gegeben.

DD 16.2 Tue 12:20 SCH/A101

Neuausrichtung vom Strahlenschutzpraktikum: Ein Design Based Research Projekt — •Charlotte Fischer[1,2], Gunnar Friege[2], Paul Hanemann[1], Tim Schmalz[1], Nils Sassenberg[1] und Clemens Walther[1] — [1]Universität Hannover, Institut für Radioökologie und Strahlenschutz, Herrenhäuser Str. 2, 30419 Hannover — [2]Universität Hannover, Institut für Didaktik der Mathematik und Physik - AG Physikdidaktik, Welfengarten 1, 30167 Hannover

Ein Praktikum zum Thema Radioaktivität und Dosimetrie ist seit Jahrzehnten weitgehend unverändert und soll überarbeitet und optimiert werden. Die Herausforderungen und Bedürfnisse von Lehrenden und Studierenden werden erforscht, um die Studierenden gezielt bei der Wissensanwendung, Durchführung der Versuche und deren Auswertung zu unterstützen. Der Ansatz des Design-Based Research wird eingesetzt, um eine moderne und zweckmäßige Lernumgebung zu entwickeln. In mehreren iterativen Zyklen soll die Lernumgebung auf die Bedürfnisse der Studierenden und die Kursanforderungen abgestimmt werden. Interviews mit Tutoren und Studierenden haben ergeben, dass die Vorbereitung unzureichend und das Skript veraltet ist. Als Lösung wurde eine digitale Lernumgebung entwickelt, welche unter anderem nicht-lineare interaktive Skripte zur Binnendifferenzierung beinhaltet. Die Skripte enthalten theoretische Hintergründe der Versuche und Sicherheitsmaßnahmen während des Praktikums. Das neue Material wird derzeit erstmals im Praktikum eingesetzt und im Hinblick auf Verständlichkeit, Nützlichkeit und Passung zum Kurs evaluiert.

DD 16.3 Tue 12:40 SCH/A101

CLEOPATRA - Teilchenforschung im Klassenzimmer — •Laura Rodríguez Gómez, Jochen Kaminski, Klaus Desch, Annika Hoverath, Ina Thierkopf, Tom Jakowetz und Johannes Streun — Physikalisches Institut, Universität Bonn

Wer wissen möchte, wie Forschung funktioniert, muss selbst messen, beobachten und auswerten - am besten an einem echten Experiment aus der Forschung. Das CLassroom Experiment On PArticle TRAcking (kurz CLEOPATRA) bietet einen Teilchendetektor als Experiment für den Physikunterricht der gymnasialen Oberstufe. In einer Unterrichtseinheit mit dem Detektor beschäftigen sich Schülerinnen und Schüler mit kosmischer Hintergrundstrahlung und vermessen die Winkelverteilung atmosphärischer Myonen. Der eingesetzte Teilchendetektor ist eine sogenannte Zeitprojektionskammer. Dies ist ein gasgefüllter Detektor, mit dem Teilchenspuren in 3 Dimensionen und quasi in Echtzeit aufgenommen und visualisiert werden können. Die so entstehenden Daten können digital ausgewertet werden, sodass anhand des Experiments Konzepte des Arbeitens mit digitalen Datenmengen vermittelt werden können. Dieser Vortrag stellt den CLEOPATRA-Detektor vor und bietet einen Einblick in seine Einsatzmöglichkeiten im Unterricht. Es werden Ergebnisse aus der Erprobung mit Schüler*innen und Lehrkräften präsentiert.

DD 17: Außerschulische Lernorte II

Time: Tuesday 12:00–13:00 Location: SCH/A252

DD 17.1 Tue 12:00 SCH/A252

Quanten auf Reisen - eine interaktive Wanderausstellung (Q-Bus) — •Jannis König, Andreas Fuchs, Andreas Buchleitner, Thomas Filk und Anja Kuhnhold — Physikalisches Institut, Albert-Ludwigs-Universität Freiburg, Hermann-Herder-Straße 3, 79104 Freiburg im Breisgau

Die Quantenphysik zählt zu den fundamentalen Säulen der modernen Physik und prägt maßgeblich unser heutiges Verständnis der Natur. Das Outreach-Projekt Quanten auf Reisen verfolgt das Ziel, die Gesellschaft durch eine interaktive Wanderausstellung mit aktuellen Quantentechnologien in Kontakt zu bringen. Die Ausstellung richtet sich an eine breite Öffentlichkeit und umfasst Messeauftritte, Schulbesuche sowie Fortbildungen für Lehrkräfte. Parallel zu den Outreach-Aktivitäten werden vertiefende Begleitmaterialien entwickelt, welche die Ausstellung unterstützen. Dazu gehören unter anderem Schulposter, Arbeitsblätter und Laufzettel. Ein zentrales Anliegen der Wanderausstellung ist es, gängige Fehlvorstellungen zur Quantenphysik zu identifizieren und aufzulösen. Zudem sollen die Lernfortschritte der Teilnehmer systematisch erfasst werden, um die Ausstellung kontinuierlich weiterzuentwickeln und besonders wirksame Vermittlungsansätze herauszuarbeiten. Die Exponate basieren überwiegend auf Analogieexperimenten zur Quantenphysik, die sich vor allem die Polarisationseigenschaften von Licht zunutze machen. Damit soll Quanten auf Reisen einen niedrigschwelligen und zugleich anschaulichen Zugang zur Quantenphysik ermöglichen und das Verständnis sowie die Neugier gegenüber Quantentechnologien stärken.

DD 17.2 Tue 12:20 SCH/A252

Raman-Spektroskopie im Schülerlabor — •Elias Oehler, Holger Cartarius und Dustin-Philipp Preissler — AG Fachdidaktik der Physik und Astronomie, Friedrich-Schiller-Universität Jena, 07743 Jena

Raman-Streuung bringt bis heute neue Verfahren zur Strukturanalyse verschiedenster Proben hervor. Obwohl sie seit langer Zeit Gegenstand der Forschung ist, findet Raman-Streuung in der Schule nur selten Erwähnung. Dabei ist sie experimentell in einer übersichtlichen Versuchsanordnung zugänglich.

In diesem Vortrag stellen wir unseren Raman-Spektroskopie-Aufbau für das Schülerlabor vor. Dieser ist kostengünstig, für Schülerinnen und Schüler sicher und liefert sowohl qualitativ als auch quantitativ bemerkenswerte Ergebnisse. Der Versuch ermöglicht dabei die Auseinandersetzung mit einer Vielzahl verschiedener Themen. Neben der Raman-Spektroskopie selbst sind das die Funktionsweise und Charakterisierung von Lasern, der Umgang mit optischen Aufbauten und Fluoreszenz. Methoden der Aufbereitung und Analyse von Messdaten und weitere Inhalte können am Rande oder intensiver behandelt werden.

DD 17.3 Tue 12:40 SCH/A252

Projektionale Augmented Reality im Schülerlabor: Lernsituationen im Spannungsfeld von Inszenierung und Propädeutik — •Fabian Bernstein[1], Thomas Wilhelm[2] und Carsten Nowak[3] — [1]TECHNOSEUM Mannheim — [2]Goethe-Universität Frankfurt — [3]Georg-August-Universität Göttingen

Projektionsbasierte Augmented-Reality-Systeme eröffnen neue Möglichkeiten für experimentelles Lernen, indem sie klassische Schülerexperimente durch digitale Overlays erweitern. Mittels Top-Down-Projektion lassen sich unsichtbare Größen visualisieren und narrative oder spielerische Zugänge zu physikalischen Phänomenen schaffen. Im Unterschied zu Head-Mounted Displays bleiben sie dabei niedrigschwellig, kollaborativ und robust.

Der Einsatz solcher Lernumgebungen bewegt sich im Spannungsfeld zwischen Zielgruppenorientierung und Wissenschaftspropädeutik: Einerseits sollen die Formate mediale Gewohnheiten von Jugendlichen berücksichtigen, andererseits an akademische Kontexte heranführen, in denen textbasierte Instruktionen dominieren. Einerseits sollen authentische Einblicke in wissenschaftliches Arbeiten ermöglicht werden; andererseits erzwingen Randbedingungen stark didaktisierte Lernsettings, die eher Inszenierungscharakter tragen.

Vor diesem Hintergrund werden am INNOVATIONlab des TECHNOSEUM sowie am XLAB der Universität Göttingen systematisch Potenziale projektionsbasierter Augmented Reality untersucht. Der Vortrag stellt die zugrunde liegenden Konzepte vor, diskutiert Herausforderungen der Umsetzung und berichtet von ersten Erfahrungen.

DD 18: BNE Workshop

Time: Tuesday 12:00–13:30 Location: SCH/A284

DD 18.1 Tue 12:00 SCH/A284

Workshop: SDGs nicht nur als Feierabendprogramm – politische Verantwortung im Physikstudium thematisieren — •Annemarie Sich[1], Barbara Obwaller[2], Manuel Längle[3], Jonathan Möller[4] und Stefan Brackertz[1] — [1]Universität zu Köln, Fachschaft Physik — [2]Universität Innsbruck, Studienvertretung Physik — [3]University Paris-Saclay, CNRS, Laboratoire de Physique des Solides Jetzt — [4]TU Dresden, Fachschaft Physik

Viele Hochschulen widmen sich vorgeblich der Realisierung der SDGs in Forschung und Lehre, während Studierende davon in den Kernveranstaltungen der Physik wenig merken. Verbreitet sind dagegen Zusatzangebote, etwa Ringvorlesungen, zu diversen Klimafragen. Parallel dazu laufen Debatten um Zivilklauseln, (Selbst-)Verpflichtungen der Hochschulen auf Frieden, Nachhaltigkeit und mehr; EU und Bundesministerien fordern explizit, dass gerade Physik eine größere Rolle bei der "Sicherheitsforschung" spielen soll, wodurch internationale Kooperation erheblich eingeschränkt wird.

Wir wollen im Workshop anhand zuvor gesammelter Beiträge diese Puzzleteile zusammenlegen und fragen, was es heißt, dies angemessen in der Studieingangsentwicklung zu berücksichtigen. Oder anders gesagt: Wie schafft man es, dass das Physikstudium nicht nur nach Feierabend im Bonusprogramm zur Realisierung der SDGs beiträgt?

Mehr: studienreform-forum.de

DD 19: Hochschuldidaktik II

Time: Tuesday 12:00–13:00 Location: SCH/A285

DD 19.1 Tue 12:00 SCH/A285

Konzeptionelles Verständnis und Vorstellungen von Studierenden zum elektrischen Stromkreis — •Bernadette Schorn[1], Florian Bernlochner[1], Benjamin Gross[2] und Jan-Philipp Burde[2] — [1]Universität Bonn — [2]Universität Tübingen

Beim Lehren grundlegender Konzepte zum elektrischen Stromkreis steht man einer Reihe sowohl sachbedingter, lehrbedingter und innenbedingter Lernschwierigkeiten gegenüber, die sich teilweise gegenseitig bedingen und überschneiden. Mit dem Ziel der (Weiter-)Entwicklung von Lehr- und Lernmaterialien für die Hochschule wurden in einem ersten Schritt an der Universität Bonn das konzeptionelle Verständnis und die Lernendenvorstellungen von Studierenden der Physik (Haupt- und Nebenfach) sowie Lehramtsstudierenden der Physik mittels eines dreistufigen Multiple-Choice-Tests (Groß et al. 2024, 2025) untersucht. Im Vortrag werden erste Ergebnisse zum konzeptionellen Verständnis und zu den Lernendenvorstellungen der Studierenden des fachlichen Studiengangs B.Sc. Physik (Ein-Fach-Bachelor) vor und nach der Behandlung von Inhalten zur Elektrizitätslehre in einer Grundvorlesung vorgestellt.

DD 19.2 Tue 12:20 SCH/A285

Ausgewählte Kapitel der Modernen Physik - Eine Spezialvorlesung für Lehramtsstudierende — •Thomas Filk — Physics Institute, Freiburg, Germany

Vor vier Jahren wurde an der Universität Freiburg eine Spezialvorlesung für Lehramtsstudierende eingerichtet, in der schulrelevante Themen aus der Physik behandelt werden, die im regulären Physikstudium für Lehramtsstudierende üblicherweise nicht angesprochen werden. Zu diesen Themen zählen Klimaphysik, Physik der Sonne und des Erde-Mond-Systems, Kosmologie und kosmologische Entfernungsleiter, Grundlagen der allgemeinen Relativitätstheorie und der Theorie Schwarzer Löcher, Gravitationswellen sowie weitere Themen, auf die Lehrkräfte häufig von Schülerinnen und Schülern angesprochen werden. Zu den einzelnen Inhalten der Vorlesung wurden sogenannte Kurztexte erstellt: Es handelt sich dabei um Texte zu einem Thema von höchstens 10-15 Seiten. Die Texte sind im Allgemeinen in sich abgeschlossen und setzen nur das Grundwissen eines Physikstudiums voraus.

In meinem Vortrag berichte ich von den Erfahrungen der ersten vier Jahre mit der Vorlesung und den Kurztexten. Die Materialien stehen zur freien Verfügung. Das Konzept dieser Vorlesung eignet sich besonders für Studiengänge, bei denen die Lehramtsstudierenden größtenteils dieselben Vorlesungen hören wie die Studierenden der Fachwissenschaft.

DD 19.3 Tue 12:40 SCH/A285

Physik als Nebenfach im Studium: Lernmotivationskonzept und weitere Entwicklung. — •Irina Schneider — IEAP CAU Leibnitzstrasse 19 24098 Kiel

Vor vier Jahren haben wir den Kurs Physik Nebenfach, der unter Kritik stand, an der Universität Kiel übernommen. Wir haben die Problematik des Kurses erforscht, verschiedene Methoden ausprobiert und ein Motivationskonzept entwickelt. Die Grundprobleme dieses großen Kurses sind: Die Studierenden kommen aus fünf unterschiedlichen Fachrichtungen (aktuell schon aus sechs), sie haben sehr unterschiedliches Vorwissen in Physik und Mathematik, hatten unterschiedliche Pflichtveranstaltungen im Kurs und nach dem Kurs geht es für sie unterschiedlich weiter. Auch Lernblockaden, die durch negative Erfahrungen mit Physik in der Schule entstanden sind, spielen hier eine wichtige Rolle. Unser Motivationskonzept beinhaltet drei Hauptrichtungen: 1. Wir unterstützen unsere Studierenden auf verschiedene Weise beim Einstieg in Physik und Mathematik und holen sie dort ab, wo sie stehen. Der Physikunterricht wird für die Studierenden interessant und attraktiv gestaltet. 2. Wir bleiben ständig im Dialog mit den Studierenden, führen oft Befragungen durch, um ihre Meinung zum Unterricht, zum Schwierigkeitsgrad der Aufgaben usw. zu erfahren, und stellen uns in gewissen Grenzen auf ihre Wünsche ein. 3. Wir arbeiten eng mit den Fachrichtungen zusammen, aus denen unsere Studierenden kommen. Unser Lernmotivationskonzept wurde von Studierenden und Fachkollegen positiv bewertet. Der Kurs hat sich fast verdoppelt.

DD 20: Poster – Lehrkräfteaus- und -fortbildung

Time: Tuesday 14:00–16:00 Location: P5

DD 20.1 Tue 14:00 P5

Erste Ergebnisse einer großen Lehrkräftebefragung zur Implementation physikdidaktischer Ideen — •Jakub Knebloch und Thomas Wilhelm — Institut für Didaktik der Physik, Universität Frankfurt

Trotz zahlreicher Entwicklungen neuer physikdidaktischer Unterrichtskonzepte und Materialien zeigt sich seit Jahrzehnten, dass ein Großteil neuer Ideen nicht, kaum oder erst sehr spät im Klassenzimmer ankommt.

In einer Vorstudie wurden explorative, halboffene Interviews mit fünfzehn Lehrkräften der Sekundarstufe I und II zu den Ursachen der beschriebenen Problematik durchgeführt und ausgewertet. Dies diente als Ausgangspunkt für die Entwicklung eines Fragebogens zur systematischen und quantitativen Analyse der möglichen Ursachen. Das Instrument wurde mehrfach pilotiert und auf vielfältige Weise validiert, u.a. mittels konfirmatorischer Faktorenanalyse. Die siebenfaktorielle Struktur (Zeit, Ideensuche, Schulausstattung, Informiertheit, Schüler*innen, Institution, physikdidaktische Ideen) konnte durch sehr gute Fit-Indizes, hohe Faktorladungen sowie zufriedenstellende Reliabilitäten und AVE-Werte empirisch bestätigt werden.

Das Poster präsentiert nun erste Ergebnisse dieser groß angelegten Befragung von Physiklehrkräften aus Hessen, Bayern und Österreich mit ca. 600 vollständig ausgefüllten Datensätzen. Die Auswertung erlaubt u.a. Einblicke in Unterschiede zwischen Subgruppen, etwa zwischen jüngeren und älteren Lehrkräften oder zwischen verschiedenen Schulformen.

DD 20.2 Tue 14:00 P5

Mit Lehrkräfte-Netzwerken zu mehr Lehrinnovationen in der Schulpraxis? — •Ramona Schauer-Bollig und Heidrun Heinke — RWTH Aachen University, I. Physikalisches Institut IA

Die Weiterentwicklung schulischen Unterrichts ist ein wichtiger Aspekt fachdidaktischer Forschung. Dafür ist neben der Entwicklung von Lehrinnovationen auch deren erfolgreiche Implementation in der Schulpraxis von Relevanz. Vor dem Hintergrund unzulänglicher Rahmenbedingungen für eine systematische Fort- und Weiterbildung für Lehrkräfte in Deutschland stellt dies eine besondere Herausforderung dar. Eine vielversprechende Strategie ist der symbiotische Implementationsansatz, der durch einen Austausch zwischen Wissenschaft und Praxis sowie eine Zusammenarbeit der Akteure auf Augenhöhe geprägt ist. Lehrkräfte-Netzwerke mit gleichzeitiger Beteiligung von Hochschulen bilden einen möglichen Rahmen, um diese Form der Kooperation zu realisieren. Mit dem Forschungsvorhaben wird den Fragen nachgegangen, ob etablierte

Netzwerke ein gangbarer Weg sind, physikdidaktische Lehrinnovationen in der Schule erfolgreich zu implementieren und wie geeignete Rahmenbedingungen für nachhaltig wirksame Lehrkräfte-Netzwerke aussehen können. In mehreren Schritten werden dazu etablierte Netzwerke von und für Lehrkräfte und deren Nutzung durch Lehrkräfte analysiert. Zudem wird anhand von zwei Beispielen untersucht, über welche Wege der Dissemination sich Lehrinnovationen in der Schulpraxis verbreitet haben.

DD 20.3 Tue 14:00 P5

Die Didaktische Vertiefung an der FAU: Konzept und Weiterentwicklung — •Antonia Bauer — FAU Erlangen-Nürnberg, Didaktik der Physik

An der Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU) wurde vor zwei Jahren damit begonnen, die Physiklehrkräftebildung zu reformieren: In einer neu gestalteten Lehrveranstaltung des ersten Fachsemesters werden fachwissenschaftliche und fachdidaktische Komponenten systematisch miteinander verknüpft. Die "Didaktische Vertiefung" greift dabei fachwissenschaftliche Inhalte auf, stellt die Verbindung zu didaktischen Konzepten her und schlägt die Brücke zum Physikunterricht. Ab dem Wintersemester 2025/26 wird diese Veranstaltung systematisch evaluiert, sodass strukturierte Rückmeldungen der Studierenden gezielt erfasst und ausgewertet werden können. Auf dem Poster wird das Konzept der Lehrveranstaltung exemplarisch vorgestellt. Es werden die bisherigen Erfahrungen zusammengefasst, und der mehrjährige Prozess der kontinuierlichen Weiterentwicklung wird skizziert.

DD 20.4 Tue 14:00 P5

Nachqualifizierung zur Unterrichtserlaubnis Physik: Erfahrungen, Herausforderungen und Perspektiven aus einer Weiterbildung als Antwort auf den Lehrkräftemangel — •Stefan Aehle, Dustin-Philipp Preissler und Holger Cartarius — AG Fachdidaktik der Physik und Astronomie, Friedrich-Schiller-Universität Jena

Der zunehmende Mangel an qualifizierten Physiklehrkräften stellt Schulen bundesweit vor große Herausforderungen. Um kurzfristig handlungsfähig zu bleiben und gleichzeitig die fachliche Qualität des Unterrichts zu sichern, bietet das Thüringer Institut für Lehrerfortbildung, Lehrplanentwicklung und Medien (ThILLM) in Kooperation mit der Friedrich-Schiller-Universität Jena eine einjährige Nachqualifizierung zum Erwerb einer Unterrichtserlaubnis für das Fach Physik an. Zielgruppe der Weiterbildung sind Lehrkräfte ohne Physik-Lehrbefähigung, die bereits im Schuldienst tätig sind und nach Abschluss eigenständig Physik in den Klassenstufen 7-10 unterrichten sollen. Der Lehrgang kombiniert fachliche Grundlagen mit physikdidaktischen Elementen, sicherheitsrelevanten Aspekten, sowie umfangreichen Praxisanteilen in Form von Experimentierwochen. Vorgestellt werden Erfahrungen aus zwei Semestern: Welche fachlichen und didaktischen Hürden zeigten sich bei den Teilnehmenden? Welche Unterstützungsformate bewährten sich? Es werden Herausforderungen für zukünftige Durchgänge benannt, Ergebnisse diskutiert und Implikationen für ähnliche Qualifizierungsprogramme vorgestellt.

DD 21: Poster – Außerschulische Lernorte

Time: Tuesday 14:00–16:00 Location: P5

DD 21.1 Tue 14:00 P5

Experimente zur Photonik im Schülerlabor — •Laureen Dänzer, Kim Kappl, Simon Koppenhöfer, Philipp Scheiger und Ronny Nawrodt — Universität Stuttgart, Physik und ihre Didaktik, Pfaffenwaldring 57, 70569 Stuttgart, Deutschland

Photonische Technologien stellen wichtige Schlüsseltechnologien in Forschung und Industrie dar und prägen vielfach unseren Alltag. Aus didaktischer Sicht sind photonische Experimente attraktiv, da vielfach ein einfacherer und visueller Zugang im Vergleich zu beispielsweise supraleitenden Komponenten in Quantentechnologien besteht. Leider bleibt in der schulischen Ausbildung zu wenig Zeit, um Grundlagen auf diesem Gebiet zu legen trotz seiner auch hohen wirtschaftlichen Bedeutung. Hierzu zählt auch die Polarisation, welche in unterschiedlichsten modernen Technologien Anwendung findet und zudem Alltagsnähe der Schülerinnen und Schülern mit sich bringt. Daher wurde ein Konzept erarbeitet, bei dem ausgewählte Themen der Photonik Schülerinnen und Schülern der Oberstufe vermittelt werden. Lehrerinnen und Lehrern, die im Rahmen eines Schülerlaborbesuchs ihr Klasse an die Universität bringen, werden mehrere Experimente angeboten. Das Konzept und ein erster Einblick in Experimente zur Polarisation werden vorgestellt, ebenso wie zukünftige Ideen.

DD 21.2 Tue 14:00 P5

Geschlechteraspekte im Blick: Interesse und Partizipation im Schülerlabor — •Simon Becher und Holger Cartarius — AG Fachdidaktik der Physik und Astronomie, Friedrich-Schiller-Universität Jena, 07743 Jena

Die physikdidaktische Forschung hat das Ungleichgewicht der Geschlechter bei der Beliebtheit des Schulfaches Physik mehrfach untersucht. Gut bekannt ist ebenfalls, dass erfolgversprechende Interventionen, dem Ungleichgewicht entgegenzuwirken, im gelegentlichen Durchführen monoedukativer Unterrichtsphasen, im Bezug zu Alltagsphänomenen und in der Wahl eines Kontextes für die Vermittlung der physikalischen Kernkompetenzen liegen. Aufbauend auf diesen Erkenntnissen wird in vielen Schülerlaboren bei der Zusammenstellung von Experimentiergruppen darauf geachtet, dass einzelne Versuche oder ganze Versuchsreihen monoedukativ durchgeführt werden – so auch im Schülerlabor Physik der Universität Jena.

Wir untersuchen, ob sich ein positiver Effekt auf das Interesse – wenn auch nur kurzfristig – bei einem Besuch des Schülerlabors einstellt. Erste Resultate einer Befragung werden vorgestellt.

DD 22: Poster – Astronomie

Time: Tuesday 14:00–16:00 Location: P5

DD 22.1 Tue 14:00 P5

The European Space Education Regional Office (ESERO) in Germany — •Ralf-Jürgen Dettmar — Ruhr University Bochum, Bochum, Germany

ESERO(European Space Education Research Office) Germany, the space education office of ESA in Germany based at Ruhr University Bochum is a joint project of the European Space Agency (ESA) and the German Aerospace Center (DLR). Space topics fascinate students and therefore provide ideal entry points for lively, competency-oriented STEM teaching. ESERO Germany aims to support teachers at all levels in harnessing this enthusiasm: with proven teaching materials, practice-oriented professional development, and exciting school projects around space, earth observation, space research, and technology. The poster introduces the various ESERO activities, such as school projects and teaching materials for different subjects (Biology, Chemistry, Physics, Geography, Mathematics, Computer Science, General Studies).

DD 22.2 Tue 14:00 P5

Geozentrisch zu heliozentrisch? - Mentale Modelle des Sonnensystems von während der Schulzeit — •Maximilian Loch[1], Emmanuel Rollinde[1] und Malte S. Ubben[2] — [1]Université Cergy-Pontoise — [2]Universität Leipzig

Neue empirische Befunde deuten darauf hin, dass gestaltliche und funktionale Aspekte mentaler Modelle klar voneinander zu unterscheiden sind. Dies ist besonders relevant für die meist gestaltorientierte Astronomiedidaktik, in der das Sonnensystem eines der zentralen Themen darstellt. Dennoch ist bislang wenig darüber bekannt, wie sich entsprechende Vorstellungen über die Schuljahre hinweg entwickeln; häufig wird lediglich das System Erde-Sonne-Mond untersucht. In unserer Studie analysieren wir eine umfangreiche Sammlung von Zeichnungen internationaler Lernender der Jahrgangsstufen 4 bis 12. Auf dieser Grundlage identifizieren wir typische strukturelle Gestalten ihrer mentalen Modelle des Sonnensystems und untersuchen deren Variation in Abhängigkeit vom Alter. Ausgewählte Ergebnisse dieser Analyse werden auf dem Poster vorgestellt.

DD 23: Poster – Bildung für nachhaltige Entwicklung

Time: Tuesday 14:00–16:00 Location: P5

DD 23.1 Tue 14:00 P5

Klimamodelle als System begreifen: Entwicklung eines Mess- und Modellsystems zur Klimaphysik für das Physikpraktikum — •Maximilian Kühlkamp, Ralf Detemple und Heidrun Heinke — RWTH Aachen University

Der Klimawandel stellt eines der größten globalen Probleme dar. Gerade der Physik kommt als einer Wissenschaft der Erkenntnisgewinnung die Aufgabe zu, das nötige Wissen und methodische Zugänge zu vermitteln, die als Grundlage zum Verständnis des Klimawandels und seiner Herausforderungen dienen können. Da das Klima ein komplexes System mit vielfältigen Komponenten und Wechselwirkungen ist, werden unterschiedliche Modelle zur Beschreibung des Klimas und des Klimawandels eingesetzt, die entweder auf Simulation oder auf experimentelle Zugänge setzen. In dem hier vorgestellten Ansatz sollen beide Zugänge miteinander verknüpft werden. Hierfür wird für eine Experimentier-Box als Analogie zum Klimasystem der Erde ein vereinfachtes Klimamodell entwickelt, mittels Python simuliert und durch Messungen überprüft. Dies wird in ein „Doing-Science"-Setting für Nebenfachstudierende im physikalischen Praktikum eingebettet. Dabei fungiert die Informatik als wichtige Schnittstelle zwischen mathematischer und physikalischer Beschreibung und deren Simulation. Dadurch entsteht ein konkreter Anwendungsfall für Python, der einerseits an die im Praktikum bereits erfolgreich eingesetzte Einführung in die datengestützte Auswertung mit Python anschließt und andererseits einen Beitrag zur Bildung für nachhaltige Entwicklung leisten soll.

DD 23.2 Tue 14:00 P5

Nachhaltiges Handeln im Physikunterricht: Das Transtheoretische Modell am Beispiel der Energiewende — •Timo Graffe, Margarete Imhof und Klaus Wendt — Johannes Gutenberg-Universität, Mainz, Deutschland

Das Transtheoretische Modell der Verhaltensänderung ermöglicht eine systematische Planung nachhaltigkeitsbezogener Lernprozesse im Physikunterricht. Das Poster beschreibt, wie Lehrkräfte die verschiedenen Stufen des Modells - von fehlender Handlungsabsicht bis hin zur Stabilisierung neuen Verhaltens - nutzen können, um Schülerinnen und Schüler beim Entwickeln nachhaltiger Handlungskompetenzen zu unterstützen. Am Beispiel des Themas "Energiewende" wird erläutert, wie sich kognitive-affektive und handlungsorientierte Strategien didaktisch verankern lassen, etwa durch das Arbeiten mit Zukunftsbildern, die kritisch-reflexive Betrachtung des eigenen Alltags oder die gezielte Förderung von Selbstwirksamkeit. Das Modell dient dabei als Orientierung, um unterschiedliche Lernvoraussetzungen einzubeziehen und Lernarrangements so zu gestalten, dass eine fundierte Auseinandersetzung mit der Klimakrise und ein Übergang zu nachhaltigem Handeln ermöglicht werden.

DD 23.3 Tue 14:00 P5

Was verstehen Schüler:innen unter dem Begriff Nachhaltigkeit? - Und hat das mit Klimabildung zu tun? — •Jarmo Günther und Stefan Heusler — Universität Münster, Institut für Didaktik der Physik

Mit der Einführung der siebzehn Sustainable Development Goals (SDGs) durch die United Nations wurde das Konzept der Nachhaltigkeit international verankert. Entsprechend hat die Bildung für nachhaltige Entwicklung (BNE) in Deutschland eine zentrale Rolle in schulischen Lehrplänen eingenommen. Damit wird von Schulen erwartet, Lernende zu einem reflektierten, handlungsorientierten und mehrdimensionalen Verständnis von Nachhaltigkeit zu befähigen.

Im Rahmen der Posterpräsentation wird dargestellt, welche Vorstellungen und Konzepte über Nachhaltigkeit bei Schülerinnen und Schülern verschiedener Altersstufen existieren. Die Methodik umfasst eine systematische Literaturrecherche, die internationale und deutschsprachige Veröffentlichungen der letzten zwei Jahrzehnte berücksichtigt. Es soll identifiziert werden, welche Dimensionen - ökologisch, ökonomisch, sozial - in Schülerkonzepten vorhanden sind, und ob Hinweise auf metakonzeptionelles Verständnis erkennbar sind.

Das Poster bietet einen strukturierten Überblick über den Forschungsstand als Ansatzpunkt für zukünftige empirische Studien.

DD 23.4 Tue 14:00 P5

Wie geht es weiter mit Labs4Future? - Klimabildung zwischen individueller und kollektiver Wirksamkeit — •Anna Herold, Jonathan Grothaus, Markus Elsholz und Thomas Trefzger — Uni Würzburg

Das interdisziplinäre Schülerlabor Labs4Future (9. Jgst., 2 Tage à 6h) zielt darauf ab, Lernende über reine Wissensvermittlung hinaus zu wirksamen Handlungsoptionen im Kontext der Klimakrise zu befähigen. Das zugrunde liegende Handlungsmodell Lessons4Action basiert auf indivdualpsychologischen Modellen wie der TBP und dem Norm Activation Model. Erste Ergebnisse der quantitativen Begleitforschung durch Grothaus et al. zeigen einen unerwarteten Befund: Während das partizipative Verhalten der Lernenden nach der Teilnahme am Labs4Future signifikant steigt, sinken die Werte der Climate Change Hope Scale, die individuelle Selbstwirksamkeit abbildet. Dies deutet darauf hin, dass individualpyschologische Modelle an ihre Grenzen stoßen und die kollektiven Dimensionen des Handelns stärker berücksichtigt werden müssen.

Vor diesem Hintergrund gewinnt die Einbindung kollektiver Handlungsmodelle wie des SIMPEA-Modells an Bedeutung, um die theoretische Grundlage um eine kollektive Ebene zu erweitern. Die geplante Forschung runtersucht, wie Jugendliche kollektives Handeln und kollektive Wirksamkeit verstehen, welche didaktisch-methodischen Elemente entsprechende Wirksamkeitserwartungen beeinflussen und welchen Beitrag (außerschulische) Bildungsangebote zur Förderung individueller und kollektiver Wirksamkeit leisten können.

DD 23.5 Tue 14:00 P5

Perspektiven von Physiklehrkräften zu politischer Klimabildung — •Niklas Kempf und Rita Wodzinski — Universität Kassel

Laut Niebert (2019) schließt effektive Klimabildung politische Bildung mit ein. Kranz et al. (2022) empfehlen daran anknüpfend, den Klimawandel im Unterricht als socio-scientific issue zu behandeln. Sie stellen allerdings fest, dass Bildungsangebote zur Klimabildung häufig politische Aspekte und die kollektive Handlungsebene des Klimawandels vernachlässigen.

Bildungsangebote in der Schule werden unter anderem von den Überzeugungen der Lehrkräfte geprägt. Deshalb soll im Rahmen dieses Projektes untersucht werden, in welches Verhältnis Physiklehrkräfte politische Bildung und Physikunterricht setzen. Welchen Beitrag schreiben sie dem Physikunterricht bei der unterrichtlichen Bearbeitung des Klimawandels als socio-scientific issue zu? Welche Faktoren hindern sie potenziell an einer Thematisierung politischer Aspekte? Diese Fragen sollen mit einer qualitativen Studie erforscht werden. Das Poster gibt erste Einblicke in die Studie.

DD 24: Poster – Digitale Medien

Time: Tuesday 14:00–16:00 Location: P5

DD 24.1 Tue 14:00 P5

Entwicklung neuartiger KI-gestützter Aufgabenformate für den Physikunterricht — •Sina Pfleiderer, Jan-Philipp Burde und Tilmann Steinmetz — Universität Tübingen, Tübingen, Germany

Die Aufgabenkultur im Physikunterricht gilt als sehr einseitig auf Routine- und Rechenaufgaben ausgelegt. Generative KI eröffnet neue Möglichkeiten zur Gestaltung neuartiger offener Aufgabenformate. Vor diesem Hintergrund wurden im Rahmen einer Bachelorarbeit verschiedene KI-basierte Aufgabenformate theoriegeleitet mit dem Ziel entwickelt, neben dem Fachwissen auch die Kompetenzbereiche Erkenntnisgewinnung, Bewertung und Kommunikation gezielt zu fördern. Der zentrale Ansatz besteht darin, dass die KI verschiedene Rollen oder historische Persönlichkeiten emuliert und so kontextreiche Auseinandersetzungen mit physikalischen Inhalten ermöglicht.

Auf dem Poster werden die folgenden beiden Aufgabenformate vorgestellt: 1) Argumentative Auseinandersetzungen mit KI-emulierten Personen, die eine Gegenposition einnehmen, etwa Befürworter oder Gegner der Windkraft. 2) Interviews mit den von der KI-emulierten historischen wissenschaftlichen Persönlichkeiten (z.B. J. Fourier und G.S. Ohm), u.a. um die historische Entwicklung von Wissen und damit auch Aspekte von Nature of Science zu adressieren. Die entwickelten CustomGPTs können von Lehrkräften unmittelbar im Unterricht eingesetzt werden und zugleich als exemplarische Vorlage für weitere KI-gestützte Lernaufgaben dienen.

DD 24.2 Tue 14:00 P5

Physik auf dem Spielplatz erleben: Entwicklung von Experimenten zur Mechanik mit phyphox — •Lena Busse, Marija Herdt, Sebastian Staacks und Heidrun Heinke — RWTH Aachen University

Im Rahmen einer Bachelorarbeit wurden Experimente für den Spielplatz entwickelt und erprobt, um zentrale mechanische Konzepte wie Geschwindigkeit, Beschleunigung und Kraft für Schüler:innen der Sekundarstufe I sowie interessierte Laien (Kinder oder Erwachsene, die sich seit der Schule nicht mehr mit Physik beschäftigt haben) erfahrbar zu machen. Mithilfe der App phyphox lassen sich alltägliche Bewegungen – etwa das Schaukeln oder das Drehen auf einem Karussell – in quantifizierbare Messprozesse überführen, wodurch eine enge Verbindung zwischen körperlicher Erfahrung und physikalischer Modellbildung hergestellt werden kann. Es wurden Anleitungen zur Durchführung der

Experimente und Aufgaben zur Auswertung und Interpretation der Messdaten unter Einbezug der Schülervorstellungsforschung erstellt. Dabei werden die Periodendauer, Geschwindigkeit und Beschleunigung an einer Schaukel und die Zentripetalbeschleunigung an einem Karussell untersucht. Erstes Feedback von 36 Schüler:innen zeigt neben einer hohen Motivation und positiver Resonanz zusätzlich ein hohes Potenzial, physikalische Phänomene anschaulich zu vermitteln und Lernprozesse nachhaltig zu unterstützen. Die Konzeption der Experimente und die Ergebnisse erster Erprobungen werden im Poster vorgestellt.

DD 24.3 Tue 14:00 P5

KI in der Schule: Nutzung, Einstellung und Kompetenzen von angehenden und praktizierenden Lehrpersonen — •Ludwig Schultz, Jens Damköhler, Wolfgang Lutz und Thomas Trefzger — Emil-Hilb-Weg 22 97074 Würzburg

Mit dem Aufkommen großer Sprachmodelle (LLMs), insbesondere seit der Veröffentlichung von ChatGPT im November 2022, dringt die Diskussion um die unterrichtliche Nutzung künstlicher Intelligenz (KI) in den Lehralltag ein. Der Einsatz von KI im Unterricht stellt angehende und praktizierende Lehrpersonen nicht nur vor technische und pädagogische Herausforderungen, sondern prägt auch deren Einstellung und Nutzungsverhalten gegenüber dieser Technologie. So hängt nach dem Technologieakzeptanzmodell (TAM) die tatsächliche Nutzung von der Einstellung zur Technologie ab. Erfahrungen beeinflussen gemäß der Selbstwirksamkeitstheorie von Bandura Selbstwirksamkeitserwartungen der Lehrpersonen und damit deren Einstellungen.

In einer Erhebung der Universität Würzburg wurden Lehramtsstudierende im Sommersemester 2025 befragt, um ihre Einstellungen gegenüber KI-Werkzeugen (GAAIS) zu ermitteln und Zusammenhänge mit der Nutzung von KI sowie der Selbsteinschätzung bezüglich AI-Literacy (MAILS) zu untersuchen. In einer zweiten Erhebung im Sommer 2025 wurden Lehrpersonen in der zweiten und dritten Phase der Lehrerbildung mit den gleichen Instrumenten befragt. Dabei wird die Untersuchung vor allem von der Frage geleitet, inwieweit sich die (selbsteingeschätzten) Kompetenzen in den Gruppen der praktizierenden und angehenden Lehrpersonen unterscheiden.

DD 24.4 Tue 14:00 P5

Ein Lehrprojekt zu KI als Forschungswerkzeug in der biologischen Physik — Yoav G. Pollack[1], Komal Bhattacharyya[1] und •Stefan Klumpp[1,2] — [1]Institut für Dynamik komplexer Systeme, Universität Göttingen, Göttingen — [2]Max Planck School Matter to Life

Generative KI-Anwendungen finden zunehmende Akzeptanz als alltägliches Werkzeug in Forschung und Lehre. Dennoch macht der effektive Einsatz dieser Werkzeuge sowohl Studierenden wie auch Lehrenden noch Schwierigkeiten. Um dies in der Lehre zu thematisieren, haben wir in einem Lehrprojekte Studierende Themen der biologischen Physik mit Hilfe von KI-Tools recherchieren lassen. Das Projekt wurde einmal mit Master- und einmal mit Bachelor-Studierenden durchgeführt. Begrenzte Instruktion zu Strategien für eine effizientere KI-Nutzung weckten Interesse und Kreativität der Studierenden und motivierten die Reflexion des eigenen KI-Einsatzes.

DD 25: Poster – Experimente und Praktika

Time: Tuesday 14:00–16:00 Location: P5

DD 25.1 Tue 14:00 P5

Physik des Frisbeeflugs im kontextorientierten Unterricht — •Dominik Dorsel, Heidrun Heinke und Bianca Watzka — I. Physikalisches Institut A, RWTH Aachen University

Der Frisbeeflug lässt sich durch zwei zentrale Prinzipien beschreiben: den aerodynamischen Auftrieb durch die gewölbte Form (Bernoulli-Effekt) und die Stabilisierung durch die Rotationsbewegung um dieeigene Achse. Mithilfe moderner Sensorik werden sowohl Druckunterschiede als auch die Rotationsrate der Scheibe während des Flugs erfasst. Die gewonnenen Messdaten werden drahtlos via Bluetooth Low Energy an die Smartphone-App phyphox übertragen und dort anschaulich visualisiert. Aus fachdidaktischer Perspektive bietet der Frisbee-Kontext einen motivierenden, lebensweltlich bedeutsamen Zugang zukomplexen physikalischen Konzepten. Lernende können reale Datenerheben, Hypothesen überprüfen und die Diskrepanz zwischen Modell und tatsächlichem Flugverhalten reflektieren. Das Poster präsentiert das Sensorsystem, exemplarische Messdaten sowie Vorschläge zur unterrichtlichen Einbettung.

DD 25.2 Tue 14:00 P5

Circuit Nodes - Modulare 3D-gedruckte Schaltungskomponenten für den Physikunterricht — Hans Kubitschke, •Fabian Hennig, Jonas Gleichmann, Jörg Schnauss und Philipp Bitzenbauer — Institut für Didaktik der Physik, Universität Leipzig, Leipzig, Deutschland

Das Poster stellt Circuit Nodes vor, ein modulares und kostengünstiges System von 3D-gedruckten Komponenten und Leiterplatinen, das elektrische Schaltungen in einer Weise abbildet, die direkt an gängige Schaltpläne anschließt. Die magnetisch koppelbaren Module ermöglichen den Aufbau von Schaltungen und zielen darauf ab, Abstraktionshürden bei der Übertragung zwischen schematischen Schaltplänen und praktischem Versuchsaufbau zu reduzieren. Der Beitrag präsentiert die technische Umsetzung und stellt einen Zugriff auf die Open-Source Bibliothek mit Materialien für den eigenen Nachbau bereit. Feedback von Lehrkräften auf Basis erster Einsätze in der Unterrichtspraxis deuten auf eine einfache Handhabung und individuelle Anpassbarkeit für den Unterricht hin.

DD 25.3 Tue 14:00 P5

INTERAPT: Laborpraktika mit interaktiven und adaptiven Skripten gestalten — •Josefine Neuhaus, Jasper Cirkel und Pascal Klein — Physik und ihre Didaktik, Göttingen

Physikalische Laborpraktika wollen einerseits Wissen vertiefen und andererseits laborpraktische Kompetenzen fördern. Eine Herausforderung, die sich Dozierenden und Betreuenden hierbei stellt, ist die Heterogenität der Studierendenschaft in unterschiedlichen Faktoren. Zu diesen Faktoren zählen Unterschiede im mathematischen und physikalischen Hintergrundwissen, aber auch unterschiedliche Interessenslagen. Der Beitrag präsentiert einen Einblick in das Projekt INTERAPT, einen Ansatz zur Gestaltung interaktiver und adaptiver Praktikumsskripte. In Rahmen eines Lernmoduls zur Vorbereitung der Studierenden auf den Versuch werden mittels diagnostischer Elemente und gezielter Verzweigungen individuelle Lernpfade eröffnet. Diese ermöglichen den Studierenden unterschiedliche Schwerpunktsetzungen, beispielsweise auf die Analyse des Versuchsaufbaus, eine ausführlichere theoretische Grundlagenfundierung oder weitergehende Auswertungsschritte mit erhöhtem Programmieranteil und eine Simulation des Experiments.

In dem Beitrag werden Einblicke in die Gestaltung eines Lernmoduls zum Pohlschen Resonator gegeben und Evaluationsergebnisse bezüglich der usability und affektiver Variablen aus einer Pilotimplementierung im Praktikumsbetrieb präsentiert.

DD 26: Poster – Hochschuldidaktik

Time: Tuesday 14:00–16:00 Location: P5

DD 26.1 Tue 14:00 P5

Experimente vom Black-Box-Typ zur Förderung der Problemlösefähigkeiten — •Hendrik Maas und Gunnar Friege — Leibniz Universität Hannover - Institut für Didaktik der Mathematik und Physik - AG Physikdidaktik, Welfengarten 1a, 30167 Hannover

Die Fähigkeit des Problemlösens gilt als eine zentrale Kompetenz im 21. Jahrhundert. Problemlöseaufgaben im Physikunterricht bestehen größtenteils aus theoretischen Aufgaben. Experimentelle Probleme sind wie Experimente aus vielerlei Hinsicht für Lernende eine große Herausforderung. Hypothesenbildung, Planung, Aufbau, Durchführung und Interpretation stellen Lernende oft vor Probleme. Experimente vom Black-Box-Typ bieten den Vorteil, dass der Aufbau weitgehend vorgegeben, aber erschlossen werden muss. Problemlöseschemata und Fachwissen müssen dafür kombiniert werden, womit inhalts- und prozessbezogene Kompetenzen gemeinsam gefördert werden. In einem von der Müller-Reitz-Stiftung geförderten Projekt werden Black-Box-Experimente für die Sekundarstufe I und II entwickelt und vervielfacht, die in diesem Beitrag vorgestellt werden.

DD 26.2 Tue 14:00 P5

Erhebung der notwendigen Komepetenzen für eine experimentelle Bachelorarbeit in Physik aus Sicht der Betreuer*innen — •Michaela Schulz[1], Dane-Vincent Schlünz[2], Daniel Laumann[2] und Lisa Stinken Rösner[1] — [1]Universität Bielefeld — [2]Universität Münster

Im physikalischen Grundpraktikum (GP) sollen Fachstudierende experimentelle Kompetenzen erwerben, die die Grundlage für eine spätere eigenständige Forschung darstellen. Dozierende bemängeln jedoch immer wieder, dass die im GP

erworbenen Kompetenzen häufig ausbaufähig oder ungenügend für die Erstellung einer Bachelorarbeit (BA) in der Experimentalphysik (EP) seien (Schlünz et al., 2024). Um diese Diskrepanz zu adressieren, wurde mittels einer Interviewstudie sowie eines darauf aufbauenden Fragebogens standortübergreifend erhoben, welche experimentellen Kompetenzen Studierende aus Sicht der Betreuer*innen benötigen, um ihre BA in der EP erfolgreich und in angemessener Zeit abschließen zu können. Die Resultate der Umfrage liefern hilfreiche Informationen, u.a. zur Überarbeitung der Konzeptionen physikalischer Grundpraktika.

DD 26.3 Tue 14:00 P5

Modellierung von Blickbewegungen bei der Beurteilung der Divergenz von Vektorfeldern — •Niklas Weiss, Larissa Hahn, Pascal Klein und Stefan Klumpp — Universität Göttingen, Institut für Dynamik komplexer Systeme

Formeldarstellungen visuell zu interpretieren ist eine grundlegende Komponente des Verständnisses von mathematischen und physikalischen Konzepten. Diese Übersetzungsleistung wird bei der Beurteilung der Divergenz zweidimensionaler Vektorfelder relevant. Bei einer Eye-Tracking Studien mit 141 Studienanfängern (Klein et al. 2021) wurde gezeigt, dass systematische Augenbewegungen in horizontale und vertikale Richtung bei der Lösung solcher Probleme ein korrektes Vorgehen andeuten. Auf diesen Beobachtungen aufbauend wurde aus den Sakkadenbewegungen ein Modell entwickelt, welches Augenbewegungen durch eine symbolische Dynamik repräsentiert und mit dem diese als diskreter Markov-Prozess simuliert werden können. Der Vergleich von Beobachtung und Simulation zeigt, dass sich wiederholende horizontale und vertikale Sakkaden in den Beobachtungen überrepräsentiert sind, und legt nahe, dass diese die korrekte Beurteilung der Divergenz unterstützen. Mit diesen Erkenntnissen wurde mit Machine-Learning ein Algorithmus trainiert, der anhand des Sakkaden-Modells die Antwort der Probanden mehrheitlich vorhersagen kann.

DD 26.4 Tue 14:00 P5

Physik-Lernen in hybriden Gruppen: Wirksamkeitsuntersuchungen nach dem ICAP-Modell mit Selbsteinschätzungen und Unterrichtsbeobachtungen — •Michael Griesbeck, Christine Lux, Julia Neubert, Martina Alles und Anja Teistler — Technische Hochschule Rosenheim, Hochschulstr. 1, 83024 Rosenheim

Hybride Gruppenarbeit ermöglicht die synchrone Zusammenarbeit von Studierenden in gemischten Gruppen aus Präsenz- und Online-Teilnehmenden, was flexible Teilnahmeszenarien unterstützt. Unabhängig von der Teilnahmeart sollen Lernerfolge wie im lernförderlichen SCALE-UP-Raum- und Lehrkonzept ermöglicht werden. Der Beitrag berichtet über eine mehrjährige Untersuchung von hybrider Gruppenarbeit im Physik- bzw. Bauphysikunterricht für Studierende der Ingenieurswissenschaften und Innenarchitektur in einem spezialisierten Lehrraum, der die hybride Zusammenarbeit mit hochwertiger Medientechnik unterstützt und damit die anspruchsvollen Bedingungen hybrider Interaktion erfüllt. Die Evaluation erfolgte anhand studentischer Selbsteinschätzungen sowie strukturierter Unterrichtsbeobachtungen nach dem ELCOT3-Protokoll, die jeweils mithilfe des ICAP-Modells ausgewertet wurden. Von besonderem Interesse war das kognitive Engagement der Studierenden, das sich nach der ICAP-Hypothese mit dem zu erwartenden Lernerfolg verknüpfen lässt und in den gemischten Teams auch separat für Präsenz- und Online-Teilnehmende erfasst wurde. Wir beobachten, dass Studierende in hybriden Teams überwiegend aktive, konstruktive und interaktive Lernaktivitäten zeigen, vergleichbar mit rein präsenzbasierten Formaten im SCALE-UP-Raum.

DD 26.5 Tue 14:00 P5

Identity Play in der Showphysik - Auswirkungen der Vorbildfunktion auf die eigene Fachidentität — •Nils Kunisch und Lisa Stinken-Rösner — Universität Bielefeld

Im Projekt „PiBonStage“ soll das Interesse von Schüler*innen am Fach Physik durch Physik-Shows entfacht bzw. gestärkt werden. Diese Shows werden in einem dafür entwickelten Seminar konzipiert und aufgeführt. Neben der Förderung experimenteller Kompetenzen steht die proaktive Wissenschaftskommunikation durch Studierende im Fokus, wodurch ein modernes Bild der Physik vermittelt werden soll. Unter fachlicher Begleitung von Expert*innen aus der Experimentalphysik, der Physikdidaktik und der Wissenschaftskommunikation entwickeln und realisieren die Seminarteilnehmer*innen eigenständig Show-Experimente, die in einer Physik-Show für Schulklassen aus der Region zusammengeführt werden. In ihrer Rolle als (Show)Physiker*innen fungieren die Studierenden in diesem Kontext als nahbare und kompetente Vorbilder für die Schüler*innen.

Die begleitende Forschung fokussiert diese Vorbildfunktion der Studierenden und untersucht vor dem theoretischen Hintergrund des *identity play*, inwiefern die Physikidentität der Studierenden durch die aktive Gestaltung und Aufführung der Show sowie die Wahrnehmung der eigenen Vorbildfunktion beeinflusst wird.

DD 27: Poster – Lehr- und Lernforschung

Time: Tuesday 14:00–16:00 Location: P5

DD 27.1 Tue 14:00 P5

Tutorial zur Mehrebenenanalyse von Daten aus quasiexperimentellen Studien — •Roland Berger[1], Maria Danzglock[2], Alina Hindriksen[1] und Florian Scharf[2] — [1]Universität Osnabrück — [2]Universität Kassel

Im Rahmen quasiexperimenteller Studien werden in der fachdidaktischen Forschung oftmals Daten in mehreren Schulklassen erhoben. Damit ergibt sich eine hierarchische Struktur der Daten. Innerhalb einer jeden Klasse besteht zum Beispiel durch unterschiedliche Lehrqualität eine mehr oder weniger große Ähnlichkeit zwischen den Schülerinnen und Schülern, hingegen ist die Ähnlichkeit zwischen den Klassen geringer. Damit ist oft eine zentrale Voraussetzung für die Anwendbarkeit einer Varianzanalyse nicht erfüllt, nämlich die Unabhängigkeit der Fehlerkomponenten. Das hat zur Folge, dass man ohne Berücksichtigung der Schachtelung in einer Varianzanalyse leichter signifikante Effekte findet, die in Wirklichkeit aber Artefakte sind (Typ-I-Fehler).

In der verfügbaren Literatur zu Mehrebenenanalysen wird selten explizit auf spezifische Besonderheiten im Kontext von quasiexperimentellen Studien eingegangen. Daher haben wir ein Tutorial verfasst, in dem geschachtelte Analysen mit Kovariate, zweifaktorielle Analysen mit einem Messwiederholungsfaktor sowie Moderatoranalysen vorgestellt werden. Im Rahmen des Tutorials werden die Quellcodes zu den entsprechenden Mehrebenenanalysen sowie Beispieldaten aus einer unserer quasiexperimentellen Studien bereitgestellt. Das Tutorial stellt somit eine praxisnahe Ergänzung zur Literatur zu Mehrebenenanalysen dar.

DD 27.2 Tue 14:00 P5

Immersives Lernen sichtbar gemacht: Eine Eye-Tracking-Studie zu einem VR-basierten Physikexperiment — •Matthias Klassen[1], Gunnar Friege[1] und Salome Flegr[2] — [1]Institut für Didaktik der Mathematik und Physik, AG Physikdidaktik, Leibniz Universität Hannover, Hannover, Deutschland — [2]Professur für Didaktik der Physik, Technische Universität Dresden, Dresden, Deutschland

Diese Studie untersucht visuelle Aufmerksamkeitsmuster während eines immersiven VR-basierten Physikexperiments zur Sammellinse. 96 Achtklässlerinnen (M = 13,65*Jahre, SD = 0,57) bearbeiteten einen Versuch an der optischen Bank, während Eye-Tracking ihre Blickbewegungen aufzeichnete. Die Analyse fokussierte auf die Verweildauer auf relevanten Bereichen, Übergänge zwischen relevanten und irrelevanten Bereichen sowie den Lösungserfolg der Aufgaben. Zur Identifikation typischer Aufmerksamkeitsprofile führten wir eine Clusteranalyse auf standardisierten Variablen durch. Die Analyse identifizierte vier Blickprofile: High Performer mit stabiler Aufmerksamkeit und bester Leistung, mittlere Performer mit moderater Fokussierung und mittlerer Performance, eine Gruppe mit selektiver, aber unstrukturierter Aufmerksamkeit, die trotz gezielter Blickbewegungen nur bedingt effizient arbeitete, sowie Low Performer mit geringer Fokussierung und schwacher Performance. Aus letzterer Gruppe gab es wenige Ausreißer (ca. 12,5*%), die trotz niedriger Ausgangsleistung besonders motiviert waren und gleichzeitig effiziente Blickstrategien sowie hohe Erfolgsraten zeigten.

DD 27.3 Tue 14:00 P5

Schülervorstellungen zum Magnetismus im Anfangsunterricht — Cliona Zechel und •Thomas Wilhelm — Institut für Didaktik der Physik, Goethe-Universität Frankfurt

Die Kenntnis konkreter Schülervorstellungen ist für das Unterrichten physikalischer Themen sehr wichtig. Wie intensiv Schülervorstellungen zu einem Thema erforscht sind, schwankt allerdings sehr stark zwischen den verschiedenen Gebieten der Physik.

Der Magnetismus ist ein Thema vom Kindergarten bis zur Hochschule. Somit ist es überraschend, dass als Literatur zu entsprechenden Schülervorstellungen stets nur eine Quelle angegeben wird, die auf eine Staatsexamensarbeit einer Grundschulstudentin aus dem Jahre 1992 zurückgeht. Allein aufgrund der vergangenen Zeit ist eine Replikation nötig.

Im Rahmen einer Staatsexamensarbeit wurde mit Hilfe von halboffenen Leitfadeninterviews untersucht, welche Vorstellungen Grundschüler*innen zum Magnetismus haben. Dabei wurden zehn Schüler*innen der 2. und 4. Jahrgangsstufe befragt. Die transkribierten Interviews wurden nach Gropengießer (2015) aufbereitet und ausgewertet. Die Ergebnisse passen teilweise zu der obigen Studie; es gibt aber auch Unterschiede. Vorgehen und Ergebnisse werden auf dem Poster dargestellt.

DD 27.4 Tue 14:00 P5

Kognitive Dimensionen mentaler Modelle Lernender zur (linearen) Polarisation von Licht — •Judith Schmid, Joaquin Veith und Philipp Bitzenbauer — Universität Leipzig, Leipzig, Germany

Lernende haben oft Schwierigkeiten, anschlussfähige mentale Modelle zur Polarisation zu entwickeln. Die zugrunde liegenden kognitiven Strukturen mentaler Modelle sind in bestehender Forschung bisher weitgehend unerforscht geblieben. Wir haben die Vorstellungen von Lernenden im Lichte des Fidelities Model of Conceptual Development (FMCD) untersucht. Das Framework unterscheidet zwei kognitive Dimensionen, die den mentalen Modellen der Lernenden zugrunde liegen: Gestalttreue (FG) und Funktionalitätstreue (FF). Das Zusammenspiel beider Dimensionen ermöglicht eine Typisierung der Denkweisen von Lernenden. Es wurde ein Testinstrument auf Basis etablierter Schülervorstellungen entwickelt. Die Dimensionen FF und FG wurden mittels Testitems operationalisiert, um sie im Kontext Polarisation messbar zu machen. Die Items des Instruments wurden durch Expertenbefragungen sowie Think-Aloud-Studien pilotiert. In einer Erhebung mit N = 178 Schüler*innen der Sekundarstufe und Studierenden bestätigte eine konfirmatorische Faktorenanalyse eine robuste Zwei-Faktoren-Struktur und Faktorreliabilität. Wir stellen die theoretische Rahmung, Entwicklung und Pilotierung des Instruments vor und zeigen, inwiefern die Ergebnisse ferner das FMCD stützen.

DD 27.5 Tue 14:00 P5

Translating Attitudes: Design and Evaluation of Interventions based on Research Findings for Physics in the 10th Grade of Cypriot Lyceums. — •Theodoros Aslanidis — Ministry of Education, Sport and Youth Cyprus

This presentation details the pivotal transition from diagnostic research to practical educational intervention within the context of Physics education in Cyprus.

Drawing on extensive quantitative and qualitative data from my recent doctoral study on 10th-grade students' attitudes and beliefs towards Physics, initial findings revealed persistent challenges. These include entrenched perceptions of the subject as rote memorization, perceived high difficulty, and a general disconnection from real-world applications.

The crux of this work lies in the design and rationale of an evidence-based teaching intervention specifically tailored to address the identified challenges.

This presentation delineates the structure of the multi-week intervention, the theoretical framework underpinning its development, and the rigorous methodology planned for its subsequent evaluation.

Ultimately, this presentation aims to demonstrate a pathway from empirical academic findings to effective classroom reform. The outcomes will provide tangible, data-driven recommendations for curriculum development and teacher professional development in Cypriot public schools, with the goal of significantly enhancing student engagement and foster a lifelong appreciation for the science of Physics.

DD 27.6 Tue 14:00 P5

Sakkadenrichtungen und Sakkadenlängen zur Beschreibung von visuellen Strategien — Paula Fehlinger[1], Berhard Ertl[2] und •Bianca Watzka[1] — [1]RWTH Aachen University — [2]Universität der Bundeswehr München

Augenbewegungen liefern zentrale Hinweise zur Beschreibung visueller Aufmerksamkeit bei der Bearbeitung von Aufgaben. Ein wesentlicher Bestandteil dieser Beschreibung ist die Analyse von Sakkaden, die den Blickwechsel zwischen relevanten Bereichen abbilden. Deren Richtung und Länge erlauben Rückschlüsse auf eingesetzte visuelle Strategien. In bisherigen Arbeiten werden Sakkadendaten häufig als diskrete Daten dargestellt, etwa durch Histogramme. Kontinuierliche Darstellungen werden teilweise mithilfe der Kerndichteschätzung realisiert, dabei jedoch häufig mit gaußschen Kernen modelliert, die für Richtungsdaten nur eingeschränkt geeignet sind. Der vorliegende Beitrag stellt einen Ansatz zur Analyse von Sakkadenrichtungen sowie zur gleichzeitigen Analyse von Richtung und Amplitude auf Basis der Kerndichteschätzung vor. Dabei werden die unterschiedlichen Datenstrukturen beider Größen berücksichtigt: Während Sakkadenrichtungen zirkuläre Daten darstellen, folgen Sakkadenlängen einer linearen Verteilung. Durch die Kombination eines von-Mises-Kerns für Richtungen mit einem gaußschen Kern für Längen entsteht eine kontinuierliche Beschreibung beider Charakteristika einer Sakkade. Diese Methode erweitert bestehende Analyseansätze, indem sie Diskretisierung vermeidet und zyklische Eigenschaften korrekt abbildet. Gleichzeitig ermöglicht sie eine integrierte Betrachtung von Richtung und Länge.

DD 27.7 Tue 14:00 P5

Lernendenvorstellungen in der E-Lehre - Welchen Einfluss haben Stromkreismodelle? — •Katharina Leibfarth[1], Jan-Philipp Burde[1], Peter Gerjets[2] und Ulrich Trautwein[1] — [1]Universität Tübingen — [2]IWM Tübingen

Viele Lernende haben auch nach dem Unterricht konzeptionelle Schwierigkeiten mit einfachen Stromkreisen. Insbesondere sind Lernendenvorstellungen verbreitet, beispielsweise die Vorstellung, dass Strom verbraucht wird oder Batterien einen konstanten Strom liefern. Gleichzeitig werden einfache Stromkreise häufig anhand von Analogien und Modellen unterrichtet, wobei verschiedenste Modelle zur Veranschaulichung eingesetzt werden. Während Lernendenvorstellungen zur Elektrizitätslehre umfassend dokumentiert sind, ist weitgehend ungeklärt, welchen Einfluss unterschiedliche schulische Modelle auf Lernendenvorstellungen zu einfachen Stromkreisen haben.

Vor diesem Hintergrund wurden Akzeptanzbefragungen mit Schüler:innen der Sekundarstufe I zu einfachen Stromkreisen anhand unterschiedlicher Modelle durchgeführt und mithilfe einer qualitativen Inhaltsanalyse ausgewertet. Auf dem Poster werden die Ergebnisse der Interviews zu den Lernendenvorstellungen vorgestellt und der Einfluss unterschiedlicher Modelle diskutiert.

DD 27.8 Tue 14:00 P5

Handlungsorientierte Elektrizitätslehre in der Sekundarstufe I: Einblicke ins Unterrichtsgeschehen — •Daniel Hecht — PH Weingarten

Handlungsorientierung gilt als ein didaktisch vielversprechender Ansatz, dessen empirische Fundierung im Physikunterricht jedoch begrenzt ist. Die Studie untersucht ein mehrwöchiges, werkstattartiges Setting der Elektrizitätslehre in mehreren Klassen, in dem Schüler*innen in Partnerarbeit praktische Mini-Experimente und ein mehrschrittiges Abschlussprojekt bearbeiteten. Die Datengrundlage umfasst umfangreiche Audioaufnahmen der Gruppenarbeit, schriftliche Schülerfeedbacks sowie abschließende Interviews. Die Audioaufnahmen werden mittels induktiver Kategorienbildung ausgewertet; Fragebögen und Interviews ergänzen die Analyse um Perspektiven der Lernenden. Die Datenerhebung ist abgeschlossen, erste Analysen liegen vor. Diese zeigen, dass die praktischen Arbeitsphasen von den Lernenden überwiegend positiv erlebt werden. Zugleich wird deutlich, dass das anspruchsvollere Abschlussprojekt trotz spürbarer Frustrationserlebnisse während der Bearbeitung rückblickend von vielen Schüler*innen als besonders motivierend und lohnend beschrieben wird. Weitere Auswertungen werden bis zur Tagung zusätzliche Einblicke in das Lern- und Interaktionsgeschehen ermöglichen. Ziel der Studie ist es, empirisch fundierte Einblicke in Potenziale und Herausforderungen handlungsorientierter Elektrizitätslehre zu gewinnen und Ansatzpunkte für vertiefende Untersuchungen zu identifizieren.

DD 28: Poster – Neue Konzepte

Time: Tuesday 14:00–16:00 Location: P5

DD 28.1 Tue 14:00 P5

Spielerische experimentelle Lerngelegenheiten zur Optik mit Rätseln für ein Escape Game — •Ludger Wirth, Ramona Schauer-Bollig und Heidrun Heinke — RWTH Aachen University, I. Physikalisches Institut IA

Educational Escape Games können für den Physikunterricht großes Potenzial bieten, wenn Inhalte und Spiel sinnvoll miteinander verbunden werden, um Motivation zu schaffen und Schüler*innen mit fachlichen Inhalten spielerisch vertraut zu machen. Dabei bieten sie die Möglichkeit, dass komplexe physikalische Inhalte kontextualisiert und erfahrbar gemacht sowie wichtige Kompetenzen, wie die Kommunikations- und Problemlösefähigkeit, gefördert werden können. Vor diesem Hintergrund wurden für ein bestehendes modulares Escape Game bildungstheoretisch geleitet Rätsel im Themenbereich Optik entwickelt und getestet. Die Inhalte orientieren sich hierbei am Kernlehrplan NRW für Physik der Sekundarstufe I. Ziel der Entwicklung war es, eine interaktive und wenig materialintensive Lernerfahrung zu ermöglichen, die das experimentelle Erkunden von Licht- und Materialeigenschaften aus dem Bereich der geometrischen Optik fördert. Die entwickelten Rätsel arbeiten deswegen unter anderem mit dem Simulationsprogramm Ar.X, welches von der Universität Mainz entwickelt wurde und auf mobilen Endgeräten mit Kamera genutzt werden kann. Hierbei werden QR-Codes als Ankerpunkte für die Simulation von optischen Bauteilen benutzt, was interaktive Lernerfahrungen bei geringem Materialaufwand ermöglicht. Auf dem Poster werden die Rätsel und erste Erfahrungen des Einsatzes mit Schüler*innen vorgestellt.

DD 28.2 Tue 14:00 P5

Predictive Coding in the Human Brain and its possible applications for a Shared Universe Engine — •André Bresges — University of Cologne, Albertus-Magnus-Platz, 50931 Cologne

Predictive coding theory proposes the brain isn't a passive receiver but an active prediction machine, constantly generating internal models to anticipate sensory input, minimizing surprise by only processing the "prediction errors" (mismatches) that occur. This leads to efficient perception, learning, and action by

updating its world model to better match reality. Predictive Coding is a Bayesian brain hypothesis where top-down predictions (expectations from past experience) meet bottom-up sensory data, with errors signaling the need for adjustment of the model. Predictive Coding explains consciousness not as a static model, but dynamically as *the brain's best guess about the world*. Educational Methods like POE (Predict Observe Explain) are in good alignment with this theoretical framework. We argue that predictive coding might also be a good theory to build a Shared Universe Engine upon because of its: Efficiency: Reduces redundant processing, saving cognitive resources. Precision: The Brain aims to minimize prediction errors. Speed: Unifies perception, cognition, and action (sensor direction and tuning) under a single principle.

DD 28.3 Tue 14:00 P5

Eine digitale adaptive Lernumgebung für geometrische Optik — •Marie Oberndorfer und Roger Erb — Goethe-Universität Frankfurt

Eine zentrale Anforderung an modernen Unterricht ist die Sicherstellung von Chancengleichheit. Hierfür müssen Lehrkräfte ihren Unterricht an die Ausgangslagen der Lernenden anpassen, indem sie Aufgaben mit entsprechendem Anforderungsniveau sowie angepasste Hilfestellungen und individuelles Feedback zur Verfügung stellen. Dabei treffen sie auf eine Bandbreite von lernrelevanten Heterogenitätsbereichen wie Vorwissen oder sprachlichen Voraussetzungen, wodurch weitere Herausforderungen hinsichtlich der Materialentwicklung und des Klassenmanagements entstehen können. So kann die Umsetzung eines bedarfsgerechten Unterrichts zur Belastung für Lehrkräfte werden. Digitale Medien können hierbei eine wertvolle Unterstützung darstellen. Vor diesem Hintergrund beschäftigt sich das vorgestellte Promotionsvorhaben mit der Entwicklung einer digitalen, adaptiven Lernumgebung in Form eines Intelligenten Tutoring Systems (ITS). Die Lernumgebung stellt für Lernende der Sekundarstufe I einen Zugang zur geometrischen Optik bereit. Bei der Gestaltung des ITS wird ein besonderer Fokus auf die Erarbeitung von Modellen und deren Charakteristika im Sinne von Nature of Science gelegt. Die Implementierung der Adaptivität in das ITS erfolgt nach dem Rahmenmodell von Sibley et al., das die Elemente Formative Diagnose sowie Mikro- und Makroadaption beinhaltet.

DD 28.4 Tue 14:00 P5

Escape Game- Erneuerbare Energien: Entwicklung eines physikdidaktischen Escape Games mit dem Double-Diamond — •Moritz Langer und André Bresges — Universität zu Köln, Deutschland

Das Poster stellt den Entwicklungsprozess eines physikdidaktischen Escape Games für Schüler*innen vor, in dessen Fokus erneuerbare Energien stehen. Im Sinne von Game Based Learning lernen die Teilnehmenden mit dem Spiel: Physikalische Inhalte zum Einsatz erneuerbarer Energien werden im Rahmen einer Geschichte über Rätsel und integrierte Experimente erschlossen. Ziel ist es unter anderem, fachliches Wissen auszubauen und die Relevanz nachhaltiger Energien im Alltag (SDG 7) aufzuzeigen.

Die Entwicklung folgt dem Double-Diamond-Modell mit den Phasen Discover, Define, Develop und Deliver, die um eine Disrupt-Phase ergänzt werden. Das Escape Game wird zunächst mit Hilfe von Studierenden entwickelt und erprobt und auf dieser Basis weiterentwickelt, bevor es in einem zweiten Schritt mit Schüler*innengruppen eingesetzt und weitererprobt wird. Als Lernort dient die Ökologische Rheinstation, die einen Bezug zu realen Anwendungen erneuerbarer Energien sowie zum Ökosystem Rhein herstellt. Das Poster diskutiert Potenziale von Escape Games für einen motivierenden und handlungsorientierten Physikunterricht zu nachhaltiger Energie.

DD 29: Poster – Nature of Science

Time: Tuesday 14:00–16:00 Location: P5

DD 29.1 Tue 14:00 P5

Was sollten Schüler:innen über Wissenschaft lernen? — •Lea Herbst und Verena Spatz — Didaktik der Physik, TU Darmstadt, Deutschland

Das Verständnis des grundlegenden Wesens naturwissenschaftlicher Arbeit (Nature of Science und Scientific Inquiry) wird bereits seit Jahrzehnten als wesentliches Bildungsziel angesehen. Die Einbettung in den Unterrichtet bereitet Lehrkräften jedoch aus unterschiedlichen Gründen Schwierigkeiten. Im Rahmen des Outreach-Projektes des Sonderforschungsbereichs 1245 in der Kern- und Astrophysik hat eine Gruppe aus Lehrkräften sowie Wissenschaftler:innen des Sonderforschungsbereichs gemeinsam ein Konzept für Schulmaterial zur Vermittlung von Nature of Science und Scientific Inquiry Aspekten entwickelt. Ziel davon ist die Unterstützung von Lehrkräften bei der Vermittlung adäquater Vorstellungen zu den ausgewählten Aspekten. In dessen Erarbeitungsprozess spielte unter anderem die Frage, welche Aspekte aus der Perspektive von Wissenschaftler:innen als besonders relevant eingestuft werden, eine Rolle. Dafür wurden Wissenschaftler:innen des Sonderforschungsbereichs befragt, was Schüler:innen über Wissenschaft lernen sollten. Diese Befragung wurde nun auf den gesamten Fachbereich Physik der TU Darmstadt ausgeweitet, um mögliche Einflüsse durch den inhaltlichen Schwerpunkt zu untersuchen und somit ein repräsentativeres Bild für das gesamte Fach Physik zu erhalten. In diesem Beitrag werden die Ergebnisse der Befragung, sowie deren Auswertung vorgestellt.

DD 30: Poster – Quantenphysik

Time: Tuesday 14:00–16:00 Location: P5

DD 30.1 Tue 14:00 P5

Die Tiefenstruktur des Interesses von Studierenden zu Quantentechnologien — •Ismet N. Dogan, Dagmar Hilfert-Rüppell und Rainer Müller — Institut für Fachdidaktik der Naturwissenschaften, TU Braunschweig, Deutschland

Interessen spielen eine bedeutende Rolle in Lernprozessen. Die Tiefenstruktur sowie Natur von Interesse wird stark in der Literatur diskutiert. Es finden sich Ansätze, die Interesse als Emotion oder als mehrteilige Struktur auffassen sowie weitere diffuse Angehensweisen. An erster Stelle ist es unser Ziel, die Tiefenstruktur des Interesses zu erforschen und zu verstehen, wie das Interesse zu Quantentechnologien aufgebaut und klassifiziert werden kann. Quantentechnologien stellen als zukünftig relevante Technologie ein spannendes Themengebiet dar, das auch einen guten Kontext zur anspruchsvollen Quantenphysik bietet. Als anspruchsvolles Themengebiet ermöglicht es uns, potentielle Verbindungen von kognitiven Komponenten zum Interesse darzulegen. Es fand eine Erhebung statt in der die Teilnehmenden - Studierende unterschiedlicher Studienrichtungen - einen Text zu Quantentechnologien gelesen und darauf folgend Items zum Interesse ausgefüllt haben. Die Items wurden auf Grundlage der Theorie nach Krapp formuliert. Hier geht man davon aus, dass das Interesse drei Komponenten besitzt: eine emotionale, eine kognitive und eine wertorientierte Komponente. Schlussendlich wurde eine explorative Faktoranalyse durchgeführt und ausgewertet. Das Poster beschäftigt sich mit dieser Erhebung des Interesses von Studierenden zu Quantentechnologien und liefert bedeutende Erkenntnisse zum Interesse von Studierenden zu Quantentechnologien.

DD 30.2 Tue 14:00 P5

Entwicklung und Erprobung einer Unterrichtseinheit zu Magnetfeldsensoren auf Basis von Quanteneffekten in NV-Zentren — •Florian Böttcher, Moritz Förster, Alexander Schuster und Gesche Pospiech — TU Dresden, Professur für Didaktik der Physik

Im Rahmen der zweiten Quantenrevolution schreitet die Forschung und Entwicklung im Bereich moderner Quantentechnologien rasant voran. Für den Schulunterricht bietet die Einbettung entsprechender Kontexte die Möglichkeit, deren gesellschaftliche Relevanz aufzuzeigen und zugleich berufsorientierende Bezüge herzustellen.

Eine der vielversprechendsten und realitätsnahesten Anwendungen moderner Quantentechnologien ist die Quantensensorik, darunter vor allem Quantenmagnetometer, die auf Basis von Stickstofffehlstellen (NV-Zentren) in Diamanten arbeiten.

In einer wissenschaftlichen Abschlussarbeit wurde eine Unterrichtseinheit zu Magnetfeldsensoren auf Basis von Quanteneffekten in NV-Zentren konzipiert sowie im Rahmen eines Ferienkurses erprobt und mit qualitativen Methoden evaluiert. Das Poster stellt die Grundkonzepte der Unterrichtseinheit vor und gibt Einblick in erste Ergebnisse der Evaluation.

DD 30.3 Tue 14:00 P5

Quantum AR Lab: Das Quantenoptik-Labor für Schule und Co. in Augmented-Reality — •Philipp Bitzenbauer, Judith Schmid und Malte Ubben — Institut für Didaktik der Physik, Universität Leipzig

Das Poster stellt Quantum AR Lab vor, eine Multiplayer-AR-App, die zentrale Experimente der Quantenoptik authentisch und interaktiv zugänglich macht. Reale quantenoptische Aufbauten bleiben im schulischen und hoch-

schulischen Alltag aufgrund hoher Kosten und technischer Komplexität meist unzugänglich; Quantum AR Lab schließt diese Lücke, indem sechs typische Einzelphotonen-Experimente - Koinzidenzmessung, Antikorrelation am halbdurchlässigen Spiegel, Einzelphotoneninterferenz, Hong-Ou-Mandel, sowie zu Verschränkung und Franson-Interferenz - in einer ortsunabhängigen, praxistauglichen AR-Umgebung erfahrbar werden. Maßstäbliche 3D-Nachbauten experimenteller Komponenten, justierbare Elemente sowie die Integration originaler Messdaten ermöglichen ein realitätsnahes Experimentieren. Drei Schwierigkeitsgrade je Experiment und ein Multiplayer-Modus unterstützen individuelles und kollaboratives Arbeiten gleichermaßen.

DD 30.4 Tue 14:00 P5

Photonenverschränkung in der Sekundarstufe II: Intervention zum Vergleich kognitiver & affektiver Variablen bei Real- vs. Bildschirmexperiment — •Josefin Metje[1], Salome Flegr[2], Marco Seiter[1] und Heiko Krabbe[1] — [1]Ruhr-Universität Bochum — [2]Technische Universität Dresden

Die Einführung von Verschränkung kann in der Schule durch reale Experimente (RE) und interaktive Bildschirmexperimente (IBE) mit verschränkten Einzelphotonen erfahrungsbasiert erfolgen. IBE sind interaktive, auf Fotos oder Videos basierende Szenarienaufnahmen des Realexperiments, die sich an Computern oder Tablets durchführen lassen und eine vereinfachte und weniger fehleranfällige Interaktion mit dem Experiment erlauben als die Durchführung des realen Experiments. Im Rahmen eines Promotionsprojekts wird untersucht, inwiefern sich diese beiden Varianten (RE und IBE) hinsichtlich Motivation, Wissenszuwachs sowie mentalem Load und Effort von Schülerinnen und Schülern unterscheiden. Die Studie ist als empirische, quasi-experimentelle Untersuchung angelegt, wobei der Einsatz von RE bzw. IBE als unabhängige Variable dient. In der Intervention sollen die Lernenden das Phänomen der Verschränkung sowie quantenmechanische Messprozesse und deren stochastische Vorhersagbarkeit am Beispiel verschränkter Einzelphotonen erschließen und beschreiben. Der Wissenszuwachs wird mit einem selbst entwickelten und evaluierten Testinstrument erfasst. Auf dem Poster wird die Übersetzung des Interventionskonzepts in das Interventionsmaterial gemäß der allgemeinen Validierungslogik für Interventionsstudien (Seiter & Krabbe, eingereicht) vorgestellt.

DD 30.5 Tue 14:00 P5

Experiment für Schüler:innen zur Quantenbildgebung mit nichtdetektiertem Licht — •Benedikt Weiss[1], Verena Spatz[1], Markus Gräfe[2] und Jens Küchenmeister[3] — [1]Didaktik der Physik, TU Darmstadt — [2]Institut für Angewandte Physik, TU Darmstadt — [3]Thorlabs GmbH

Die Quantenphysik zählt zu den faszinierendsten und zugleich herausforderndsten Bereichen der modernen Physik und bestimmt nicht nur maßgeblich unsere aktuelle wissenschaftliche Weltsicht, sondern auch unseren Alltag. Quantentechnologien (LASER, PV-Anlagen, Mikrochips, etc.) sind längst etabliert und noch immer fließen Forschungsgelder in Milliardenhöhe in die Entwicklung von Quantentechnologien der zweiten Generation (Quantencomputer, Sensortechnik und Kommunikation). Angesichts dieser Entwicklung ist es wichtig, dass nicht nur Schüler:innen, sondern auch die Öffentlichkeit im allgemeinen mit den Grundprinzipien dieser Technologien vertraut gemacht werden.

Ziel des Projekts ist ein Nachbau des Experiments zur Quantenbildgebung von Zeilinger et. al. (Nobelpreis für Physik 2022) und die Erforschung, inwiefern das Experiment für die Lehre sinnvoll eingesetzt werden kann, welche Lernziele mithilfe des Experiments angestrebt werden können, an welchen Stellen des Experiments Lernende Quantenphysik erkennen (können) und ob sich der Aufwand für dieses Realexperiment im Gegensatz zu einer Simulation lohnen kann. Auf dem Poster werden das Experiment und das geplante Studiendesign vorgestellt.

DD 30.6 Tue 14:00 P5

Ein Experiment zum Welle-Teilchen-Dualismus aus dem 3D-Drucker — •Norman Thimm, Nele Hötte, Sebastian Nell, Ralf Detemple und Heidrun Heinke — RWTH Aachen University, Aachen, Germany

In der Quantenmechanik fällt es Schüler:innen oft schwer, die zugrunde liegenden Phänomene anschaulich zu begreifen, auch weil es im Vergleich zur klassischen Mechanik deutlich weniger leicht nachvollziehbare Experimente gibt. Bekannt sind etwa der Doppelspaltversuch, der die Wellennatur von Quantenteilchen demonstriert, oder der Photoeffekt, der die Teilchennatur von Photonen illustriert.

Der Aufbau PHODE verfolgt das Ziel, beide Aspekte, Wellen- und Teilcheneigenschaften von Photonen, in einem einzigen Experiment anhand des sich entwickelnden Beugungsbildes bei der Beugung von Photonen am Doppelspalt sichtbar zu machen. So wird deutlich, dass Photonen und andere Quantenobjekte nicht „entweder ... oder“ sind, sondern gleichzeitig durch Eigenschaften von Wellen und Teilchen beschrieben werden müssen.

PHODE besteht überwiegend aus kostengünstigen 3D-gedruckten DIY- Komponenten auf der Basis der O3Q-Optikwürfel und ermöglicht es Schüler:innen, selbstständig ein eigenes Quantenexperiment zu realisieren. Auf dem Poster stellen wir den weiterentwickelten Aufbau und seine didaktischen Potentiale vor.

DD 30.7 Tue 14:00 P5

Der quantenmechanische Potentialtopf und sein didaktisches Konzept — •Simon Koppenhöfer, Kim Kappl, Laureen Dänzer, Johannes Funk, Anja Galm, Philipp Mauz, Felix Fritschle, Nils Kugler, Ronny Nawrodt und Philipp Scheiger — 5. Physikalisches Institut, Abt. Physik und ihre Didaktik, Pfaffenwaldring 57, 70569 Stuttgart

In aktuellen Bildungs- und Lehrplänen, sowie in den KMK-Standards, wird unter anderem der Potentialtopf stärker betont. Im erhöhten Anforderungsniveau soll dieser mit Schülerinnen und Schülern quantitativ besprochen werden, was beispielsweise experimentell mit Farbzentren in Alkalihalogeniden begleitet werden kann. Für das Basisniveau ist eine qualitative Behandlung vorgesehen, die mindestens die Begriffe Emission, Absorption, diskrete Spektren und Energieniveauschema erarbeiten soll. Ziel ist es hierbei, über das Bohrsche Atommodell hinaus den Aufbau von Atomen näherzubringen.

Dieser Beitrag stellt verschiedene Möglichkeiten vor, die Unterrichtsgänge beider Niveaus sowohl mit Demonstrations- als auch mit Schülerexperimenten zu begleiten. Diese optisch ansprechend aufbereiteten und erprobten Experimente verorten sich dabei in technischen, typisch physikalischen als auch biologischen Kontexten, um eine diverse interessierte Schülerschaft zu adressieren.

DD 30.8 Tue 14:00 P5

Quantensensorik im Schülerlabor: Experimente und didaktische Materialien zu NV-Zentren in Diamant — Simon Koppenhöfer, Kim Kappl, Laureen Dänzer, Johannes Funk, Anja Galm, Philipp Mauz, Felix Fritschle, Nils Kugler, Ronny Nawrodt und •Philipp Scheiger — 5. Physikalisches Institut, Abt. Physik und ihre Didaktik, Pfaffenwaldring 57, 70569 Stuttgart

Quantensensoren auf Basis von Stickstoff-Fehlstellen-(NV-)Zentren in Diamant ermöglichen es, quantenphysikalische Phänomene mit hoher Anschaulichkeit und zugleich fachlicher Authentizität zugänglich zu machen. Für außerschulische Lernorte wie Schülerlabore stellen sie damit ein vielversprechendes Medium dar, um moderne Quantentechnologien erfahrbar zu machen. Im vorgestellten Projekt werden niedrigschwellige Experimente entwickelt, die die Fluoreszenz der Farbzentren sowie magnetische Feldmessungen mittels Optisch Detektierter Magnetresonanz (ODMR) demonstrieren und sich mit kostengünstigen Komponenten umsetzen lassen.

Der Beitrag skizziert den Entwicklungsprozess der Experimente sowie des didaktischen Begleitmaterials und diskutiert, wie NV-basierte Quantensensorik nachhaltig in Angebote außerschulischer Lernorte integriert werden kann.

DD 30.9 Tue 14:00 P5

Schalten mit Licht - Entwicklung und Durchführung einer Versuchsreihe für Schülerlabore — •Dennis Lafeld und Holger Cartarius — AG Fachdidaktik der Physik und Astronomie, Friedrich Schiller Universität Jena

Im Rahmen des Graduiertenkollegs PhInt (Photo-Polarizable Interfaces and Membranes) erfolgt die Erforschung der Photoaktivität von Oberflächen und Membranen.

Ein zentraler Bestandteil von PhInt ist die didaktische Aufarbeitung der Forschungsergebnisse und deren Kommunikation an die breite Öffentlichkeit. Hierfür wurde eine Versuchsreihe für Schülerlabore mit dem Ziel der Vermittlung grundlegender Eigenschaften und Funktionsweisen von Photoschaltern entwickelt. Die Versuchsreihe wurde anschließend im Rahmen des MINT-Festivals 2025 in Jena mit fünf Schulklassen der Thüringer Oberstufe erprobt.

In diesem Beitrag sollen die entwickelte Versuchsreihe sowie die Erprobung und Erfahrungen bei der Durchführung mit Schulklassen vorgestellt werden.

DD 30.10 Tue 14:00 P5

Versuchsangebote für Schulen im Rahmen von MasterClass-Workhops — •Tim Overwin, Azadeh Ghanbari und Rainer Müller — Institut für Fachdidaktik der Naturwissenschaften, Abt. Physik und Physikdidaktik, TU Braunschweig, Deutschland

MasterClass-Workshops bieten Schulklassen aus Braunschweig und Umgebung seit 2019 die Möglichkeit, einen Einblick in aktuelle physikalische Versuche und Forschung zu bekommen. Dabei sollen Interesse, Motivation und das Verständnis von, meist quantenmechanischen, Phänomenen gefördert werden. Die Workshops werden mit höheren Klassenstufen von Gymnasien oder Gesamtschulen entweder mobil in den Schulen oder in der TU durchgeführt. Aktuelle Versuche beschäftigen sich unter anderem mit Quantenkryptographie, -computing und -sensorik.

DD 31: Poster – Physikdidaktik und Inklusion

Time: Tuesday 14:00–16:00 Location: P5

DD 31.1 Tue 14:00 P5

Inklusives Experimentieren mit Forscherboxen: Die Ansichten der Lernenden. — •Giulia Pantiri[1], Lea Mareike Burkhardt[2], Thomas Wilhelm[1], Volker Wenzel[2], Arnim Lühken[3], Dieter Katzenbach[4] und Fatime Beka[3] — [1]Institut für Didaktik der Physik, Uni Frankfurt — [2]Abteilung Didaktik der Biowissenschaften, Uni Frankfurt — [3]Institut für Didaktik der Chemie, Uni Frankfurt — [4]Institut für Sonderpädagogik, Uni Frankfurt

In dem Design-Based-Research-Projekt E2piMINT ist ein inklusives und fächerübergreifendes Unterrichtskonzept für die Sekundarstufe I entstanden. Zentrales Ziel des Projektes war es, Lehrkräfte mit geeigneten Unterrichtsmaterialien und -konzepten zu unterstützen, um Schüler*innen gemeinsames Lernen zu ermöglichen und ihr Interesse an den Naturwissenschaften und an experimentellen Aktivitäten zu fördern. Dafür wurden zwei Sets von Forscherboxen entwickelt, die Experimente aus Physik, Biologie und Chemie enthalten und sich auf die Themen "Farben" sowie "Kleben und Haften" beziehen. Die Erprobung und Evaluation des Konzepts und der Forscherboxen erfolgte in den Schülerlaboren der Goethe-Universität Frankfurt sowie an Schulen und wurde durch Forschung mit quantitativen und qualitativen Methoden begleitet (Mixed Methods). Der Vortrag stellt zunächst kurz das Konzept und seine inklusiven Merkmale vor und präsentiert dann ausgewählte Ergebnisse aus den Interviews mit den teilnehmenden Schüler*innen.

DD 32: Poster – Sprache und Physikunterricht

Time: Tuesday 14:00–16:00 Location: P5

DD 32.1 Tue 14:00 P5

Ist Sprache Nebensache? - Wirkung von Fachsprache in Erklärvideos — •Heiko Krabbe, Sebastian Kröger und Marco Seiter — Didaktik der Physik, Ruhr-Universität Bochum

Immer mehr Jugendliche nutzen Erklärvideos zum Lernen. Die wahrgenommene Qualität und Verständlichkeit der Erklärvideos kann allerdings stark variieren. Als Einflussfaktor wird häufig die Verwendung von Fachsprache diskutiert. In einer experimentellen Studie wurde untersucht, wie sich Fach- gegenüber Alltagssprache auf die Wahrnehmung eines Videos durch SchülerInnen und das Verständnis auswirkt. Hierzu wurde ein online verfügbares Video zur "Goldenen Regel der Mechanik" mit zwei Tonspuren neu vertont (Fachsprache vs. Alltagssprache). Alle übrigen Gestaltungsmerkmale (z. B. Animationen, Dauer, Sprechtempo) blieben konstant. Die SchülerInnen im Alter von 13 bis 15 Jahren wurden randomisiert einer der beiden Version zugewiesen. Erfasst wurden (a) die wahrgenommene Qualität getrennt nach sprachlichen und nichtsprachlichen Aspekten, (b) das selbstberichtetes Verständnis sowie (c) das tatsächliche Verständnis mittels eines Fachwissenstests. Auf dem Poster berichten wir die Ergebnisse der Studie und diskutieren Implikationen für die Gestaltung von sprachsensiblen und lernförderlichen Erklärvideos im Physikunterricht.

DD 33: Poster – Sonstiges

Time: Tuesday 14:00–16:00 Location: P5

DD 33.1 Tue 14:00 P5

My Freiwilliges Wissenschaftliches Jahr at the University of Oldenburg — •Katrin Nagel, Daniel Timmer, and Christoph Lienau — Institut für Physik, Carl von Ossietzky Universität Oldenburg, Oldenburg, Germany

Many highschool graduates face the difficult question of what they want to do. The variety of courses of study can be intimidating and few have an idea of what to do after their Abitur. These people have the opportunity to do a Bundesfreiwilligendienst (BFD). A BFD is a voluntary gap year between school and study as a self-discovery phase. The Carl von Ossietzky University Oldenburg offers a special yet lesser known version as one of very few universities called Freiwilliges Wissenschaftliches Jahr (FWJ, voluntary scientific year). I am doing my FWJ in the physics department, specifically in the research group Ultrafast Nano-Optics, where I gain an insight into scientific work as well as first lab experiences by building an interferometer. Interferometers are highly used in current research, e.g. ultrafast coherent spectroscopy. On my poster, I will report on my experiences with the FWJ in Oldenburg and show first results of my experiments. Increased awareness of this program would be particularly helpful for future Abitur graduates who are not sure what field of study they want to choose.

DD 34: Mitgliederversammlung

Time: Tuesday 18:00–20:00 Location: SCH/A101

Alle Mitglieder des Fachverbands Didaktik der Physik sind herzlich eingelanden.

DD 35: Kerschensteiner-Preisvortrag

Time: Wednesday 9:30–10:30 Location: HÜL/S386

Prize Talk DD 35.1 Wed 9:30 HÜL/S386

Die Bonner Physikshow – ein Öffentlichkeitsprojekt mit Studierenden — •Herbi Dreiner — Physikalisches Institut, Universität Bonn — Träger des Georg-Kerschensteiner-Preises 2026

Die Bonner Physikshow wurde im Dez. 2001 von Michael Kortmann und Herbi Dreiner gegründet. Bei dem Projekt entwickeln Physikstudierende der Uni Bonn am Ende ihres ersten Studienjahrs eine etwa 2h Show mit Live Experimenten und führen es auch selber für Schulklassen und allg. Publikum auf. Die Experimente sind dabei in ein Theaterstück mit Handlung eingebettet. Die Shows sollen unterhaltsam und lehrreich sein. Alle Experimente werden erklärt.

Alle 2 Jahre wird eine neue Gruppe rekrutiert. Bisher gab es 14 Jahrgänge. Die erfahrenen Studierenden weisen die Neuen jeweils ein. Sie nehmen dann auch an vielen fortgeschrittenen Projekten Teil. Mit einer Show über Elementarteilchenphysik sind wir schon durch Deutschland: AC, B(3x), BK, BO, BOH, DO, FR, GÖ, HAL, HH(3x), K, LEV(2x), M(4x), MZ, OB, SG, SON, SU, TÜ, W; und ganz Europa gereist: CH, DK, E(2x), I(2x), NL, P, PL, SI, SLO, UK. 2019 haben wir ein erstes Musical entworfen: Planetamos; 2025 ein zweites: Zukunftsenergien - Zukunftsmusik?

Es gibt jährlich eine Weihnachtsphysikshow, wo alle Jahrgänge mitmachen. 2021 wurde dies in 25 Einzelfilmen als Adventskalender bei YouTube veröffentlicht.

Das Zielpublikum sind zu allererst die Studierenden der Uni Bonn und dann das Publikum bei den Aufführungen. Es ist also ein Bildungsprojekt an der Uni und ein Öffentlichkeitsprojekt.

DD 36: Quantenphysik III

Time: Wednesday 10:45–11:45 Location: SCH/A101

DD 36.1 Wed 10:45 SCH/A101

Schüler- und Lehrkräfteperspektiven auf Smartphone-gestützte Schülerexperimente zur Quantenphysik — •Johannes Schlaf, Dominik Dorsel, Sebastian Staacks, Christoph Stampfer und Heidrun Heinke — I. & II. Physikalisches Institut A, RWTH Aachen University, Deutschland

Schulexperimente zur Quantenphysik sind oft komplex und benötigen teures Equipment. Dies erschwert die Einbindung von Realexperimenten in den Unterricht. Daher wurden zwei Schülerexperimente zur Quantenphysik entwickelt, die durch den Einsatz von Smartphones zur Messdatenerfassung übersichtlich und schülernah gestaltet sind: (i) ein Analogieexperiment zum BB84-Protokoll und (ii) ein Experiment zur Bestimmung des Planckschen Wirkungsquantums mit einem als DIY-Projekt (do it yourself) konzipierten Aufbau. Seit dem WS 2024/25 wurden die Experimente in Studierenden-, Schüler- und Lehrkräftegruppen hinsichtlich ihrer Usability evaluiert und optimiert. Seit Mai 2025 wurden in Workshops gemeinsam mit Lehrkräften Konzepte für den Einsatz und die Verbreitung der Experimente an Schulen entwickelt. Seit November 2025 wurden zusätzlich Schülerworkshops zur Bestimmung des Planckschen Wirkungsquantums ausgerichtet, um so die Verbreitung der DIY-Aufbauten an Schulen zu fördern. Im Vortrag werden die Experimente sowie deren Entwicklungsprozess vorgestellt und Ergebnisse aus Lehrkräfte- und Schülerworkshops präsentiert.

DD 36.2 Wed 11:05 SCH/A101

Didaktische Aufbereitung von Realexperimenten zur Quantenoptik in der Schule — •Nico Ammon, Julius Hlawatsch und Axel Enders — Universität Bayreuth, Bayreuth, Deutschland

Die Quanteninformationstechnologie ist ein Zukunftsfeld der Natur- und Ingenieurswissenschaften und hat als solches Einzug in den gymnasialen Physikunterricht gehalten. Darum ist es wichtig, die Grundlagen der Quantenoptik zu behandeln und so die Anwendung zugänglich zu machen.

Während quantenoptische Realexperimente für die meisten Schulen zu teuer sind, stellt das Lehrmittel "Quantenkoffer" eine Möglichkeit dar, ein geteiltes Gerät an mehreren Bildungsreinrichtungen zu nutzen. Damit kann man Experimente der Quantenoptik auf Schulniveau demonstrieren und diskutieren.

Unter Fachlehrern besteht bei diesem Thema ein enormes Interesse an Weiterbildung, didaktischer Aufbereitung, Schulmaterialien und Experimenten. In diesem Beitrag wird ein Vorschlag für ein entsprechendes Fortbildungskonzept für Physiklehrer unter Verwendung des Quantenkoffers präsentiert. Dabei wird eine didaktische Rekonstruktion der grundlegenden Quantenoptik vorgenommen. Erste empirische Ergebnisse einer Akzeptanzbefragung von den teilnehmenden Lehrkräften werden vorgestellt.

DD 36.3 Wed 11:25 SCH/A101

Quantum Dice: An Open Source a Haptic Analogy for Teaching Quantum Entanglement — •Bart Folkers, Aernout van Rossum, Alexander Brinkman, and Kirsten Stadermann — University of Twente, Enschede, the Netherlands

We developed an open source electronic analogy designed to simulate quantum physics (QP) concepts, including quantum entanglement. This electronic analogy consists of two 3D printed dice with embedded electronics and small displays, collectively referred to as Quantum Dice. Quantum Dice supports a range of educational scenarios, from basic entanglement demonstrations to quantum key distribution experiments. In this presentation, we share insights into the design and development of Quantum Dice. We also report on their implementation in diverse educational settings. In addition, we situate the project within ongoing educational design research in quantum education, in which we investigate what teachers and students need to work effectively with haptic analogies. Attendees will have the opportunity to interact with Quantum Dice prototypes, explore integration into their own teaching, and discuss how such analogies support reasoning about abstract quantum phenomena. More information is available at ut.onl/quantumdice.

DD 37: Lehr- und Lernforschung

Time: Wednesday 10:45–11:25 Location: SCH/A252

DD 37.1 Wed 10:45 SCH/A252

Entwicklung und Evaluation eines LLM-basierten Feedbacksystems für das physikalische Problemlösen — •Fabian Kieser[1], Paul Tschisgale[2], Holger Maus[2], Stefan Petersen[2], Marcus Kubsch[1] und Peter Wulff[3] — [1]FU Berlin, Berlin, Deutschland — [2]IPN, Kiel, Deutschland — [3]PH Ludwigsburg, Ludwigsburg, Deutschland

Künstliche Intelligenz eröffnet neue Möglichkeiten für individualisiertes und adaptives Lernen. Besonders Feedbacksysteme auf Basis großer Sprachmodelle (LLMs) versprechen flexible Lernunterstützung. Während sich bisherige Forschung vornehmlich darauf konzentriert, konzeptuelles Verständnis zu fördern, adressiert dieser Beitrag die Frage inwieweit LLM-basierte Feedbacksysteme auch bei komplexeren Fähigkeiten wie dem physikalischen Problemlösen reliabel und valide funktionieren. Zugleich sind LLMs als probabilistische Systeme nicht frei von Risiken: Sie können fehlerhafte Antworten erzeugen und ihre Nutzung zu einer übermäßigen Abhängigkeit der Lernenden führen. Um das Potenzial und die Grenzen solcher KI-basierten Feedbacksysteme unter anspruchsvollen Bedingungen zu untersuchen, haben wir unser System mit hochmotivierten Teilnehmenden des deutschen Auswahlwettbewerbs der Internationalen PhysikOlympiade erprobt. Ziel ist es, zu untersuchen, unter welchen Bedingungen solche Systeme Lernprozesse unterstützen können. Im Beitrag wird die oben gestellte Forschungsfrage mit Hilfe von empirischen Daten aus einer Erprobung einer solchen LLM-basierten Webanwendung im Projekt WasP beantwortet und zur Diskussion gestellt.

DD 37.2 Wed 11:05 SCH/A252

Oberflächenmerkmal oder Tiefenstruktur - worauf fokussieren Lernende und ExpertInnen bei Physikaufgaben? — •Marco Seiter und Heiko Krabbe — Ruhr-Universität Bochum

Chi (1981) hat gezeigt hat, dass NovizInnen Aufgaben mehr nach Oberflächenmerkmalen und ExpertInnen nach Tiefenstrukturmerkmalen in Form von konzeptionellen Prinzipien zusammenordnen. Darauf aufbauend untersucht diese Studie die Kriterien, nach denen Aufgaben gruppiert werden und wie sich diese Kriterien durch gezielte konzeptionelle Prompts verändern. ProbandInnen sollten in vier Runden Aufgaben nach selbstgewählten Kriterien gruppieren. Die erste Runde dient der Replikation der Befunde von Chi mit erweiterter Stichprobe. In den Runden zwei bis vier wurden die Probanden zusätzlich auf die Bewegungsarten (2), den Zusammenhang zwischen Kraft und Bewegung (3) und die Schlussrichtung (Kraft auf Bewegung; Bewegung auf Kraft) (4) gepromted. Die Stichprobe umfasste SchülerInnen, Studierende und wissenschaftliche ExpertInnen aus der Physik. Analysiert wurden die gebildeten Gruppierungen und die Begründungen hinsichtlich Oberflächenmerkmalen vs. Tiefenstruktur (konzeptionelle Prinzipien). Es zeigen sich Übergänge von oberflächen- zu prinzipiengeleiteten Gruppierungen und Verschiebungen durch unterschiedliche Prompts. Daraus können Indikatoren für möglichen Wissens- und Strategietransfer zwischen Aufgaben abgeleitet werden. Der Beitrag diskutiert Implikationen für die Gestaltung aufgabenbasierter Lernumgebungen in Hinblick auf das Prompting und die Explikation von Tiefenstrukturen zur Förderung von konzeptionellem Verständnis in Schule und Hochschule.

DD 38: Nature of Science

Time: Wednesday 10:45–11:45 Location: SCH/A284

DD 38.1 Wed 10:45 SCH/A284

Media competences of physics education students — •Kathleen Falconer, Laura Schäfer, Stefan Hoffmann, and André Bresges — Universität zu Köln, Institut für Physikdidaktik, Gronewaldstr. 2, 50931 Köln

A random selection of physics education students were interviewed on their perception of their media competences referring to the "Medienkompetenzrahmen NRW" for teachers. The students were selected from three groups: first group were first-year students, second group were currently at the end of a problem-based media lab and the third group were students that had finished at least one semester of a project-based media lab before covid. The analysis of the interview data showed that there was a clear path from the new students through the more experienced students. The two main themes found were the development of media competences of the students and the students' expectations from the university to help them develop their media competences.

DD 38.2 Wed 11:05 SCH/A284

INSIGHT: Historische Instrumente in Schulen nachbauen und nutzen — •Peter Heering[1] und Vasiliki Psoma[2] — [1]Europa-Universität Flensburg — [2]National and Kapodistrian University of Athens

Im Rahmen eines ERASMUS+ Projektes werden Materialien entwickelt, die es einerseits ermöglichen sollen, historische Geräte mit zeitgenössischen Materialien nachzubauen bzw. derart nachgebaute Geräte im Unterricht zu verwenden. Dabei ist ein Ziel, forschende Unterrichtsansätze zu unterstützen und gleichzeitig sowohl eine Kompetenzentwicklung im Bereich Nature of Science ebenso zu ermöglichen wie auch die Wahrnehmung von Physik als eine kulturelle Errungenschaft, die durch sehr verschiedene Menschen entwickelt wurde. Dabei ist die Mehrzahl der entwickelten Materialien für den Einsatz in der Sekundarstufe I gedacht, einige Beispiele sind aber explizit für die Sekundarstufe II konzipiert. Aus unserer Gruppe werden hierbei Materialien für vier historische Instrumente entwickelt: den Schweiggerschen Multiplikator, das Sykes Hydrometer, Youngs Eriometer und die Camera Lucida. Im Rahmen dieses Beitrags wird nach einer knappen Vorstellung des Projekts insbesondere auf die durch unsere Gruppe entwickelten Materialien sowie auf die Erfahrungen in einer ersten Sommerschule mit Lehrkräften eingegangen werden. Die Ergebnisse dieser Evaluatoin legen nahe, dass historische wissenschaftliche Instrumente in dieser Form als wirkungsvolle Vermittler zwischen wissenschaftlicher Erkenntnis, Kulturgeschichte und moderner MINT-Bildung dienen können.

DD 38.3 Wed 11:25 SCH/A284

Nature of Science im Lehramtsstudium — •Markus Obczovsky[1] und Kristina Fricke[2] — [1]Universität Frankfurt, Deutschland — [2]Berlin, Deutschland

Ein Ziel des Physikunterrichts ist die Entwicklung eines Nature of Science (NOS)-Verständnisses. Studien zeigen jedoch, dass (angehende) Lehrkräfte oft selbst ein nicht belastbares NOS-Verständnis haben und NOS-Aspekte in Ressourcen für Lehrpersonen, wie Schulbüchern, häufig nicht explizit und fachlich nicht belastbar sind. Daraus folgt das Desiderat für das Lehramtsstudium, dass Studierende ein angemessenes NOS-Verständnis entwickeln sowie lernen verschiedene Ressourcen zu analysieren und zu adaptieren. Zu diesem Zweck schlagen wir vor, zwei komplementäre NOS-Konzeptualisierungen für den Unterricht zu kombinieren und als Werkzeuge zur Analyse von Ressourcen anzubieten: den Consensus View (CV) und den Family Resemblance Approach (FRA). Während der CV sieben explizite, disziplinübergreifende NOS-Aspekte auflistet (z. B. Wissen ist vorläufig), umfasst der FRA Kategorien von NOS-Aspekten (z. B. Wissen), die für unterschiedliche Forschungskontexte kontextualisiert werden können. Es zeigte sich jedoch, dass die Akzeptanz solcher Werkzeuge eine zentrale Voraussetzung für deren Nutzung darstellt. In einem Design-based Research Ansatz untersuchen wir in einem ersten Erprobungszyklus, inwieweit Studierende CV und FRA als Werkzeug zur Analyse von Ressourcen verstehen und den komplementären Einsatz der beiden als nützlich beschreiben. Der Beitrag diskutiert die Konzeption der Lehrveranstaltung sowie die Ergebnisse des Erprobungszyklus.

DD 39: Interesse II

Time: Wednesday 10:45–11:45 Location: SCH/A285

DD 39.1 Wed 10:45 SCH/A285

Science Identity von Studienanfänger*innen im Fach Physik — •Lisa Stinken-Rösner[1], Nils Kunisch[1], Laura Pannullo[1], Thorid Rabe[2] und Inka Haak[2] — [1]Universität Bielefeld, Bielefeld, Germany — [2]Universität Halle, Halle, Germany

Die Entscheidung für eine physikalische Laufbahn genauso wie das Durchhaltevermögen und die Leistungen im Studium sind eng mit der Science Identity verbunden - also der Frage, inwiefern sich Personen als Teil der physikalischen Gemeinschaft wahrnehmen und von anderen als zugehörig anerkannt werden (Carlone & Johnson, 2007; Chen et al., 2020; Hazari et al., 2010). Im Rahmen der präsentierten Studie wurde an zwei Standorten die Science Identity von Physikstudierenden im ersten Fachsemester fragebogenbasiert erhoben. Untersucht wird unter anderem, ob die Science Identity von verschiedenen Personenmerkmalen abhängig ist, z. B. dem gewählten Studienfach (Physik, Medizinphysik, Lehramt) oder dem Geschlecht. Zusätzlich wurden für die Subgruppe der Lehramtsstudierenden die Teacher Identity und Science Teacher Identity erfasst, da insbesondere diese Studierenden sich im Spannungsfeld zwischen zwei beruflichen Identitäten als Physiker*in und als Lehrer*in bewegen.

DD 39.2 Wed 11:05 SCH/A285

'Die Projektwoche hat mir gezeigt, dass ich viel mehr kann als gedacht' - Ergebnisse einer Intervention zur Förderung der Physikidentität junger Frauen — •Paula Becker[1], Annelie Schulze[2], Andrea Westphal[3] und Peter Wulff[1] — [1]Pädagogische Hochschule Ludwigsburg — [2]Universität Potsdam — [3]Universität Greifswald

Es bestehen weiterhin geschlechtsspezifische Disparitäten in der Präferenz, das Fach Physik zu wählen. Physikidentität, d. h. inwiefern Personen sich mit dem Fach positiv in Beziehung setzen können, wurde als eine zentrale Ursache identifiziert. Außerschulische Programme bieten die Möglichkeit, identitätsfördernde Faktoren gezielt aufzugreifen. Um den Bedarf einer gezielten Integration motivationstheoretischer und fachdidaktischer Befunde zur Förderung von Schülerinnen zu addressieren, wurde ein fünftägiges Interventionsprogramm für Schülerinnen ab 17 Jahren theoriebasiert entwickelt und mithilfe eines Mixed-Method-Designs evaluiert. Insgesamt nahmen N = 40 Schülerinnen an dem Interventionsprogramm teil. Untersucht wurde, inwiefern sich Konstrukte der Physikidentität und die Studienintention über die Zeit veränderten und welche Gestaltungselemente von den teilnehmenden Schülerinnen als besonders wirksam wahrgenommen wurden. Im Rahmen des Vortrags werden die Ergebnisse der längsschnittlichen Evaluation präsentiert und Implikationen diskutiert.

DD 39.3 Wed 11:25 SCH/A285

Erfahrungen von Studienanfänger*innen mit der Physik-Community - Zusammenhang mit dem Zugehörigkeitsgefühl — •Inka Haak[1], Thorid Rabe[1] und Markus S. Feser[2] — [1]MLU Halle-Wittenberg, Institut für Physik, Hoher Weg 8, 06120 Halle — [2]IPN Kiel, Didaktik der Physik, Olshausenstr. 62, 24118 Kiel

Das Physikstudium mit einem ausgeprägten Gefühl dazuzugehören zu bestreiten, ist ein bedeutsamer Prädiktor für den Studienerfolg. Weitgehend ungeklärt ist bisher, wie sich ein Zugehörigkeitsgefühl zur Physik-Community, also der Gruppe von Menschen, die sich beruflich/akademisch mit Physik beschäftigen, in der Studieneingangsphase entwickelt. Es ist jedoch plausibel anzunehmen, dass Erfahrungen mit der Physik-Community hier eine tragende Rolle spielen. Im Rahmen der VeSP-Be Studie wurden unter anderem das Zugehörigkeitsgefühl zur Physik-Community und individuellen Erfahrungen mit dieser von N=216 Studienanfänger*innen der Physik verschiedener Studiengänge mithilfe eines Online-Fragebogens erhoben. Die offenen Antworten zu Erfahrungen mit der Physik-Community wurden mithilfe einer evaluativen Inhaltsanalyse ausgewertet und deren Zusammenhang mit dem Zugehörigkeitsgefühl zur Physik-Community statistisch mittels einer Odds-Ratios-Analyse quantifiziert. Erste Ergebnisse zeigen, dass die Äußerungen von positiven bzw. negativen Erfahrungen stark mit dem Zugehörigkeitsgefühl zusammenhängen. In weiteren Analysen soll exploriert werden, inwiefern die geäußerten Erfahrungen mit der Physik-Community, das Zugehörigkeitsgefühl zur Physik-Community und weitere Personenmerkmale statistisch zusammenhängen.

DD 40: Quantenphysik IV

Time: Wednesday 12:00–12:40 Location: SCH/A101

DD 40.1 Wed 12:00 SCH/A101

Insights into an International Year of Quantum Secondary STEM Teacher Professional Development Initiative — Angela M. Kelly[1], •Carsten Albert[1,2,3], Dominik Schneble[1], Tzu-Chieh Wei[1], and Zijian Song[1] — [1]The State University of New York - Stony Brook University, USA — [2]Leibniz Institute for Solid State and Materials Research Dresden, Germany — [3]TUD Dresden University of Technology, Germany

To meet the growing need for quantum information science and technology (QIST) workforce development, precollege students need to be exposed to QIST. However, quantum topics are not often taught in high school classrooms in the United States.

This research reports outcomes from a university-based International Year of Quantum Science teacher leadership initiative designed to promote QIST education in U.S. secondary schools in the New York area. A one-day conference was held in June 2025, aiming to build motivation for middle and high school STEM teachers to incorporate quantum ideas, QIST curricular developments, and the QIST research and workforce landscape in their disciplinary instruction. Following the conference, 12-hour professional development workshops were offered.

This presentation will give insights into the general approach of the project and highlight best practices for facilitating teachers' motivation and QIST pedagogical self-efficacy.

DD 40.2 Wed 12:20 SCH/A101

Warum steht die imaginäre Einheit in der Schrödingergleichung? — •Oliver Passon — Bergische Universität Wuppertal

Die (zeitabhängige) Schrödingergleichung enthält die imaginäre Einheit i und ihre Lösungen sind im Allgemeinen komplexwertige Funktionen. Dies ist allem Anschein nach ein weiterer Hinweis auf die Neuartigkeit der Quantentheorie, denn in anderen Bereichen der Physik werden komplexe Zahlen bloß verwendet, um sich einen Rechenvorteil zu verschaffen. Von physikalischer Bedeutung sind dann lediglich der Real- und/oder der Imaginärteil der Lösung.

Aus didaktischen Gründen ist die Motivation dieser Neuartigkeit sicherlich von Bedeutung. Noch wichtiger ist die Frage, ob nicht auch eine "reelle" Quantenmechanik formuliert werden könne. Mein Vortrag betrachtet didaktische, fachliche und historische Aspekte dieser Debatte.

DD 41: Lehrkräfteaus- und -fortbildung II

Time: Wednesday 12:00–13:00 Location: SCH/A252

DD 41.1 Wed 12:00 SCH/A252

Wie unsere Schüler:innen denken: Ein kognitiv fundiertes Modell zur Vorhersage typischer Denkprozesse und zur Entwicklung passender Handlungsstrategien im Physikunterricht — •Sergio Rivera Hernandez — FU Berlin, Berlin, Germany — Gabriele-von-Bülow-Gymnasium, Berlin, Germany

Eine der größten Herausforderungen im Physikunterricht besteht in der Planung von Unterrichtseinheiten, die es der Mehrheit der Lernenden ermöglichen, das angestrebte Lernziel zu erreichen. Aufgrund der Heterogenität der Lerngruppen ist hierfür eine präzise Diagnose typischer Denkprozesse notwendig, die bei der Bearbeitung einer Physikaufgabe auftreten und zu Fehlern führen können. Gerade Referendar:innen und Berufsanfänger:innen stehen dabei häufig vor der Schwierigkeit, diese Denkprozesse vorherzusagen und passende Handlungsalternativen zu entwickeln.

Dieser Beitrag präsentiert ein theoretisches Modell sowie ein konkretes Planungsinstrument, die auf den Dual-Prozess-Theorien der Kognitionspsychologie basieren. Sie dienen Lehrkräften als Orientierung zur systematischen Fehleridentifikation und als Grundlage für die Entwicklung passender Unterstützungsmaterialien. Dieser Ansatz wird derzeit in der Berliner Physiklehrkräfteausbildung erprobt. Vorgestellt werden das Modell und die entwickelten Planungsraster anhand konkreter Beispiele sowie erste Ergebnisse der praktischen Erprobung.

DD 41.2 Wed 12:20 SCH/A252

Eine detaillierte Analyse eines großen Aktionsforschungszyklus im Rahmen des Learning-by-Teaching-Ansatzes im Rahmen der Ausbildung von Physiklehrer*innen an der Universität zu Köln — •Stefan Hoffmann, Kathleen Falconer und André Bresges — Universität zu Köln, Institut für Physikdidaktik, Gronewaldstr. 2, 50931 Köln

Das Learning-by-Teaching Konzept an der Universität zu Köln stützt sich mittlerweile auf eine mehr als 17-jährige Erfahrung. Seit der Entwicklung und Implementierung wurde es kontinuierlich weiterentwickelt im Sinne der partizipativen Aktionsforschung. Dadurch ist man im Stande sowohl auf kleinere im Lehralltag auftretende Probleme und Herausforderungen als auch auf größere die Studierendenpopulation betreffende äußere Gegebenheiten zu reagieren. In dem Vortrag soll ein großer Zyklus aus mehreren Semestern im Rahmen der kontinuierlichen Weiterentwicklung des Lehr-Lern-Konzeptes vorgestellt werden.

DD 41.3 Wed 12:40 SCH/A252

Fallanalysen zur Gestaltung von Experimentierphasen: Ergebnisse einer empirischen Längsschnittuntersuchung — •Teresa Tewordt und Lisa Stinken-Rösner — Universität Bielefeld

Experimentieren im Physikunterricht fördert konzeptuelles Verständnis und experimentelle Fähigkeiten der Lernenden (Idris, 2022; Kreitler & Kreitler, 1974; Li et al., 2023). Damit diese Potenziale wirksam werden, müssen Experimentierphasen von Lehrkräften gezielt geplant und in den Unterricht eingebettet werden. Zentrale Einflussfaktoren, die den Gestaltungsprozess beeinflussen, sind im Modell zum Designen von Experimentierphasen (DEP Modell) beschrieben (Tewordt & Stinken-Rösner, 2025).

Auf Basis dieses Modells wurde eine Längsschnittstudie mit Masterstudierenden im Physiklehramt durchgeführt, um deren Professionalisierung im Verlauf zweier Semester zu untersuchen. Hierbei wurden die Entwicklung des professionellen Wissens, der Selbstwirksamkeitserwartung und der Entscheidungsstrategien beim Planen und Durchführen von Experimenten erfasst. Anhand von Fallanalysen wird gezeigt, inwiefern sich die Fähigkeiten der Studierenden zur Gestaltung von Experimentierphasen im Verlauf des Masterstudiums entwickeln.

DD 42: Neue Konzepte II

Time: Wednesday 12:00–13:00 Location: SCH/A285

DD 42.1 Wed 12:00 SCH/A285

EVAnova: (Meta-)kognitive Unterstützung für eigenverantwortliches Arbeiten im Physikunterricht – Erste Ergebnisse aus der Lehrkräfte-Evaluation — •Julius Hlawatsch, Heiko Müller und Axel Enders — Universität Bayreuth, Bayreuth, Deutschland

Im bayerischen LehrplanPlus für das Fach Physik an Gymnasien ist ab der Jahrgangsstufe 11 ein Lernbereich "Eigenverantwortliches Arbeiten (EVA)" zu ausgewählten Inhaltsbereichen verpflichtend verankert. Ziel von EVA ist dabei, dass sich die Schüler Fachwissen selbstständig aneignen, die dazu notwendigen Quellen erschließen und auswerten und die eigenen Ergebnisse in geeigneter Form darstellen. Die Umsetzung stellt für die überwiegende Mehrheit sowohl der bayerischen Lehrkräfte als auch der Schüler eine große Herausforderung dar, unter anderem, weil der hohe Anteil von Schüleraktivität und -verantwortung von der gängigen Unterrichtspraxis abweicht. Davon sind insbesondere leistungsschwächere Schüler betroffen, wie eine explorative Vorstudie unter Gymnasiallehrkräften im Rahmen dieses Projekts zeigte. Basierend auf den gewonnenen Erkenntnissen wurde das Unterrichtskonzept EVAnova entwickelt, das die Schüler bei EVA (meta-)kognitiv unterstützt, z. B. durch gezieltes Methodentraining, Prompting und Reflexionsbögen. Dieses Konzept sowie erste Ergebnisse einer evaluativen Interviewstudie unter den Lehrkräften, die EVAnova in ihrem Unterricht bereits eingesetzt haben, sollen in diesem Vortrag vorgestellt werden.

DD 42.2 Wed 12:20 SCH/A285

Mit Kugelbahnen MINT-Kompetenzen fördern und den Unterricht ins Rollen bringen — •Luca Goroncy und Angela Fösel — Didaktik der Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg

Kugelbahnen finden sich in vielen Kindergärten und Kinderzimmern wieder, jedoch kann dieses pädagogische Werkzeug auch für den MINT-Unterricht verwendet werden. Mit ihrer Hilfe können physikalische Konzepte und ebenso naturwissenschaftliche Arbeitsweisen gefördert werden.

Im Rahmen einer Zulassungsarbeit wurden Kugelbahnstrukturen, hier insbesondere Low-Cost-Messwerterfassungssysteme, neu konzipiert und realisiert.

Ziel ist es, diese Bauelemente in bereits bestehende kommerzielle Kugelbahnsysteme zu integrieren für die Anwendung von Kugelbahnen im MINT-Unterricht. Der Fokus liegt auf den Experimenten und der Exploration von Kugelbahnelementen durch Schülerinnen und Schülern.

Vorgestellt werden das Konzept und ausgewählte Experimente sowie Aktivitäten.

DD 42.3 Wed 12:40 SCH/A285

Konstruktion eines Halbach-Arrays für die Optimierung von Versuchsaufbauten mit homogenen Magnetfeldern — •Deniz C. Senel[1], Konstantin Gerstenberger[2], Günter Auernhammer[2] und Bianca Watzka[1] — [1]I. Physikalisches Institut (IA), RWTH Aachen University, Sommerfeldstraße 16, 52074 Aachen, Deutschland — [2]Leibniz-Institut für Polymerforschung Dresden e.V., 01069 Dresden, Deutschland

Im Rahmen eines kooperativen Forschungsprojekts zu strukturierten magnetischen Elastomeren (DFG FOR 5599) werden Halbach-Arrays eingesetzt, die durch die gezielte Anordnung von Permanentmagneten besonders starke und zugleich homogene Magnetfelder erzeugen. Schultypische Experimentieraufbauten mit Hufeisenmagneten oder Helmholtzspulen liefern demgegenüber häufig nur Magnetfelder mit begrenzter Feldstärke oder eingeschränkter Homogenität, sodass zentrale Konzepte und Eigenschaften magnetischer Felder – wie Superposition, Homogenität und die vom Feld vermittelten Kräfte – oftmals nur eingeschränkt betrachtet werden können. Mithilfe des Arrays wird ein experimenteller Zugang zu diesen Aspekten deutlich erleichtert. Dieser Beitrag beschreibt die Konstruktion eines solchen Halbach-Arrays, die didaktische Hinführung und experimentelle Anwendungen. Dazu gehören ein optimierter Leiterschaukelversuch sowie ein Versuch zur Visualisierung der Superposition von Magnetfeldern.

DD 43: Abschlussplenum

Time: Wednesday 13:00–13:30 Location: SCH/A101

30 min

Quantum Information Division
Fachverband Quanteninformation (QI)

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Overview of Invited Talks and Sessions

(Lecture halls BEY/0137, BEY/0245, and BEY/0E17; Poster P4)

Invited Talks

QI 2.1	Mon	9:30–10:00	BEY/0245	**Advances in Frequency-Multiplexed Readout and Subsequent Qubit-State Reset** — •Benjamin Lienhard, Shivang Arora, Emily Guo, Priyanka Yashwantrao, Patryk Dabkowski, Stefan Filipp
QI 4.1	Mon	15:00–15:30	BEY/0245	**Reducing Noise, Complexity, and Optimization Barriers in Quantum Simulations of Strongly Correlated Systems** — •Werner Dobrautz
QI 6.1	Tue	9:30–10:00	BEY/0245	**Erbium dopants for quantum networks** — •Andreas Reiserer
QI 11.1	Wed	9:30–10:00	BEY/0245	**Nb-trilayer Josephson junction based parametric amplifiers for microwave frequency signals** — •Lukas Grünhaupt
QI 15.7	Thu	11:30–12:00	BEY/0137	**Robust shadow tomography: from quantum simulation to high-energy physics** — •Hai-Chau Nguyen
QI 16.1	Thu	9:30–10:00	BEY/0245	**Measurement-free universal fault-tolerant quantum computation** — •Friederike Butt, Ivan Pogorelov, Alex Steiner, Marcel Meyer, Thomas Monz, Markus Müller, Robert Freund
QI 18.1	Thu	15:00–15:30	BEY/0245	**Multipartite Quantum states from guided-wave structures** — •Virginia D'Auria, Adrien Bensemhoun, Silvia Cassina, Carlos Gonzalez-Arciniegas, Mohamed Fauzi Melalkia, Giuseppe Patera, Jonathan Faugier-Tovar, Quentin Wilmar, Ségolène Olivier, Alessandro Zavatta, Anthony Martin, Jean Etesse, Laurent Labonté, Sébastien Tanzilli
QI 21.1	Fri	9:30–10:00	BEY/0245	**Non-Hermitian topology and directional amplification** — •Clara Wanjura

Sessions

QI 1.1–1.11	Mon	9:30–12:45	BEY/0137	**Quantum Computing and Algorithms I**
QI 2.1–2.10	Mon	9:30–12:45	BEY/0245	**Implementations I**
QI 3.1–3.12	Mon	15:00–18:30	BEY/0137	**Quantum Simulation**
QI 4.1–4.11	Mon	15:00–18:30	BEY/0245	**Quantum Manybody Systems (joint session QI/TT)**
QI 5.1–5.10	Tue	9:30–12:30	BEY/0137	**Quantum Computing and Algorithms II**
QI 6.1–6.10	Tue	9:30–12:45	BEY/0245	**Implementations II**
QI 7.1–7.6	Tue	9:30–11:00	BEY/0E17	**Quantum Thermodynamics**
QI 8.1–8.6	Tue	14:00–15:30	BEY/0137	**Implementations III**
QI 9.1–9.6	Tue	14:00–15:30	BEY/0245	**Decoherence and Open Systems I**
QI 10.1–10.11	Wed	9:30–12:45	BEY/0137	**Quantum Information: Concepts and Methods I**
QI 11.1–11.10	Wed	9:30–12:45	BEY/0245	**Implementations IV**
QI 12.1–12.10	Wed	15:00–18:00	BEY/0137	**Quantum Foundations**
QI 13.1–13.10	Wed	15:00–18:00	BEY/0245	**Quantum Control**
QI 14.1–14.28	Wed	18:00–21:00	P4	**Quantum Information Poster Session**
QI 15.1–15.9	Thu	9:30–12:30	BEY/0137	**Quantum Information: Concepts and Methods II**
QI 16.1–16.10	Thu	9:30–12:45	BEY/0245	**Quantum Software**
QI 17.1–17.8	Thu	15:00–17:30	BEY/0137	**Decoherence and Open Systems II**
QI 18.1–18.9	Thu	15:00–18:00	BEY/0245	**Quantum Communication**
QI 19	Thu	18:00–19:00	BEY/0245	**Members' Assembly**

QI 20.1–20.8	Fri	9:30–12:00	BEY/0137	**Metrology and Sensing**
QI 21.1–21.10	Fri	9:30–12:45	BEY/0245	**Quantum Information: Concepts and Methods III**

Members' Assembly of the Quantum Information Division

Thursday 18:00–19:00 BEY/0245

Sessions

– Invited Talks, Contributed Talks, and Posters –

QI 1: Quantum Computing and Algorithms I

Time: Monday 9:30–12:45 Location: BEY/0137

QI 1.1 Mon 9:30 BEY/0137

The Complexity of Simulating Inertially Coupled Bosonic Hamiltonians — •Refik Mansuroglu[1], Lilith Zschetzsche[1], and Norbert Schuch[1,2] — [1]University of Vienna, Faculty of Physics, Boltzmanngasse 5, 1090 Vienna, Austria — [2]University of Vienna, Faculty of Mathematics, Oskar-Morgenstern-Platz 1, 1090 Vienna, Austria

The computational complexity of simulating physically natural quantum systems is a central question at the interface of quantum physics and computer science. While recent work has established the BQP-completeness of simulating an exponential number of coupled classical oscillators [Babbush et al.], the complexity of more general bosonic dynamics has remained unresolved. Here we prove that simulating inertially coupled bosonic systems, a broad class that includes quantum harmonic oscillators as a special case, is BQP-complete. In the Hamiltonian framework, we consider the problem of deciding whether the expectation value of an R-local observable is polynomially separated from zero, given only polynomially many nonzero initial amplitudes $q_j(0)$ and $p_j(0)$. We show that the Hamiltonians governing continuous-time quantum walks can be expressed as inertially coupled bosonic systems, thereby unifying two paradigms of quantum dynamics within a single complexity-theoretic classification.

QI 1.2 Mon 9:45 BEY/0137

Equivalence of Quantum Walk and Coupled Classical Oscillator Simulation — •Lilith Zschetzsche[1], Refik Mansuroglu[1], András Molnár[1,2], and Norbert Schuch[1,2] — [1]University of Vienna, Faculty of Physics, Boltzmanngasse 5, 1090 Wien, Austria — [2]University of Vienna, Faculty of Mathematics, Oskar-Morgenstern-Platz 1, 1090 Vienna, Austria

We present direct and physically well-motivated reductions between the simulation of quantum walk Hamiltonians and the simulation of exponentially many coupled classical oscillators, problems that are known to be BQP-complete. Mapping the complex amplitudes of the quantum walk to the displacements and conjugate momenta of the classical oscillators allows us to identify the equations of motions of the quantum walk with those of the harmonic oscillators. That is, we construct a classical Hamiltonian of harmonic oscillators from a quantum walk Hamiltonian (and vice versa), such that energy terms for oscillators and vertex populations of the quantum walk are identified as measurement outcomes on the time-evolved state. Given the BQP-completeness of one of those problems, our reduction can be seen as an alternative proof for BQP-hardness of the other, although the reduction reaches beyond BQP-complete versions of the problem.

QI 1.3 Mon 10:00 BEY/0137

Block encoding and QSVT for solving differential equations — •Abhishek Setty — Forschungszentrum Jülich, Germany — University of Cologne, Germany

We present a unified framework for efficient block encoding of arbitrary sparse matrices, addressing the key barriers to practical quantum algorithms: multi-controlled gate overhead, amplitude reordering, and hardware connectivity. Our method combines a combinatorial-optimization strategy for control-qubit assignment with coherent permutation operators, yielding explicit gate-level constructions with reduced depth. Building on this, we outline a quantum linear systems pathway for solving differential equations within the QSVT paradigm. We demonstrate this on a complex linear system and extend it to CFD problems, including the heat equation and Carleman-linearized Burgers equation. These results highlight both the potential and limitations of current methods, underscoring the need for efficient estimation of minimum singular value, depth-reduction techniques, and benchmarks against classical reachability. This pathway lays a foundation for advancing quantum linear system methods toward large-scale applications.

QI 1.4 Mon 10:15 BEY/0137

Exploring Variational Entanglement Hamiltonians — •Yanick S. Kind[1,2] and Benedikt Fauseweh[1,2] — [1]TU Dortmund, Dortmund, Germany — [2]German Aerospace Center, Cologne, Germany

Recent advances in analog and digital quantum-simulation platforms have enabled exploration of the spectrum of entanglement Hamiltonians via variational algorithms. We investigate the convergence properties of a variational algorithm and benchmark the results against numerically exact calculations. By interpreting the cost function as an integral, we employ an iterative quadrature scheme, reducing the measurement overhead by several orders of magnitude. We further demonstrate that a modified Bisognano-Wichmann ansatz allows better convergence in lattice models and provides a diagnostic for quantum phase transitions. Finally, we show that a lower cost function does not necessarily lead to a lower trace distance. However, it still faithfully reproduces degeneracies in the entanglement spectrum, which are essential for topological applications. Y. S. Kind, B. Fauseweh, arXiv:2505.10530, 2025

QI 1.5 Mon 10:30 BEY/0137

The sub-Riemannian geometry of measurement based quantum computation — •Lukas Hantzko — Leibniz Universität, Hannover, DE

The computational power of symmetry-protected phases of matter can be accessed through local measurements, but what is the most efficient way of doing so? In this work, we show that minimizing operational resources in measurement-based quantum computation (MBQC) on subsystem symmetric resource states amounts to solving a sub-Riemannian geodesic problem between the identity and the target logical unitary. This reveals a geometric structure underlying MBQC and offers a principled route to optimize quantum processing in computational phases.

QI 1.6 Mon 10:45 BEY/0137

Entanglement-informed construction of variational quantum circuits — Alina Joch[1,2], Götz Uhrig[1], and •Benedikt Fauseweh[1,2] — [1]Condensed Matter Theory, TU Dortmund University, Otto-Hahn-Straße 4, 44227 Dortmund, Germany — [2]Institute of Software Technology, German Aerospace Center (DLR), 51147 Cologne, Germany

The variational quantum eigensolver is a promising tool for simulating ground states of quantum many-body systems on noisy quantum computers. Its effectiveness relies heavily on the ansatz, which must be both hardware-efficient for implementation on noisy hardware and problem-specific to avoid local minima and convergence problems. Here, we explore entanglement-informed ansatz schemes that naturally emerge from specific models, aiming to balance accuracy with minimal use of two-qubit entangling gates. We investigate quasi-1D Hamiltonians focusing on entanglement barriers and long-range interactions. We find that including the entanglement structure in the parameterized quantum circuit reduces the resources necessary to achieve a given accuracy. A better assessment is obtained by analyzing how the ansatz captures the entanglement spectrum. Our comprehensive analysis provides a new perspective on the design of ansätze based on the expected entanglement structure of the approximated state.

Quantum Sci. Technol. 10 035032 (2025)

30min. break

QI 1.7 Mon 11:30 BEY/0137

Measurement-driven Quantum Approximate Optimization — •Tobias Stollenwerk[1] and Stuart Hadfield[2,3] — [1]Institute for Quantum Computing Analytics (PGI-12), Jülich Research Centre, Wilhelm-Johnen-Straße, 52428 Jülich, Germany — [2]Quantum Artificial Intelligence Lab (QuAIL), NASA Ames Research Center, Moffett Field, CA 94035, USA — [3]USRA Research Institute for Advanced Computer Science (RIACS), Mountain View, CA 94043, USA

Algorithms based on non-unitary evolution have attracted much interest for ground state preparation on quantum computers. In this work we specialize and extend one recently proposed approach that employs mid-circuit measurements and control to the setting of constrained and unconstrained combinatorial optimization. For this we compare and contrast both penalty-based and feasibility-preserving approaches, elucidating the significant advantages of the latter approach. We show how to select parameters such that the success probability of each measurement step is bounded away from 1/2. Our approach is general and may be applied to easy-to-prepare initial states as a standalone algorithm, or deployed as a quantum postprocessing stage. We then propose a more sophisticated variant of our algorithm that adaptively applies a mixing operator or not, based on the measurement outcomes seen so far, as to speeds up the algorithm and helps the system evolution avoid slowing down or getting stuck suboptimally. In particular, we show that mixing operators from QAOA can be imported directly, both for the necessary eigenstate scrambling operator and for initial state preparation, and discuss quantum resource tradeoffs.

QI 1.8 Mon 11:45 BEY/0137

Greens Function on Quantum Computers: Error Mitigation and application in Dynamical Mean Field Theory — •Jannis Ehrlich[1], Aljoscha F. Baumann[1], Daniel F. Urban[1,2], and Christian Elsässer[1,2] — [1]Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg, Germany — [2]Freiburger Materialforschungszentrum, Universität Freiburg, Germany

Dynamical Mean Field Theory (DMFT) has become a powerful tool for investigating the physics of materials that exhibit strong electronic correlations, like high-temperature superconductivity or metal-insulator transitions. The numerically challenging part is the calculation of the Greens function (GF) of the underlying Anderson impurity auxiliary model due to the explicit treatment of electron interactions, which is also directly connected to the energy of the system and the spectral function.

We present a time-evolution approach for extracting the GF by simulating the quantum system on a quantum computer and show its performance for the auxiliary Anderson impurity model of DMFT on real quantum processors with systems of increasing sizes. We further investigate the relevance of accuracy in the ground-state preparation and demonstrate possibilities to reduce and mitigate errors of current quantum devices.

QI 1.9 Mon 12:00 BEY/0137

Generation of Fermionic Gaussian States: Optimal and Approximate Matchgate Circuits — •Marc Langer[1,2], Raúl Morral-Yepes[1,2], Adam Gammon-Smith[3,4], Frank Pollmann[1,2], and Barbara Kraus[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany — [3]School of Physics and Astronomy, University of Nottingham, Nottingham, NG7 2RD, UK — [4]Centre for the Mathematics and Theoretical Physics of Quantum Non-Equilibrium Systems, University of Nottingham, Nottingham, NG7 2RD, UK

Fermionic Gaussian states (FGS), and the related matchgates, play an important role in the study of various phenomena. Despite being able to represent highly entangled states, they are still tractable on classical computers. A naturally arising question is how to optimally create such states, for instance when using matchgate circuits acting on product states. In this work, we present algorithms for explicitly constructing such circuits that provably yield the minimal number of gates. Our techniques furthermore allow us to characterize which states can be represented exactly with a low depth matchgate circuit. Some applications of these results include approximate state preparation, robust disentangling algorithms and classical simulation methods.

QI 1.10 Mon 12:15 BEY/0137

Adaptive, efficient and provable energy estimation on noisy intermediate-scale quantum computers — •Bruno Murta[1], Alexander Gresch[2], and Martin Kliesch[1] — [1]TUHH - Hamburg University of Technology — [2]eleQtron GmbH

Estimating the energy of a prepared quantum state from measurements is a central subroutine in quantum simulation algorithms. In a noisy intermediate-scale quantum (NISQ) setting, this estimation must be carried out with shallow readout circuits. In this work, we introduce an energy estimation framework that both tightens theoretical guarantees and reduces the cost of measuring molecular and solid-state Hamiltonians on NISQ devices. Our protocol exploits empirical (co)variance information gathered during measurement collection to adapt the estimation to the specific state, interpolates between qubit-wise and global commutativity to provide a trade-off between circuit depth and shot efficiency, and is supported by rigorous error bounds. Numerical benchmarks on molecular and lattice models indicate that the resulting scheme achieves a significant suppression of shot noise for a fixed measurement budget, while keeping quantum resources compatible with current NISQ hardware.

QI 1.11 Mon 12:30 BEY/0137

A Constant Measurement Quantum Algorithm for Graph Connectivity — •Maximilian Balthasar Mansky[1], Chonfai Kam[2], and Claudia Linnhoff-Popien[1] — [1]LMU Munich — [2]Palermo University

We introduce a novel quantum algorithm for determining graph connectedness using a constant number of measurements. The algorithm can be extended to find connected components with a linear number of measurements. It relies on non-unitary abelian gates taken from ZX calculus. Due to the fusion rule, the two-qubit gates correspond to a large single action on the qubits. The algorithm is general and can handle any undirected graph, including those with repeated edges and self-loops. The depth of the algorithm is variable, depending on the graph, and we derive upper and lower bounds. The algorithm exhibits a state decay that can be remedied with ancilla qubits. We provide a numerical simulation of the algorithm.

QI 2: Implementations I

Time: Monday 9:30–12:45 Location: BEY/0245

Invited Talk QI 2.1 Mon 9:30 BEY/0245

Advances in Frequency-Multiplexed Readout and Subsequent Qubit-State Reset — •Benjamin Lienhard[1,2], Shivang Arora[1,2], Emily Guo[1,2], Priyanka Yashwantrao[1,2], Patryk Dabkowski[1,2,3], and Stefan Filipp[1,2] — [1]Technical University of Munich, Garching 85748, Germany — [2]Walther-Meißner-Institut, Garching 85748, Germany — [3]Zurich Instruments, 8005 Zürich, Switzerland

In scalable, resource-efficient quantum processors with large numbers of superconducting qubits, readout performance often becomes a key limitation for overall system fidelity. Achieving fast, high-fidelity simultaneous measurement—critical for quantum error correction—typically relies on frequency-multiplexed readout to reduce resource overhead. However, crosstalk and other nonidealities pose significant challenges for conventional signal processing and state discrimination. Emerging machine learning (ML) approaches provide efficient, low-complexity mappings from measurement signals to qubit states, reducing error rates and enabling real-time scalability. In this talk, I will present recent advances in ML-based readout and reset techniques, along with their implementation on dedicated hardware. By combining scalable algorithms with compact, ML-driven discriminators deployed on FPGAs, we can address the readout bottleneck and substantially improve both fidelity and speed.

* funded through the EQuIPS Quantum Futur project from the Federal Ministry of Education and Research (BMBFTR) under funding number 13N17232.

QI 2.2 Mon 10:00 BEY/0245

Environment-assisted Cross-Resonance gate — •Radhika Hemant Joshi[1], Alwin van Steensel[1], Julian Rapp[2], and Mohammad Ansari[1] — [1]Peter Grunberg Institute, PGI-2, Forschungszentrum Julich, 52428 Julich, Germany — [2]Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany

Superconducting qubits have emerged to become a promising platform for quantum computing [1]. A cross-resonance (CR) gate is a particularly important two-qubit gate, which enables CNOT operation. In CR gate, two qubits, the so-called control and target, are coupled and the control qubit is driven at frequency of the target qubit [2,3]. However, the operation of these gates is affected by their environment[4]. To quantify this effect, we consider a Cross-Resonance (CR) gate connected to external reservoirs and evaluate the entangling interaction.

[1] J. Clarke, F. Wilhelm, Superconducting quantum bits, Nature453, 1031-1042 (2008)

[2] Xuexin Xu, M.H. Ansari, ZZ freedom in two qubit gates, Phys.Rev. Applied 15, 064074(2021), arXiv:2009.00485

[3] Xuexin Xu, M. Ansari, Parasitic-Free Gate: An Error-Protected Cross-Resonance Switch in Weakly Tunable Architectures, Phys.Rev. Applied 19, 024057, arXiv:2212.05519

[4] Radhika H. Joshi, Mohammad H. Ansari, Environment-assisted Cross-Resonance gate, in preparation.

QI 2.3 Mon 10:15 BEY/0245

Robust universal gate set for neutral-atom qudits — Amir Burshtein[1], •Shachar Fraenkel[1], Moshe Goldstein[1], and Ran Finkelstein[1,2] — [1]School of Physics and Astronomy, Tel Aviv University, Tel Aviv 6997801, Israel — [2]The Center for Nanoscience & Nanotechnology, Tel Aviv University, Tel Aviv 6997801, Israel

Quantum devices comprised of native qudits, instead of qubits, offer promising advantages for quantum simulation and fault-tolerant quantum computation, yet efficient schemes for the control and entanglement of qudits in quantum hardware remain scarce. In particular, no experimental demonstration of multi-qudit control has been achieved to date in neutral-atom arrays. We propose a universal control scheme for qudits encoded in ground and metastable states of neutral atoms. Within this scheme, single-qudit gates are implemented efficiently via the simultaneous driving of multiple transition frequencies. For entangling operations, we provide a recipe implementing any symmetric controlled-phase gate (e.g., controlled-Z) for any qudit dimension d. The recipe relies on a global drive, a key requirement for high experimental fidelity, and involves pulses that simultaneously drive two different Rydberg transitions, which we prove to be the minimal number generally necessary for realizing such global-drive phase gates. This underlines a more general need for adjusting the notion of a universal gate set to the practical limitations of the hardware of interest. The gates we design are easy to calibrate and robust to realistic experimental imperfections, as we demonstrate via extensive noise simulations.

arXiv:2508.16294

QI 2.4 Mon 10:30 BEY/0245

Hyperfine spectroscopy of rare-earth ions in $CaWO_4$ using broadband electron spin resonance — •Georg Mair[1,2], Ana Strinić[1,2,3], Achim Marx[1], Kirill Fedorov[1,2,3], Hans Huebl[1,2,3], Rudolf Gross[1,2,3], and Nadezhda Kukharchyk[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]School of Natural Sciences, Technische Universität München, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology, 80799 München, Germany

The spin states of rare-earth ions doped into crystals provide a promising platform for quantum memories, owing to their long coherence times and frequency compatibility with superconducting quantum circuits. We investigate dilute ensembles of erbium and ytterbium ions in $CaWO_4$ crystals at millikelvin temperatures using broadband electron spin resonance spectroscopy based on superconducting coplanar waveguides. This approach enables the precise detection of zero-field and low-field spin transition spectra. Hyperfine and quadrupolar interactions emerging from the nuclear spins of ^{167}Er, ^{171}Yb, and ^{173}Yb give rise to a rich microwave spectrum below 4 GHz, from which we identify Zero First-Order Zeeman (ZEFOZ) shift transitions. By measuring coherence properties of individual hyperfine spin transitions, we find Hahn echo coherence times of tens of microseconds to milliseconds. Our broadband spectroscopy approach thus enables not only the fitting of full spin Hamiltonians, but also the identification and validation of long-lived spin transitions.

QI 2.5 Mon 10:45 BEY/0245

shaping free electron wavepackets with plasmonic near-field — •Fatemeh Chahshouri[1] and Nahid Talebi[1,2] — [1]Institute of Experimental and Applied Physics, Kiel University, 24098 Kiel, Germany — [2]Kiel, Nano, Surface, and Interface Science * KiNSIS, Kiel University, 24098 Kiel, Germany

Free-electron interactions with light and matter have long served as a cornerstone for exploring the quantum and ultrafast dynamics of material excitation. Here, we investigate how the plasmonic near-fields of gold nanorods and dimers modulate slow-electron wavepackets and result in controlled elastic and inelastic interactions beyond the nonrecoil approximation. We first show that tailoring the geometry, polarization, and near-field topology of the nanorod, together with adjusting the phase offset between sequential near-field components through phase-locked gating, enables deterministic control over momentum transfer to the electron, including both inelastic longitudinal energy exchange and transverse recoil of the electron beam. We then study electron shaping under rotating plasmonic fields generated either by two orthogonally polarized pulses with controlled phase delay or by circularly polarized light with defined handedness, which leads to angular-momentum transfer and a strong handedness-dependent electron modulation in both real- and reciprocal space. These results underscore the versatility of engineered plasmonic near-fields for shaping free-electron beams and open new opportunities for ultrafast interferometry and quantum-coherent electron microscopy.

30min. break

QI 2.6 Mon 11:30 BEY/0245

A Free-Electron-Driven Quantum Light Source — •Armin Feist[1,2], Guanhao Huang[3,4], Germaine Arend[1,2], Yujia Yang[3,4], Jan-Wilke Henke[1,2], Zheru Qiu[3,4], Hao Jeng[1,2], Arslan Sajid Raja[3,4], Rudolf Haindl[1,2], Rui Ning Wang[3,4], Tobias J. Kippenberg[3,4], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, DE — [2]4th Physical Institute, University of Göttingen, DE — [3]Institute of Physics, EPFL, Lausanne, CH — [4]Center for Quantum Science and Engineering, EPFL, Lausanne, CH

Tailored nonclassical light is essential for photonic quantum technologies, yet generating complex optical states remains challenging. Inelastic free-electron scattering offers a promising new method for creating parametric and wavelength-tunable quantum light, particularly through coherent cathodoluminescence.

Here, we present a novel platform that efficiently couples free-electron beams to silicon nitride integrated photonics [1], enabling the generation of electron-photon pair states [2]. By post-selecting electrons with quantized energy loss, we can herald nonclassical single and multi-photon states [2,3]. This establishes a versatile source of tailored quantum light, potentially leading to a new class of hybrid quantum technology that combines electrons and photons.

[1] J.-W. Henke *et al.*, Nature **600**, 653 (2021)
[2] A. Feist *et al.*, Science **377**, 777 (2022)
[3] G. Arend *et al.*, Nat. Phys. **21**, 1855 (2024)

QI 2.7 Mon 11:45 BEY/0245

Fast Monitoring of Qubit T1 Fluctuations from Single-Shot Readout — •Julian Englhardt[1,2], Emily Wright[1,2], Niklas Glaser[1,2], Leon Koch[1,2], Christian Schneider[1,2], Benjamin Lienhard[1,2], Max Werninghaus[1,2], and Stefan Filipp[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Department of Physics — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften

Temporal fluctuations in energy relaxation times (T1) on superconducting qubits can occur on fast and irregular timescales. A quantitative understanding of the underlying relaxation dynamics is important for improving qubit stability and therefore advancing the development of fault-tolerant superconducting quantum processors. We employ a new method by monitoring the qubit continuously and determining the average decay and excitation rates. Simulations suggest that the decay constant can be extracted on timescales significantly shorter than conventional T1 measurements, allowing for monitoring of relaxation dynamics two orders of magnitude faster than conventional approaches. Preliminary experimental results demonstrate the feasibility of this technique and its potential for identifying fast fluctuations in qubit performance. As we extract the information directly from single-shot data, we do not require any additional classical logic beyond active reset, making the method easily integrable into existing setups. We acknowledge financial support from GeQCoS, MUNIQC-SC, MCQST, OpenSuperQPlus100, Munich Quantum Valley, and Deutsche Forschungsgemeinschaft (DFG, German Research Foundation).

QI 2.8 Mon 12:00 BEY/0245

Towards measurement based quantum computation with multipods — Claire Benjamin[1,2], Dániel Varjas[3,4], Gábor Széchenyi[5,6], Judit Romhányi[1], and •László Oroszlány[2,6] — [1]Department of Physics and Astronomy, University of California, Irvine — [2]Department of Physics of Complex Systems, Eötvös Loránd University — [3]Department of Theoretical Physics, Institute of Physics, Budapest University of Technology and Economics — [4]Institute for Theoretical Solid State Physics, IFW Dresden and Würzburg-Dresden Cluster of Excellence; — [5]Department of Materials Physics, ELTE Eötvös Loránd University — [6]HUN-REN Wigner Research Centre for Physics

We propose a Hubbard-star construction at half filling as a route to realizing Affleck-Kennedy-Lieb-Tasaki (AKLT) physics. By connecting star-shaped clusters of quantum dots, we derive low-energy effective Hamiltonians that reproduce the S=1 and S=3/2 AKLT models. Using exact diagonalization and quasi-degenerate perturbation theory, we identify the coupling regimes in which these models emerge. Since AKLT ground states are known resources for measurement-based quantum computation, our scheme offers a feasible path toward quantum computational phases in recently fabricated, highly tunable quantum dot arrays.

QI 2.9 Mon 12:15 BEY/0245

Local isotopic enrichment of ^{28}Si for quantum applications — •Lukas Prager[1], Ewelina Gacka[1], Priyal Dadhich[1], Stefan Findeisen[2], Nico Klingner[1], and Gregor Hlawacek[1] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Bautzner Landstr. 400, 01328 Dresden, Germany — [2]Department of Mechanical Engineering, HZDR, Bautzner Landstr. 400, 01328 Dresden, Germany

Donor spin qubits in silicon are a promising candidate in the search for a qubit that can be fabricated in a scalable way while exhibiting long coherence times. Achieving minimal decoherence requires a magnetic moment-free environment, called *spin vacuum*, which, in case of silicon, necessitates the suppression of the nuclear spin-bearing isotope ^{29}Si (4.7%). We perform this task by ^{28}Si focused ion beam (FIB) implantation with energies larger than 45 keV to implant more atoms than removing by sputtering. The usage of a FIB offers a time efficient and spatially resolved way to achieve the necessary fluences (>10^{19} ions/cm^2), while the spatial confinement leaves the surrounding semiconductor materials and devices untouched. Our aim is to ultimately achieve remaining concentrations of ^{29}Si that are lower than centrifuge-based approaches (<10 ppm). The resulting spin vacuum areas are one of the fundamental building blocks of a scalable qubit platform based on bismuth donor spin qubits embedded into silicon. The bismuth atoms will be precisely implanted in a deterministic way. Besides that, our device will feature qubits coupled via mechanical modes and single electron transistor governed readout.

QI 2.10 Mon 12:30 BEY/0245

A heat-resilient hole spin qubit in silicon — Victor Champain[1], Gabriele Boschetto[2], Heimanu Niebojewski[2], Benoit Bertrand[2], Lorenzo Mauro[2], Marion Bassi[1], Vivien Schmitt[1], Xavier Jehl[1], Simon Zihlmann[1], Romain Maurand[1], Yann-Michel Niquet[3], •Clemens Winkelmann[1], Silvano De Franceschi[1], Biel Martinez[2], and Boris Brun[1] — [1]Univ. Grenoble Alpes, CEA, Grenoble INP, IRIG-Pheliqs, Grenoble, France — [2]Univ. Grenoble Alpes, CEA, Leti, F-38000 Grenoble, France — [3]Univ. Grenoble Alpes, CEA, IRIG-MEM-L Sim, Grenoble, France

Recent advances in scaling up spin-based quantum processors have revealed unanticipated issues related to thermal effects. Microwave pulses required to manipulate and read the qubits are found to overheat the spins' environment, which unexpectedly induces Larmor frequency shifts, reducing thereby gate fidelities. In this study, we shine light on these elusive thermal effects, by experimentally characterizing the temperature dependence of the Larmor frequency for a single hole spin in silicon. Our results unambiguously reveal an electrical origin underlying the thermal susceptibility, stemming from the spin-orbit-induced electric susceptibility. We perform an accurate modeling of the spin electrostatic envi-

ronment and gyromagnetic properties, allowing us to pinpoint electric dipoles as responsible for these frequency shifts, that unfreeze as the temperature increases. Surprisingly, we find that the thermal susceptibility can be tuned with the magnetic field angle and can even cancel out, unveiling a sweet spot where the hole spin is rendered immune to thermal effects. arXiv:2509.15823

QI 3: Quantum Simulation

Time: Monday 15:00–18:30 Location: BEY/0137

QI 3.1 Mon 15:00 BEY/0137

Real-Time Dynamics in a (2+1)-D Gauge Theory: The Stringy Nature on a Superconducting Quantum Simulator — Jesús Cobos[1], Joana Fraxanet[2], César Benito[3], Francesco di Marcantonio[1], Pedro Rivero[2], Kornél Kapás[4], •Miklós Antal Werner[4], Örs Legeza[4,5,6,7], Alejandro Bermudez[3], and Enrique Rico[1,8,9,10] — [1]EHU QC, Bilbao, Spain — [2]IBM Quantum, New York, USA — [3]UAM-CSIC, Madrid, Spain — [4]Wigner RCP, Budapest, Hungary — [5]Dynaflex LTD, Budapest, Hungary — [6]TUM IAS, Garching, Germany — [7]Parmenides St., Pöcking, Germany — [8]DIPC, San Sebastián, Spain — [9]IKERBASQUE, Bilbao, Spain — [10]CERN, Geneva, Switzerland

We probe string modes of motion with dynamical matter in a digital quantum simulation of the $\mathbb{Z}_2$-Higgs model with an optimized embedding into a heavy-hex organized superconducting quantum processor with up to 144 qubits. Using local gauge symmetries, we implement various error suppression, mitigation, and correction strategies to enable high control of electric strings connecting dynamical charges and to observe longitudinal oscillations and transverse bending at the endpoints of the string, which are precursors to hadronization and rotational spectra of mesons. To validate our error-aware protocols, we employ extensive tensor network simulations: the relevant parameter regimes of the model are determined by large-scale DMRG simulations. The dynamics are classically simulated by the basis update and Galerkin (BUG) method, and the agreement with hardware results is remarkable.

QI 3.2 Mon 15:15 BEY/0137

Braiding of Majorana zero modes on the digital IBM quantum processor — •Stefan Schmitz[1,2], Kevin Lively[3], Maike Drieb-Schön[4], Tim Bode[1], Benedikt Fauseweh[3,5], and Dmitry Bagrets[1,2] — [1]Peter Grünberg Institute, Quantum Computing Analytics (PGI-12), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany — [3]Institute for Software Technology, German Aerospace Center (DLR), 51147 Cologne, Germany — [4]Institute for Theoretical Physics, University of Innsbruck, 6020 Innsbruck, Austria — [5]Department of Physics, TU Dortmund University, 44227 Dortmund, Germany

The search for elusive Majorana fermions in solid-state devices has occupied the scientific community for more than a decade. Their unambiguous detection is expected to rely on a braiding protocol that can verify their non-Abelian statistics. We have emulated one variant of this protocol using digital quantum simulations performed on IBM quantum processors. Remarkably, only 12 Trotter steps are sufficient to reproduce a theoretically predicted Majorana braiding operation with a fidelity exceeding 99.9 % in the absence of decoherence and noise. In experiment, this upper bound can not be reached due to the lack of topological protection for the virtual Majoranas. However, we show that applying error mitigation techniques can restore experimental fidelity to values close to the ideal limit.

QI 3.3 Mon 15:30 BEY/0137

How compactness curbs entanglement growth in bosonic systems — •Stefan Aimet[1], Philipp Schmoll[1], Jens Eisert[1], and Spyros Sotiriadis[2] — [1]Freie Universität Berlin, Dahlem Center for Complex Quantum Systems and Institut für Theoretische Physik, 14195 Berlin, Germany — [2]Institute of Theoretical and Computational Physics, University of Crete, 71003 Heraklion, Greece

Zero modes, degrees of freedom with vanishing frequency, play a crucial role in the non-equilibrium dynamics of bosonic systems. In Gaussian models, such zero modes are known to drive unbounded, logarithmic growth of entanglement entropy. We show that this divergence is not an inherent feature of zero modes per se, but arises only for non-compact zero modes whose continuous spectrum and non-normalisable eigenstates allow unbounded position-space spreading and momentum-space dephasing. By contrast, compact zero modes occurring in compact bosonic systems behave fundamentally differently: spreading and dephasing are eventually halted, and compactness caps the entanglement entropy at a finite value. We demonstrate this mechanism using a minimal toy model comparing two coupled harmonic oscillators with two coupled quantum rotors, and show that the same underlying physics carries over to many-body settings by comparing an N-site compact rotor chain with the non-compact harmonic chain. Finally, we relate these insights to ultracold-atom realisations of compact quantum field theories, clarifying when the compact free boson (Tomonaga-Luttinger liquid) description is required and when the commonly used non-compact massless Klein-Gordon model fails.

QI 3.4 Mon 15:45 BEY/0137

A Parametrically-Driven High-Q Multimode Cavity for Analog Quantum Simulations — •Johannes Schading[1], Ian Yang[1], Joao C. Pinto Barros[2], Thea Budde[2], Raquel Garcia-Belles[3], Alexander Anferov[3], Yiwen Chu[3], Marina Marinkovic[2], and Alexander Grimm[1] — [1]Bosonic Quantum Information Group (LNQ/CPS), Paul Scherrer Institute, Switzerland — [2]High Performance Computational Physics Group, ETH Zürich, Switzerland — [3]Hybrid Quantum Systems Group, ETH Zürich, Switzerland

Analog quantum simulations offer a powerful route to study real-time dynamics in systems such as lattice gauge theories or quantum synchronization of nonlinear oscillators. However, these simulations require interaction strengths to exceed decoherence rates by a large margin. Our approach to address this challenge is to encode the system degrees of freedom in high-Q bosonic modes and activating strong parametric interactions in an all-to-all-connected multimode architecture coupled to a superconducting qubit. By applying a microwave drive, we use a qubit-mediated fourth-order parametric process to realize a three-bosonic-mode interaction with a hopping rate of $J/2\pi > 50$ kHz, significantly larger than typical decay rates in high-purity aluminum cavities [1]. Our multimode architecture allows for in-situ connectivity that enables simulations of high-dimensional systems, such as a (2+1)D lattice formulation of the Schwinger model. In this talk, I will discuss our progress towards implementing analog quantum simulations with parametrically-activated bosonic-mode interactions. [1] Chakram, S. *et al. Physical Review Letters* **127**, 107701 (2021).

QI 3.5 Mon 16:00 BEY/0137

Effective Hamiltonians for Measurement Protocols in Quantum Circuits — •Manuel Freudig[1], Davide Bincoletto[2], Francesco Diotallevi[1], Leander Reascos[1], Mónica Benito[1], and Jakob Kottmann[2] — [1]Institute of Physics, University of Augsburg, Augsburg, Germany — [2]Institute for Computer Science, University of Augsburg, Augsburg, Germany

A significant drawback for the realization of Variational Quantum Eigensolvers (VQEs), is the overhead due to measurement repetitions. Addressing this bottleneck, an iterative measurement protocol, designed for molecular Hamiltonians, was introduced [1]. It relies on cheaply measuring commuting groups of operators, while the residual (non-commuting) elements are grouped in a different basis and then measured. Our work proposes an enhanced measurement strategy by integrating the iterative measurement protocol [1] with perturbative and non-perturbative techniques for the derivation of effective Hamiltonians [2,3]. This combination aims to further reduce measurement overhead and increase the accuracy of the approximated expectation value, providing a more viable path for practical VQE implementations.

[1] Bincoletto, D.; Kottmann, J. S.; arXiv:2504.03019. [2] Li, B.; Calarco, T.; Motzoi, F.; PRX Quantum 3, 030313. [3] Schrieffer, J. R.; Wolff, P. A.; Phys. Rev. 149, 491-492.

QI 3.6 Mon 16:15 BEY/0137

Hamiltonian simulation with explicit formulas for Digital-Analog Quantum Computing — Mikel Garcia de Andoin[1,2], Thorge Müller[3], and •Gonzalo Camacho[3] — [1]University of the Basque Country UPV/EHU, Leioa, Spain — [2]EHU Quantum Center, Leioa, Spain — [3]Deutsches Zentrum für Luft- und Raumfahrt (DLR), Köln, Germany

In Hamiltonian simulation, modifying a given source Hamiltonian is often required to engineer a desired target Hamiltonian. In this work, we provide an exact solution for the problem of expressing arbitrary target two-body Hamiltonians as the sum of local unitary transformations of an arbitrary source Ising Hamiltonian, with the total number of required terms being at most quadratic in system size. This allows us to design an efficient digital-analog compilation protocol for Hamiltonian simulation that avoids employing numerical optimization over a large parameter space, minimizes computational resources and allows for further scaling.

30min. break

QI 3.7 Mon 17:00 BEY/0137

Barren-plateau free variational quantum simulation of Z2 lattice gauge theories — •Fariha Azad[1], Matteo Inajetovic[1], Stefan Kühn[2], and Anna Pappa[1] — [1]Electrical Engineering and Computer Science Department, Technische Universität Berlin, 10587 Berlin, Germany — [2]Deutsches Elektronen-Synchrotron DESY, Platanenallee 6, 15738 Zeuthen, Germany

In this work, we design a variational quantum eigensolver (VQE) suitable for investigating ground states and static string breaking in a Z2 lattice gauge theory (LGT). We consider a two-leg ladder lattice with Kogut-Susskind staggered fermions and verify the results of the VQE simulations using tensor network methods. We find that for varying Hamiltonian parameter regimes and in the presence of external charges, the VQE is able to arrive at the gauge-invariant ground state without explicitly enforcing gauge invariance through penalty terms. Additionally, experiments showing string breaking are performed on the IBM quantum platform. Thus, VQEs are seen to be a promising tool for Z2 LGTs, and could serve as a stepping stone toward studies of other gauge groups. We find that the scaling of gradients with the number of qubits is favorable for avoiding barren plateaus. Furthermore, strategies that avoid barren plateaus arise naturally as features of LGTs, such as choosing the initialization by setting the Gauss law sector and restricting the Hilbert space to the gauge-invariant subspace.

QI 3.8 Mon 17:15 BEY/0137

Efficient Quantum and Classical Simulation of the Non-Uniform Wave Equation — •Kevin Lively, Vittorio Pagni, and Gonzalo Camacho — Deutsches Zentrum für Luft- und Raumfahrt, Quantum Computing Applications, Sankt Augustin

We present an efficient algorithm based on the construction of a unitary quantum circuit for simulating the non-uniform wave equation in one, two or three dimensions. We utilize the first-order-in-time-derivative form of the wave equation alongside Pauli four-vectors to embed and manipulate vector quantities in a language which translates naturally to quantum simulation. We exploit this to create an efficient quantum-inspired classical tensor-network algorithm to inject and propagate waveforms through inhomogeneous media far beyond the memory limitations of naive finite difference methods. We explore applications of this algorithm in real world data-sets of complex media.

QI 3.9 Mon 17:30 BEY/0137

Quantum Simulation of Electron-Phonon Interactions in Circuit QED — •Riccardo Roma[1,2], Tim Bode[1], Dmitriy S. Shapiro[1], Alessandro Ciani[1], Dmitry Bagrets[1,3], and Frank Wilhelm-Mauch[1,2] — [1]Institute for Quantum Computing Analytics (PGI-12), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Theoretical Physics, Saarland University, 66123 Saarbrücken, Germany — [3]Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

Electron-phonon interaction is a fundamental process in condensed-matter physics, responsible for a variety of phenomena ranging from polaron formation in semiconductors and molecules to charge-density waves, (high-temperature) superconductivity or the Hubbard-Holstein (HH) and the Yukawa-Sachdev-Ye-Kitaev (YSYK) models.

Leveraging physical resonators for emulating bosonic degrees of freedom allows to circumvent the considerable overhead associated with their encoding in qubits. It also avoids the necessity of truncating the bosonic Fock space, which is an inherent limitation of current qubit encodings.

We extend the standard gate set available for superconducting qubits by entangling gates between a transmon and a microwave resonator, showing how this can be achieved experimentally via flux tuning or microwave driving. We then derive the digital simulation circuits for the HH and YSYK models. Our work concludes with a minimal electron-phonon model for which we demonstrate a Dicke-type superradiant transition that is robust to noise and thus experimentally feasible.

QI 3.10 Mon 17:45 BEY/0137

Discrete local dynamics in globally driven dual-species Rydberg atom arrays — Francesco Cesa[3,4], Andrea di Fini[1,2], •David Korbany[1,2], Roberto Tricarico[3,4], Hannes Pichler[3,4], Hannes Bernien[3,5,6], and Lorenzo Piroli[1,2] — [1]DIFA, Universit'a di Bologna — [2]INFN, Sezione di Bologna — [3]IQOQI Innsbruck — [4]Institute for Theoretical Physics, University of Innsbruck — [5]Pritzker School of Molecular Engineering, University of Chicago — [6]Institute for Experimental Physics, University of Innsbruck

We present a simple construction to implement a family of one- and two-dimensional discrete dynamics using dual-species Rydberg atom arrays. The discrete dynamics that we consider are special examples of quantum cellular automata (QCA) and include the exact Floquet dynamics of the kicked Ising model, as well as the Trotterized evolution of translation-invariant nearest-neighbor Hamiltonians. In our scheme, one of the two species of atoms represents the physical qubits, while the other species plays an auxiliary role, mediating the interactions. Our construction only requires global driving, with no local addressing of the qubits, and assumes an ideal blockade regime. Importantly, when the inter-species interactions are dominant over the intra-species one, we give a simple argument showing that, both in the one- and two-dimensional case, the deviations from the ideal blockade regime are at least as small as for established single-species implementations in one-dimensional arrays. Finally, we illustrate applications of our constructions in the study of chaotic features of QCA dynamics. Our results may be relevant for near-term experimental implementations.

QI 3.11 Mon 18:00 BEY/0137

Extracting transport properties using zero noise extrapolations of noisy quantum dynamics — •Hansveer Singh[1], Pieter Claeys[1], Sarang Gopalakrishnan[2], and Anushya Chandran[3] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden, DE — [2]Princeton University, Princeton, New Jersey USA — [3]Boston University, Boston, Massachusetts, USA

We examine extrapolating transport coefficients of quantum systems subjected to weak noise. Though noise generally breaks conservation laws of a quantum system, we show for weak noise strengths it is still possible to define an effective notion of transport. For chaotic diffusive quantum systems, we provide a protocol to extrapolate diffusion constants and argue that the effective diffusion constant in the weak noise limit can be decomposed into two parts: an analytic function of the noise strength and a function determined by non-linear corrections to diffusive hydrodynamics. We support our findings with tensor network simulations of a dissipative version of the staggered field spin-1/2 XXZ chain.

QI 3.12 Mon 18:15 BEY/0137

Scrambling the Information of Transmons using Interaction by Metamaterials — •Arne Schlabes and Mohammad Ansari — Forschungszentrum Jülich

Transmission lines made of capacitors in series and inductors to the ground form so called metamaterials with inverse dispersion relations. These Left-Handed materials allow for a multi-mode interaction of transmons coupled to the resonator. We use flux tunable qubits and parametric driving to excite resonator mode states. This occupation can be spread controllably from the resonator to a qubit and back to other resonator states. With this we realize a scrambling of information which started locally in one resonator state but is then encoded non-locally in multiple states. The precise composition of the final state depends on the parameters used to encode it, without them the initial state can not be recovered.

QI 4: Quantum Manybody Systems (joint session QI/TT)

Time: Monday 15:00–18:30 Location: BEY/0245

Invited Talk QI 4.1 Mon 15:00 BEY/0245

Reducing Noise, Complexity, and Optimization Barriers in Quantum Simulations of Strongly Correlated Systems — •Werner Dobrautz — Center for Advanced Systems Understanding (CASUS), Görlitz, Germany — Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany — Center for Scalable Data Analytics and Artificial Intelligence (ScaDS.AI) Dresden/Leipzig, Dresden, Germany — Technical University Dresden, Dresden, Germany

Near-term quantum hardware poses severe constraints for quantum chemistry and quantum many-body simulations due to noise, limited coherence, and challenging optimization landscapes. We present a unifying set of algorithmic strategies to address these bottlenecks, combining transcorrelated Hamiltonians, spin-adapted representations, and advanced variational optimization techniques. By embedding electronic correlations directly into the Hamiltonian, transcorrelated methods yield compact, noise-resilient quantum circuits and improved convergence for both molecular systems and lattice models. Spin-adapted formulations further reduce Hilbert space complexity and enable efficient simulations of correlated spin systems. To enhance robustness and trainability, we introduce multireference error mitigation strategies and qBang, a momentum-aware variational optimization scheme that effectively navigates flat and ill-conditioned energy landscapes. Together, these approaches establish a scalable and hardware-aware framework for accurate quantum simulations of strongly correlated systems on current and near-term quantum devices.

QI 4.2 Mon 15:30 BEY/0245

Hybrid superconducting devices — •Anamaria Ghihor[1], Yejin Lee[1], Haolin Jin[1], Markus König[1], Andreas Leithe-Jasper[1], Roemer Hinlopen[1,2], Carsten Putzke[2], Philip Moll[2], Uri Vool[1], and Eteri Svanidze[1] — [1]MPI CPfS - Nothnitzer Str. 40, Dresden, Germany — [2]MPI MPSD - Luruper Chaussee 149, Hamburg, Germany

Superconducting resonators are highly tunable, low-loss coherent macroscopic devices, making them ideal for quantum technology and sensing applications. Recently, these resonators have been paired with van der Waals (vdW) materials to explore their microwave losses, dielectric properties and kinetic inductance. However, creating a hybrid device that only integrates a superconduct-

ing resonator with a vdW flake limits the range of materials that can be used. To overcome this limitation, we fabricate a lamella using a focused ion beam (FIB), effectively replicating the flake. This approach offers the added benefit of precise dimensional control, something that is difficult to achieve with exfoliated flakes. The lamella can then be attached in situ to the resonator using a micro-manipulator. In this talk we will show preliminary hybrid devices with lamella developed from conventional and unconventional superconductors.This approach greatly expands the range of materials that can be explored and enables detailed studies of their superfluid density.

QI 4.3 Mon 15:45 BEY/0245

Hybrid Monte Carlo enhanced by exact diagonalization: simulating interacting Hubbard systems — •Martina Gisti[1], Finn Temmen[2], Thomas Luu[1], David Luitz[2], and Johann Ostmeyer[3] — [1]Institute of Physics, University of Bonn, Nußallee 12, 53115 Bonn — [2]Forschungszentrum Jülich GmbH Wilhelm-Johnen-Straße 52428 Jülich — [3]Helmholtz Institute for Radiation and Nuclear Physics, University of Bonn

We present a hybrid simulation framework that integrates the hybrid Monte Carlo method with exact diagonalization techniques to study Hubbard chains coupled through many-body interactions. Within a path integral formulation, thermal expectation values are expressed and evaluated exactly along the chains. We study the impact of the hybrid method on persistent challenges in the application of stochastic simulations, such as the sign problem and ergodicity violations. The approach mitigates the sign problem that hampers conventional simulations, providing a feasible path for studying strongly correlated quantum systems beyond one dimension.

QI 4.4 Mon 16:00 BEY/0245

Topological properties of coupled superconducting chains in the presence of interactions — •Frederick Del Pozo — aboratoire Kastler Brossel, Sorbonne Universite, CNRS, ENS-PSL Research University, Coll'ege de France; 4 Place Jussieu, 75005 Paris, France

We investigate the topological and critical properties of coupled and interacting superconducting wires.

As a prototype of superconductors with topological order, the Kitaev chain model is a perfect testing ground for novel theoretical and numerical tools, including the density-matrix-renormalization-group (DMRG) algorithm and bipartite entanglement entropy.

In the following talk we report on the results of several recent works, which have lead to a deeper understanding of the topological and critical properties of coupled and interacting Kitaev chains, also in the presence of real-space disorder. We reveal that the usual topological invariant, defined in the absence of interactions, remains a sensible marker for the topology when two wires are brought into close proximity of each other where interaction effects and inter-wire hopping processes become relevant. We also reveal the appearance of a many-body entangled ground state, and interaction reinforced critical region in the wires' phase diagram.

Our results highlight the rich physics present in quasi one-dimensional quantum systems, and motivates the further research into properties relevant for applications in superconducting qubits and topological quantum computation protocols.

QI 4.5 Mon 16:15 BEY/0245

Quantum Assisted Ghost Gutzwiller Ansatz — •PV Sriluckshmy, Francois Jamet, and Fedor Simkovic — IQM Quantum Computers, Georg-Brauchle-Ring 23-25, 80992 Munich, Germany

The ghost Gutzwiller ansatz (gGut) technique was shown to achieve accuracy comparable to dynamical mean-field theory at a much lower computational cost. However, gGut is limited by the bottleneck of computing the density matrix. We develop a hybrid quantum-classical gGut technique that computes ground state properties of embedding Hamiltonians on a quantum computer using the quantum-selected configuration interaction (QSCI) algorithm. We find that the ground states of interest become sufficiently sparse as the number of ghost orbitals increases. We investigate QSCI's performance using local unitary cluster Jastrow (LUCJ) ansatz with circuit cutting on IQM's quantum hardware for up to 24 qubits. Our converged gGut calculations correctly capture the metal-to-insulator phase transition in the Fermi-Hubbard model. This was achieved using quantum samples to build a basis with as little as 1% of the total CI states.

30min. break

QI 4.6 Mon 17:00 BEY/0245

Measurement-Based Quantum Computation in Symmetry-Enriched Topological Phases — •Paul Herringer[1,2,3], Vir B. Bulchandani[4,5], Younes Javanmard[1], David T. Stephen[6,7], and Robert Raussendorf[1,3] — [1]Leibniz Universität Hannover, Hannover, Germany — [2]University of British Columbia, Vancouver, Canada — [3]Stewart Blusson Quantum Matter Institute, Vancouver, Canada — [4]Rice University, Houston, USA — [5]National University of Singapore, Singapore — [6]University of Colorado Boulder, Boulder, USA — [7]California Institute of Technology, Pasadena, USA

We present the first examples of topological phases of matter with uniform power for measurement-based quantum computation. This is possible thanks to a new framework for analyzing the computational properties of phases of matter that is more general than previous constructions, which were limited to short-range entangled phases in one dimension. We show that ground states of the toric code in an anisotropic magnetic field yield a natural, albeit non-computationally-universal, application of our framework. We then present a new model with topological order whose ground states are universal resources for MBQC. Both topological models are enriched by subsystem symmetries, and these symmetries protect their computational power. Our framework greatly expands the range of physical models that can be analyzed from the computational perspective.

QI 4.7 Mon 17:15 BEY/0245

Many-body localization in the Sherrington-Kirkpatrick model — •Gergo Dénes[1], Balázs Hetényi[1], Márton Kormos[1], Angelo Valli[1], Pascu Moca[1,2], and Gergely Zaránd[1] — [1]Department of Theoretical Physics, Institute of Physics, Budapest University of Technology and Economics, Muegyetem rkp. 3., H-1111 Budapest, Hungary — [2]Department of Physics, University of Oradea, Str. Universitatii nr. 1 Oradea, 410087, Romania

The Sherrington-Kirkpatrick (SK) model has been extensively studied for more than 50 years [1]. In the context of optimization problems, it represents one of the most difficult paradigmatic optimization problems, the MAXCUT problem. Its quantum extension, the transverse field SK model (TFSK model) is therefore a paradigmatic model for the Quantum Adiabatic Optimization Approach (QAOA).

We performed extensive finite-size numerical simulations of the TFSK model at different transverse field strengths to extract various many-body localization (MBL) indicators, such as inverse participation ratio, Shannon entropy, and level spacing ratio. Our numerical and analytical analysis suggest the presence of an MBL transition as a function of the transverse field at certain energy densities, different from the spin-glass transition, and in contrast to the findings of Ref. [2]. In the MBL phase, states do not seem to be exponentially localized, rather, our data suggest the presence of power-law MBL.

[1] M. Mezard, G. Parisi, M. A. Virasoro Spin Glass Theory and Beyond, ISBN: 978-9971-5-0116-7 (1986).

[2] S. Mukherjee, S. Nag, A. Garg, Phys. Rev. B 97, 144202 (2018).

QI 4.8 Mon 17:30 BEY/0245

Typical entanglement entropy of anyon chains — Yale Yauk[1,2], •Alexander Hahn[1,3,2], and Lucas Hackl[4,5] — [1]Max-Planck-Institut für Quantenoptik, Hans-Kopfermann-Straße 1, D-85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstraße 4, D-80799 Munich, Germany — [3]Technical University of Munich, TUM School of Natural Sciences, Physics Department, D-85748 Garching, Germany — [4]School of Mathematics and Statistics, The University of Melbourne, Parkville, VIC 3010, Australia — [5]School of Physics, The University of Melbourne, Parkville, VIC 3010, Australia

Random-state entanglement serves as a key probe of quantum chaos, thermalization, and information scrambling, but its behavior in topologically ordered systems remains unclear. Here we study the statistical properties of bipartite entanglement in one-dimensional anyon chains, where the Hilbert space is constrained by the fusion rules. In such systems, the conventional trace must be replaced by the quantum trace, requiring a consistent redefinition of density matrices and entanglement measures that incorporates topological data. We compute the average bipartite entanglement entropy and its variance for both open and periodic boundary conditions. The resulting average anyonic entanglement entropy reproduces the Page curve exactly, revealing that topological constraints modify the normalization but not the universal form of typical entanglement. Despite topological charge conservation, the average entanglement shows no symmetry-related correction of the kind that appears in systems with Lie group symmetries.

QI 4.9 Mon 17:45 BEY/0245

Thermal Entanglement and Out-of-Equilibrium Thermodynamics in 1D Bosonic Systems — •Julia Mathe, Nicky Kai Hong Li, Pharnam Bakhshinezhad, and Giuseppe Vitagliano — TU Wien, Atominstitut, Stadionallee 2, 1020 Vienna, Austria

We investigate entanglement in- and out-of equilibirum in harmonic chains, with direct relevance to low-energy descriptions of paradigmatic models, like 1D Bose-Einstein condensates. Working in a regime where all states are Gaussian, we employ the logarithmic negativity and the covariance matrix criterion (CMC) as known entanglement quantifiers. For thermal states, we extensively characterize entanglement and its scaling behaviour, including in the massless (critical) limit. We extract the optimal entanglement witness coming from the CMC and uncover a simple mode-resolved structure underlying the entanglement-to-separability transition. At finite temperature, the optimal witnesses are diagonal in the normal-mode basis, allowing to characterize entanglement from a few normal mode uncertainties, which are physically related to static susceptibilities. We then investigate out-of-equilibrium dynamics arising from a time-dependent

coupling and analyze entanglement growth, suppression, and transport. Based on this, we construct a full Gaussian framework for studying entanglement in thermodynamic cycles. Our results give a unified and physically intuitive picture of how entanglement emerges and evolves in 1D Gaussian many-body systems and show that thermal separability and entanglement are mainly governed by the low-energy (infrared) sector that also underlies the continuum field-theory description.

QI 4.10 Mon 18:00 BEY/0245

Symmetry-preserving warm starts for variational ground state preparation — •Ivana Miháliková — Matej Bel University, Národná ulica 12, Banská Bystrica, 97401, Slovakia — Institute of Physics, Slovak Academy of Sciences, Bratislava 84511, Slovakia

Enforcing physical symmetries can dramatically simplify ground-state preparation in the variational quantum eigensolver (VQE). This work considers a 12-spin all-to-all neutrino-inspired model and a 4×3 Heisenberg lattice. In both systems, simple product states are projected onto symmetry subspaces with fixed total spin J and J_z (and, for the Heisenberg lattice, translation and mirror symmetries), then refined using swap-based entangling layers that generate only symmetry-compatible correlations. The resulting warm starts lie well within previously established worst-case upper bounds on the energy error normalized by system size and interaction-graph degree, showing that symmetry-aware initialization can substantially outperform generic guarantees. For the Heisenberg lattice, the symmetry-preserving construction reduces the relevant search space from 4096 basis states to just 9 symmetry-compatible states and increases the effective spectral gap from about 7 to about 28 energy units. Within a VQE setting this yields a smoother optimization landscape and faster convergence with shallow circuits. In practice, the neutrino-inspired model reaches $\sim$ 98.8% fidelity within the $J = 0$ subspace, and the Heisenberg lattice exceeds 98.0% fidelity once translation and mirror symmetries are enforced.

QI 4.11 Mon 18:15 BEY/0245

An emerging generator of rotations for a 1- or many-particle Hofstadter problem on a lattice pierced by magnetic field — •Arabi Seshappan[1,2], Tangi Morvan[2], Alberto Nardin[2], and Leonardo Mazza[2] — [1]Department of Physics, University of California, Merced, CA 95343, USA — [2]Université Paris-Saclay, CNRS, LPTMS, 91405, Orsay, France

Topological quantum computation is an exciting direction for development of fault-tolerant qubits—a quintessential example being manipulation of excitations in fractional quantum Hall (FQH) systems. As recent cold-atom and photonic experiments have realized few-particle FQH states in small lattices, and theoretical results have shown spectra of specific lattice sizes to exhibit exactly flat-bands in momentum space, we have theoretically studied similar FQH lattices for 1- and many-particle bosonic cases. Our construction is that of a two-dimensional (2D) square lattice, with nearest-neighbor hopping, pierced by a perpendicular, uniform magnetic field. We vary the magnetic field such that, for lattice edge length L, the flux per plaquette ranges between $\alpha = 1/L$ and $\alpha = 1/4$, and analyze the resultant spectra. We have found that, for low energy levels, measurements of density are an excellent proxy for defining a gauge-invariant generator of rotations (GIGR) and can make order in the spectra. This removes any need for assumption of circular droplet invariance, and provides a useful characterization technique for cold-atom experiments.

QI 5: Quantum Computing and Algorithms II

Time: Tuesday 9:30–12:30 Location: BEY/0137

QI 5.1 Tue 9:30 BEY/0137

Transcorrelated Method with Quantum Computing : Quasi-Hermitian Hamiltonian Simulation — •Cheng-Lin Hong[1,2] and Werner Dobrautz[1,2,3,4] — [1]Center for Advanced Systems Understanding, 02826 Görlitz, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [3]Center for Scalable Data Analytics and Artificial Intelligence Dresden/Leipzig, 01069 Dresden, Germany — [4]Technical University Dresden, 01069 Dresden, Germany

A major challenge in quantum chemistry on quantum computers is the large number of qubits required to achieve accurate results near the complete basis set (CBS) limit. The transcorrelated (TC) method addresses this issue by using a non-unitary similarity transformation to incorporate electron-correlation effects, such as the cusp condition, directly into the Hamiltonian. This method accelerates convergence toward the CBS limit even with smaller basis sets, thereby reducing the number of qubits required. However, the non-unitary nature of the transformation leads to a non-Hermitian Hamiltonian, whose structure and its corresponding physical quantities depend sensitively on the chosen Jastrow factor. The choice of the Jastrow factor governs the final form of this Hamiltonian and its corresponding physical quantities.

We investigate such non-Hermitian transcorrelated Hamiltonians in a quantum-computing context. We analyze how different single-parameter Jastrow factors affect the structure of the final qubit Hamiltonian and evaluate the quantum resources required to solve them. Finally, we employ perturbation theory to derive an approximate solution for these non-Hermitian transcorrelated systems.

QI 5.2 Tue 9:45 BEY/0137

Optimal Embedded Ising Problem — •Elisabeth Lobe — German Aerospace Center (DLR), Braunschweig, Germany

Suitable Ising problems for quantum annealers need to be formulated such that they respect the specific hardware restrictions and at the same time represent the original problems which shall actually be solved. This requires to find an embedding into the hardware graph and choose the parameters of the embedded Ising problem in accordance with the precision of the machine. We have developed a method to provide provably equivalent embedded Ising problems with optimal parameters for a given arbitrary Ising problem and a corresponding embedding. The thus formulated optimal embedded Ising problems are compared to the state-of-the-art embedding transformation implemented in the D-Wave API. We investigate the Ising formulations in different scenarios to evaluate the performance of both methods. We show that our method provides better embedded Ising Problems in terms of coefficient distributions and more stable solution quality.

QI 5.3 Tue 10:00 BEY/0137

Verifiable End-to-End Delegated Variational Quantum Algorithms — •Matteo Inajetovic[1], Petros Wallden[2], and Anna Pappa[1] — [1]Technische Universität Berlin, Berlin, Germany — [2]Quantum Software Lab, School of Informatics, University of Edinburgh, Edinburgh, UK

Variational quantum algorithms (VQAs) have emerged as promising candidates for solving complex optimization and machine learning tasks on near-term quantum hardware. However, executing quantum operations remains challenging for small-scale users because of several hardware constraints, making it desirable to delegate parts of the computation to more powerful quantum devices. In this work, we introduce a framework for delegated variational quantum algorithms (DVQAs), where a client with limited quantum capabilities delegates the execution of a VQA to a more powerful quantum server. In particular, we introduce a protocol that enables a client to delegate a variational quantum algorithm to a server while ensuring that the input, the output and also the computation itself remain secret. Additionally, if the protocol does not abort, the client can be certain that the computation outcome is indeed correct. Our approach first proposes a verifiable protocol for delegating the quantum computation at each optimization step of a VQA, and then combines the iterative steps into an error-resilient optimization process that offers end-to-end verifiable algorithm execution, paving the way for practical quantum cloud computing applications.

QI 5.4 Tue 10:15 BEY/0137

Quantum algorithm for one quasi-particle excitations in the thermodynamic limit via cluster-additive block-diagonalization — •Sumeet Sumeet, Max Hörmann, and Kai Phillip Schmidt — Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), 91058 Erlangen, Germany

We present a hybrid quantum-classical algorithm for computing one quasi-particle excitation energies in the thermodynamic limit by combining the variational quantum eigensolver (VQE) with numerical linked-cluster expansions (NLCEs) [1], extending our NLCE+VQE approach for ground states [2] to excitations. We minimize variance (or trace) cost functions with VQE to block-diagonalize the Hamiltonian, then extend to the thermodynamic limit with NLCE. The central challenge is ensuring cluster additivity for degenerate subspaces, essential for NLCE convergence. We address this by integrating the projective cluster-additive transformation (PCAT) with VQE: PCAT constructs the cluster-additive unitary from a polynomial number of measurements on the quantum device. Benchmarking on the transverse-field Ising model demonstrates NLCE convergence with circuit depth scaling linearly with system size. We analyze cost function robustness for models with broken symmetry. The PCAT post-processing framework applies to any quantum eigenstate preparation method, demonstrated via VQE and adiabatic sweeps on real quantum hardware.

[1] Sumeet, M. Hörmann, and K. P. Schmidt, arXiv:2511.06623 (2025).
[2] Sumeet, M. Hörmann, and K. P. Schmidt, Phys. Rev. B 110, 155128 (2024).

QI 5.5 Tue 10:30 BEY/0137

Scalable Generic State Preparation through Tensor Cross Interpolation and Binary Trees — •Vittorio Pagni[1,2], Kevin Lively[1], Peter Ken Schuhmacher[1], and Michael Felderer[1,2] — [1]Institute of Software Technology German Aerospace Center (DLR) Sankt Augustin, Germany — [2]University of Cologne, Cologne, Germany

Efficient preparation of generic quantum states remains a major computational bottleneck in many quantum protocols. We introduce a deterministic and scalable method that employs tensor cross interpolation to construct a tensor-train representation of high-dimensional, queryable functions beyond what can be stored directly in memory and maps it onto a sequence of single-qubit and controlled rotations. This mapping is achieved through an intermediate binary-tree representation, which systematically exploits the underlying data structure to minimize circuit depth under various connectivity constraints. The approach offers a transparent and structured alternative to variational methods.

QI 5.6 Tue 10:45 BEY/0137

Quantum-inspired space-time PDE solver and dynamic mode decomposition — •Raghavendra Dheeraj Peddinti[1], Stefano Pisoni[1,2], Narsimha Rapaka[3], Mohamed K. Riahi[3], Egor Tiunov[1], and Leandro Aolita[1] — [1]Quantum Research Center, Technology Innovation Institute, Abu Dhabi, UAE — [2]Hamburg University of Technology, Institute for Quantum Inspired and Quantum Optimization, Germany — [3]Emirates Nuclear Technology Center, Khalifa University of Science and Technology, Abu Dhabi, UAE

Numerical solutions of partial differential equations (PDEs) are central to the understanding of dynamical systems. Space-time methods that treat the combined space-time domain simultaneously offer better stability and accuracy than standard time-stepping schemes. Interestingly, data-driven approaches, such as dynamic mode decomposition (DMD), also employ a combined space-time representation. However, the curse of dimensionality often limits the practical benefits of space-time methods. In this work, we investigate quantum-inspired methods for space-time approaches, both for solving PDEs and for making DMD predictions. We achieve this goal by treating both spatial and temporal dimensions within a single matrix product state (MPS) encoding. First, we benchmark our MPS space-time solver for both linear and nonlinear PDEs, observing that the MPS ansatz accurately captures the underlying spatio-temporal correlations while having significantly fewer degrees of freedom. Second, we develop an MPS-DMD algorithm for accurate long-term predictions of nonlinear systems, with runtime scaling logarithmically with both spatial and temporal resolution.

30min. break

QI 5.7 Tue 11:30 BEY/0137

Probabilistic imaginary-time evolution on the ion-trap quantum computer — •Satoshi Ejima[1,2], Kazuhiro Seki[2], Benedikt Fauseweh[1,3], and Seiji Yunoki[2,4] — [1]German Aerospace Center (DLR), Cologne, Germany — [2]RIKEN, Wako, Japan — [3]TU Dortmund University, Dortmund, Germany — [4]RIKEN, Kobe, Japan

Imaginary-time evolution (ITE) is a classical method for projecting ground states of quantum many-body systems. Probabilistic imaginary-time evolution (PITE) adapts this idea to quantum hardware, providing a pathway to low-energy state preparation. We formulate PITE within a state-vector simulation framework and use it to optimize initial algorithm parameters.

We benchmark the approach on the spin-1/2 Heisenberg chain and the transverse-field Ising model (TFIM). With optimized parameters, the success probability quickly approaches unity within only a few iterations, and the energy expectation converges to the exact ground-state value.

Finally, we implement PITE for the TFIM on a trapped-ion device. Although hardware noise distorts raw outcomes, a simple global depolarizing model significantly improves agreement with ideal, noise-free behavior.

Phys. Rev. Research **7**, 043182 (2025).

QI 5.8 Tue 11:45 BEY/0137

From gradients to curvature: tensor-network Hessian-vector products for second-order Riemannian quantum circuit compression — •Isabel Nha Minh Le[1,2], Roeland Wiersema[3], and Christian B. Mendl[1,2,4] — [1]Technical University of Munich, School of Computation, Information and Technology, Boltzmannstraße 3, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstrasse 4, 80799 Munich, Germany — [3]Center for Computational Quantum Physics, Flatiron Institute, 162 Fifth Avenue, New York, NY 10010, USA — [4]Technical University of Munich, Institute for Advanced Study, Lichtenbergstraße 2a, 85748 Garching, Germany

Riemannian optimization, combined with tensor network techniques, has shown strong potential for quantum circuit compression. However, existing approaches either rely solely on first-order gradient information [1] or are restricted to symmetry-invariant systems [2]. We introduce a tensor-network-based framework for efficiently computing second-order derivatives on Riemannian manifolds. By integrating these curvature estimates with in- and out-of-distribution generalization strategies from quantum machine learning [3], we develop a scalable second-order Riemannian optimization method for compressing quantum circuits.

[1] Quantum 9, 1833 (2025).
[2] J. Phys. A: Math. Theor. 57 135303 (2024).
[3] arXiv preprint arXiv:2409.16346 (2024).

QI 5.9 Tue 12:00 BEY/0137

Identifying optimal non-classicality witnesses — •Martina Jung[1], Suchitra Krishnaswamy[2], Jan Sperling[2], Timon Schapeler[3], Tim Bartley[3], Annabelle Bohrdt[4], and Martin Gärttner[1] — [1]Institute of Condensed Matter Theory and Optics, Friedrich-Schiller-University, Jena, Germany — [2]Institute for Photonic Quantum Systems, Theoretical Quantum Science, Paderborn University, Germany — [3]Department of Physics, Paderborn University, Germany — [4]Munich Center for Quantum Science and Technology (MCQST), München, Germany

Non-classicality, defined and understood in the quantum optical sense, acts as a resource for photon-based quantum technologies. Therefore, certifying the non-classicality of a quantum state is crucial to gauging its potential for quantum advantage. However, traditional non-classicality witnesses often fail in realistic scenarios involving finite-resolution photon detectors and limited statistics.

Here, we train a variational model using finitely many snapshots, measured with different detection schemes, to learn an optimal non-classicality witness for a given set of physically relevant states. The model is both device-agnostic and interpretable; the optimal witness can be extracted once the model has been trained. Training the model on experimental data measured with (i) a superconducting nanowire single-photon detector and (ii) a time-bin multiplexing detection scheme demonstrates the versatility of the approach, paving the way for efficient non-classicality certification in the lab.

QI 5.10 Tue 12:15 BEY/0137

A hybrid learning agent approach for solving the flight trajectory optimization — •Marcel Schindler[1], Rouven Kanitz[2], and Sabine Wölk[1] — [1]Institute of quantum technologies, DLR, Ulm, Germany — [2]Institute of air transport, DLR, Hamburg, Germany

It is believed that combinatorial optimization is to be among the first applications where quantum computers can demonstrate a practical advantage over classical systems. One such problem is the flight trajectory optimization, which aims to find the optimal path between two airports for an aircraft under given conditions. Due to non-local constraints of the flight path, the problem is part of complexity class NP-hard and becomes difficult to solve for classical algorithms. To address this, we employ a reinforcement learning algorithm in which the learning process of an agent is sped up by using a quantum communication channel.

QI 6: Implementations II

Time: Tuesday 9:30–12:45 Location: BEY/0245

Invited Talk QI 6.1 Tue 9:30 BEY/0245

Erbium dopants for quantum networks — •Andreas Reiserer — Technical University of Munich, TUM Center for Quantum Engineering (ZQE), Am Coulombwall 3A, 85748 Garching, Germany

Despite decade-long research into different physical systems, demonstrating a scalable platform for quantum networks and distributed quantum information processing remains an outstanding challenge. In this context, our group investigates the use of erbium dopants in silicon and silicate crystals. This platform offers unique potential for up-scaling: First, erbium dopants can exhibit second-long coherence in a temperature range accessible with 4He cryocoolers. Second, the optical transition of erbium is among the narrowest spectral features ever measured in a solid. Thus, frequency-multiplexed addressing of individual dopants gives access to an unprecedented qubit density. Finally, by embedding the dopants into slow-light waveguides or optical resonators with a high quality factor, the optical lifetime can be reduced via the Purcell effect. This has enabled lifetime-limited photon emission in the telecommunications C-band, where optical fiber losses are minimal. Furthermore, it has paved the way for the optical spin readout of erbium dopants and for spectroscopy of their surrounding nuclei. Taken together, our results thus establish erbium dopants as a promising new hardware platform that may facilitate the implementation of scalable quantum networks and repeaters based on single emitters at telecommunications wavelengths.

QI 6.2 Tue 10:00 BEY/0245

Shadow Wall Epitaxy: All-in-situ fabrication of ZnSe-based Quantum Devices — •Christine Falter[1,2], Yurii Kutovyi[1,2], Nils von den Driesch[1,2], Denny Dütz[2,3], Lars R. Schreiber[2,3], and Alexander Pawlis[1,2] — [1]Peter Grünberg Institute, Forschungszentrum Jülich GmbH, 52428 Jülich, Germany — [2]JARA-FIT, Jülich Aachen Research Alliance, Forschungszentrum Jülich and RWTH Aachen University, Germany — [3]JARA-Institute for Quantum Information, RWTH Aachen University, 52074 Aachen, Germany

The wide band-gap semiconductor ZnSe offers a wide range of unique optical and electrical properties, which make it a promising candidate for a variety of quantum devices. In standard fabrication schemes, device performance is often limited by surface states and defects introduced during ex-situ applied processing steps. With this in mind, we have developed a Shadow Wall technique for molecular beam epitaxy (MBE), which allows for all-in-situ device fabrication making all post processing steps obsolete. The technique relies on the pre-patterning of vertical walls on the substrate and the precise alignment of material fluxes during deposition. Using our technique we have realized an all-in-situ ZnSe-based field effect transistor (FET). In our contribution, we demonstrate the MBE growth of high quality ZnSe layers on pre-patterned substrates, the optimization of the electronic band-structure and the electrical characterization of the final device. The optimization of the ZnSe FET platform is a first step towards the realization of qubits based on gate defined quantum dots in ZnSe.

QI 6.3 Tue 10:15 BEY/0245

Harnessing the non-Abelian Berry phase for universal control of zero-field spin qubits — •Baksa Kolok[1,2], Csongor Hunyady[1], and András Pályi[1,2] — [1]Department of Theoretical Physics, Institute of Physics, Budapest University of Technology and Economics — [2]HUN-REN-BME-BCE Quantum Technology Research Group, Budapest University of Technology and Economics

Spin qubits in semiconductor quantum dots achieve their longest coherence times at zero magnetic field when nuclear spins are suppressed, making zero-field operation attractive. It also promises reduced control complexity by removing the need for magnets and enabling electrical, baseband manipulation. In this talk, I present a control framework that realizes universal quantum computation in sparse quantum-dot arrays operating entirely at zero magnetic field. Initialization and readout rely on singlet-triplet energy separation and Pauli spin blockade. Single-qubit gates emerge geometrically: when a qubit is shuttled around closed loops in the array, it accumulates a non-Abelian Berry phase that implements a deterministic SU(2) rotation. Although the number of accessible loops, and thus the native gate set, is discrete, we show that in generic devices two loops already provide full single-qubit controllability. Moreover, the same pair of loops suffices for complete quantum process tomography, enabling characterization of decoherence in zero-field architectures. Combined with exchange-based entangling gates, these results position sparse quantum-dot arrays as a promising platform for high-coherence, all-electric quantum computation without magnetic fields or microwave pulses.

QI 6.4 Tue 10:30 BEY/0245

Modelling readout of spin qubits using a single electron transistor — •Domonkos Svastits[1,2], Sudipto Das[1], Aritra Sen[1], and András Pályi[1,3] — [1]Budapest University of Technology and Economics, Budapest, Hungary — [2]Qutility @ Faulhornlabs, Budapest, Hungary — [3]HUN-REN-BME-BCE Quantum Technology Research Group, Budapest, Hungary

Spin qubits in semiconductor quantum dots are a promising platform for scalable quantum computing. However, current qubit operations remain too noisy for practical applications, with qubit readout often being the noisiest operation. Readout typically uses Pauli blockade spin-to-charge conversion combined with charge sensing. In this work, we present a microscopic model of charge sensing implemented by a single-electron transistor (SET), intended to guide improvements in spin-qubit readout, focusing on an n-type Silicon double quantum dot equipped with a micromagnet. Our model provides a microscopic, dynamical description of the measurement process. We show the measurement induces unwanted back-action in the form of incoherent transitions between qubit energy eigenstates, similar to predictions for a QPC (D. Svastits et al., arXiv:2505.15878 [quant-ph]). We also calculate how the measurement rate, i.e. the speed of the measurement, depends on the qubit Hamiltonian. We find that the parameter dependence of readout infidelity, post-measurement state mixedness and leakage are well explained by the transition rates and the measurement rate. Finally, we propose experimentally practical strategies to increase the measurement rate while suppressing the transition rates.

QI 6.5 Tue 10:45 BEY/0245

Ge-based qubit heterostructure: A 3-in-1 photoelectron spectroscopy study — •Andreas Fuhrberg[1], Maximilian Oezkent[2], Kevin-P. Gradwohl[2], Sergii Chernov[4], Volkmar Koller[4], Christoph Schlueter[4], Hans-Joachim Elmers[3], and Martina Müller[1] — [1]Universität Konstanz — [2]IKZ, Berlin — [3]Universität Mainz — [4]DESY, Hamburg

Semiconductor spin qubits are a key component in quantum information processing. Ge-based hole spin qubits have also proven to be a suitable system for realizing spin qubits. Strain-induced $Ge_{0.8}Si_{0.2}$/Ge/$Ge_{0.8}Si_{0.2}$ heterostructures are a common way to build such components. At both interfaces, holes are confined by a strain-induced valence band offset (VBO) - an essential device parameter. A set of three synchrotron-based photoemission experiments are performed to investigate the interfaces of Ge-based qubit heterostructures by varying the thickness of (i) the central Ge-layer and (ii) $Ge_{0.8}Si_{0.2}$ overlayer. Using hard X-ray momentum microscopy (MM), the valence band along the symmetry points Γ, X and L is characterized, and the VBO near both interfaces is quantized. MM reveals an increased energy shift of ≈ 50 meV between the heavy/light hole band and the spin-orbit band for (i) Ge and (ii) $Ge_{0.8}Si_{0.2}$ bands near the respective interface. An MM-based diffraction experiments and hard X-ray photoelectron spectroscopy further analyse the interface structure and chemistry. Together, this three-in-one photoelectron spectroscopy technique provides a nearly full characterization of the Ge-hole spin qubits main structure and supports the qubit optimization process.

30min. break

QI 6.6 Tue 11:30 BEY/0245

The flopping-mode exchange-only spin qubit — •Simon Stastny[1] and Guido Burkard[2] — [1]Universität Konstanz, Konstanz, Germany — [2]Universität Konstanz, Konstanz, Germany

Electron or hole spin qubits in quantum dots coupled to a microwave cavity are an established platform to realize spin qubits. One promising qubit is the exchange-only spin qubit, that allows for full baseband control, without magnetic fields. In this work we propose a spin qubit, that couples exchange-only qubit states to a cavity by adding a charge degree of freedom to the established three dot exchange-only qubit. The proposed qubit is a generalized flopping mode qubit: It comprises four quantum dots with three electrons, operating near the $(0,1,1,1) \leftrightarrow (1,0,1,1) \leftrightarrow (1,1,0,1)$ charge transition. The qubit as well as its resulting transversal and longitudinal spin photon couplings allow for full baseband control. the couplings and quasi static noise of the qubit are analyzed. We find dephasing times exceeding the estimated gates times, thus the proposed qubit is a promising system to realize baseband-controlled resonator-mediated (longitudinal) two qubit gates.

QI 6.7 Tue 11:45 BEY/0245

Reinforcement learning entangling operations on spin qubits — •Mohammad Abedi[1,2] and Markus Schmitt[1,3] — [1]PGI-8 (Quantum Control), Forschungszentrum Jülich, Wilhelm-Johnen-Straße, 52428, Jülich — [2]Fakultät für Physik, Universität Regensburg, Universitätsstraße 31, D-93051, Regensburg — [3]Fakultät für Informatik und Data Science, Universität Regensburg, Universitätsstraße 31, D-93040, Regensburg

High-fidelity control of one- and two-qubit gates past the error correction threshold is an essential ingredient for scalable quantum computing. We present a reinforcement learning (RL) approach to find entangling protocols for semiconductor-based singlet-triplet qubits in a double quantum dot. Despite the presence of realistically modelled experimental constraints, such as various noise contributions and finite rise-time effects, we demonstrate that an RL agent can yield performative protocols, while avoiding the model-biases of traditional gradient-based methods. We optimise our RL approach for different regimes and tasks, including training from simulated process tomography reconstruction of unitary gates, and investigate the nuances of RL agent design.

QI 6.8 Tue 12:00 BEY/0245

Spin Qubit Leapfrogging: Dynamics of shuttling electrons on top of another — •Nicklas Meineke and Guido Burkard — Faculty of Physics, University of Konstanz, 78464 Konstanz, Germany

In recent years spin shuttling has distinguished itself as a promising candidate for achieving high fidelity medium range interactions between spin qubits and presents a powerful tool for enabling scalable semiconductor spin quantum computing architectures in the future.

Modelling the process of a shuttled spin qubit encountering a stationary quantum dot, we investigate the dynamics of the (1,1)-(0,2) charge transition in a silicon double quantum dot with non-vanishing inter-valley coupling. This enables us to describe the process of the mobile electron leapfrogging over the stationary one i.e. transitioning from a (1,1,0)- to a (0,1,1)-charge state, occupying a (0,2,0) state inbetween. Here the triplets will occupy a valley excited state to circumvent Pauli-Spin-Blockade leading to a S*T0 splitting approximately equal to the valley splitting in the stationary dot. Consequently this protocol will implement an entangling gate, which can be tuned by waiting in this configuration. For the gate to be noise-resistant and controllable the valley splitting at the location of the middle dot needs to be very low. Therefore this opens up the possibility to make practical use and isolate low-valley splitting hotspots on a wafer, which would otherwise act as error sources.

QI 6.9 Tue 12:15 BEY/0245

Highly crystalline superconducting resonators grown on reconstructed sapphire via Thermal Laser Epitaxy and Molecular Beam Epitaxy — •Thomas J. Smart[1], Marc Neis[2], Roudy Hanna[1,2], Marcello Gaurdascione[2], Michael Schleenvoigt[1], Joscha Domnick[1], Benjamin Bennemann[1], Janine Lorenz[3], Jin Hee Bae[1], Abdur R. Jalil[1], Pavel A. Bushev[2], Felix Lüpke[3], Peter Schüffelgen[1], Detlev Grützmacher[1], and Rami Barends[2] — [1]Peter Grünberg Institute of Semiconductor Nanoelectronics (PGI-9), Forschungszentrum Jülich & Jülich Aachen Research Alliance; 52425, Jülich, Germany — [2]Peter Grünberg Institute of Functional Quantum Systems (PGI-13), Forschungszentrum Jülich, Campus-Boulevard 79, 52074, Aachen, Germany — [3]Peter Grünberg Institute of Quantum Nanoscience (PGI-3), Forschungszentrum Jülich, 52425, Jülich, Germany

In the ongoing search for optimizing quantum computing hardware, many alternative superconducting materials are being investigated, including nitrogen-based compounds with large superconducting band gaps, high Tc values, and resistance to oxidation. Concurrently, thermal reconstruction of substrates via Thermal Laser Epitaxy enables enhanced epitaxial growth and pristine interface quality. We demonstrate the growth of highly crystalline TiN on reconstructed sapphire via Molecular Beam Epitaxy, subsequently fabricated into superconducting resonators. These resonators produce internal quality factors greater than 2e6 at single-photon values, among the highest recorded for crystalline TiN on sapphire.

QI 6.10 Tue 12:30 BEY/0245

Characterization of driven unwanted state transitions in superconducting circuits — •Sumeru Hazra, Wei Dai, Daniel. K. Weiss, Pavel D. Kurilovich, Thomas Connolly, Harsh K. Babla, Shraddha Singh, Vidul R. Joshi, Andy Z. Ding, Pranav D. Parakh, Jaya Venkatraman, Xu Xiao, Luigi Frunzio, and Michel H. Devoret — Department of Applied Physics, Yale University, New Haven, CT, USA

Microwave drives are essential for the control and readout of superconducting quantum circuits. Ideally, strong drive increases the speed and fidelity of such operations, however, in practice, strong drives also induce unwanted state transitions that corrupt these operations. In this talk, I will present a comprehensive investigation of drive-induced transitions in a fixed-frequency qubit subjected to microwave tones over a broad 9 GHz range. By combining a pump-probe spectroscopy with driven Hamiltonian simulations, we identify the physical origins of these transitions and group them into three mechanisms: (i) Resonant interactions with parasitic two-level systems activated by drive-induced ac-Stark shifts, (ii) Intrinsic multi-photon transitions out of the computational subspace, and (iii) Inelastic scattering processes where the qubit exchanges energy with spurious electromagnetic modes or TLS defects. I will show that Floquet steady-state simulations, supplemented with finite-element electromagnetic modeling, accurately predict all transitions that do not involve TLSs. These results establish a unified framework for predicting and eliminating drive-induced unwanted transitions.

QI 7: Quantum Thermodynamics

Time: Tuesday 9:30–11:00 Location: BEY/0E17

QI 7.1 Tue 9:30 BEY/0E17

Probes of Full Eigenstate Thermalization in Ergodicity-Breaking Quantum Circuits — •Gabriel O. Alves, Felix Fritzsch, and Pieter W. Claeys — Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

The eigenstate thermalization hypothesis (ETH) is the leading interpretation in our current understanding of quantum thermalization. Recent results uncovered strong connections between quantum correlations in thermalizing systems and the structure of free probability theory, leading to the notion of full ETH. However, most studies have been performed for ergodic systems and it is still unclear whether or how full ETH manifests in ergodicity-breaking models. We fill this gap by studying standard probes of full ETH in ergodicity-breaking quantum circuits, presenting numerical and analytical results for interacting integrable systems. These probes can display distinct behavior and undergo a different scaling than the ones observed in ergodic systems. For the analytical results we consider an interacting integrable dual-unitary model and present the exact eigenstates, allowing us to analytically express common probes for full ETH. We discuss the underlying mechanisms responsible for these differences and show how the presence of solitons dictates the behavior of ETH-related quantities in the dual-unitary model. We show numerical evidence that this behavior is sufficiently generic away from dual-unitarity when restricted to the appropriate symmetry sectors.

QI 7.2 Tue 9:45 BEY/0E17

Exploring Noisy Quantum Thermodynamical Processes via Global Depolarizing Approximation — Jian Li[1], Xiaoyang Wang[2], Marcus Huber[1], Nicolai Friis[1], and •Pharnam Bakhshinezhad[1] — [1]Atominstitut, TU Wien, Stadionallee 2, 1020 Vienna, Austria — [2]RIKEN Center for Interdisciplinary Theoretical and Mathematical Sciences (iTHEMS), Wako 351-0198, Japan

Noise is an unavoidable challenge for quantum thermodynamical protocols in deep circuits [1]. To overcome the difficulty of analytically characterizing cumulative, gate-dependent errors, we introduce the Global Depolarizing Approximation (GDA), a scalable framework. The GDA approximates complex local noise channels with a single, system-wide depolarizing channel, requiring only a moderate circuit depth that approximates a unitary 2-design [2].

Applying the GDA to the Two-Sort Algorithmic Cooling (TSAC) protocol [3], we derive a novel analytical expression for its asymptotic cooling limit under realistic noise. This analysis reveals a fundamental noise-induced trade-off: the ideal exponential gain from increasing the qubit number is counteracted by an exponential increase in noise accumulation, which dictates an optimal qubit number and a sharp upper bound on the achievable cooling performance. We validate the GDA's accuracy against detailed physical noise simulations for both TSAC and Dynamic Cooling (DC) protocols [4]. Our framework offers a powerful tool for quantifying the thermodynamic cost of imperfect control in noisy quantum systems.

QI 7.3 Tue 10:00 BEY/0E17

Exact heat currents for multi-bath open quantum systems — •Matteo Garbellini[1], Valentin Link[2], and Walter Strunz[1] — [1]Institut für Theoretische Physik, Technische Universität Dresden, Dresden, Germany — [2]Technische Universität Berlin, Berlin, Germany

I present a numerically exact method for computing stationary heat currents in small quantum systems coupled to multiple bosonic reservoirs at different temperatures. Our approach leverages the recently introduced uniTEMPO method [1], which efficiently generates compressed auxiliary environments for non-Markovian Gaussian baths. Building upon this, we are able to efficiently compute heat currents into the reservoirs in both transient and steady-state regimes.

We apply our method to a single qubit strongly coupled to two baths and analyze how different coupling operators and the structure of the environments affect heat transport. Finally, we apply the method to quantum refrigeration. For a three-level system coupled to two reservoirs, we find that although autonomous global refrigeration does not occur, a frequency-resolved analysis reveals local cooling of specific environmental modes, suggesting a route to exploiting this localized effect with additional weakly coupled modes.

[1] V. Link, H.-H. Tu, and W. T. Strunz, Phys. Rev. Lett. 132, 200403 (2024)

QI 7.4 Tue 10:15 BEY/0E17

Local energy assignment for two interacting quantum thermal reservoirs — •Alessandra Colla[1,2], Bassano Vacchini[2], and Andrea Smirne[2] — [1]Institute of Physics, University of Freiburg, Hermann-Herder-Straße 3, D-79104 Freiburg, Germany — [2]Dipartimento di Fisica "Aldo Pontremoli", Università degli Studi di Milano, Via Celoria 16, I-20133 Milan, Italy

Understanding how to assign internal energy, heat, and work in quantum systems beyond weak coupling remains a central problem in quantum thermodynamics, particularly as the difference between competing definitions becomes increasingly relevant. In this work [1], we identify two common sets of definitions for first law quantities that are used in the literature to describe the thermodynamics of quantum systems coupled to thermal environments. Both are conceptually non-symmetric, treating one part of the bipartition (the "system") differently from the other (the "bath"). We analyze these in a setting where such roles are not easily assigned, namely two large sets of thermal harmonic oscillators interacting with each other. We further compare them with a third set of definitions based on a local, conceptually symmetric open-system approach ("minimal dissipation") and discuss their quantitative and structural differences. We observe that all three sets of definitions differ substantially even in the dispersive regime, and that the minimal dissipation approach features distinct work peaks that increase with coupling strength.

[1] A. Colla, B. Vacchini and A. Smirne, New Journal of Physics 10.1088/1367-2630/ae24a0 (2025)

QI 7.5 Tue 10:30 BEY/0E17

Symmetry-Aware Cooling Protocols for High-Fidelity Initialization of Many-Body Spin Networks — •Durga Dasari[1], Saikat Sur[2], and Gershon Kurizki[3] — [1]3. Physics Institute, University of Stuttgart, Stuttgart, GERMANY — [2]Institute of Mathematical Sciences, Chennai, India — [3]Weizmann Institute of Science, Israel

Interacting quantum spin networks are central to many-body quantum simulations, sensing, and quantum computation, all of which demand a highly polarized initial state. However, cooling such networks to their ground state is impeded by interaction-induced correlations and symmetry-protected subspaces. Resetting a mixed many-body state to the computational-zero state thus remains an open challenge. We present a universal cooling strategy that couples the network collectively to an ancilla spin that periodically dumps entropy into an ultracold bath. Using graph-theoretic analysis of the network*capturing connectivity, symmetry sectors, and correlation flow*we bypass the intractability of full quantum dynamics. This analysis reveals a unique coherent control sequence that deliberately breaks graph-imposed symmetry constraints and unlocks otherwise inaccessible cooling pathways. The resulting protocol provides a general and experimentally realistic route to high-fidelity purification of complex spin networks.

QI 7.6 Tue 10:45 BEY/0E17

Local and global thermodynamics of pure decoherence processes — •Irene Ada Picatoste[1], Alessandra Colla[2], and Heinz-Peter Breuer[1] — [1]Physikalisches Institut, Universität Freiburg, Hermann-Herder-Straße 3, D-79104 Freiburg, Germany — [2]Dipartimento di Fisica Aldo Pontremoli, Università degli Studi di Milano, via Celoria 16, I-20133 Milan, Italy

We study the thermodynamics of pure decoherence processes in open quantum systems coupled to a thermal reservoir. We perform a comparison between two viewpoints: a local approach [1] which is based on the system's degrees of freedom alone, and global approaches [2, 3] which require knowledge about the degrees of freedom of the bath. We also employ a specific model and, in calculating entropy production, internal energy, heat and work, we find substantial differences between the formulations. Concretely, in the global approaches we observe a large heat exchange, that refers in this particular case to the rearranging of the energy in the degrees of freedom of the reservoir, rather than to energy entering or leaving the system [4].

[1] A. Colla and H.-P. Breuer, Phys. Rev. A 105, 052216 (2022).

[2] M. Esposito, K. Lindenberg, and C. V. den Broeck, New J. Phys. 12, 013013 (2010).

[3] G. T. Landi and M. Paternostro, Rev. Mod. Phys. 93, 035008 (2021).

[4] I. A. Picatoste, A. Colla, and H.-P. Breuer, Phys. Rev. A 112, 022210 (2025).

QI 8: Implementations III

Time: Tuesday 14:00–15:30 Location: BEY/0137

QI 8.1 Tue 14:00 BEY/0137

Proposal of multi-mode couplers for all-to-all connectivity and long distance couplings for superconducting qubits — •Zhongyi Jiang[1,2], Mira Sharma[2], Simon Geisert[3], Sören Ihssen[3], Ioan Pop[3,4,5], and Mohammad Ansari[1] — [1]Peter Grünberg Institute PGI-12, Forschungszentrum Jülich, Jülich 52425, Germany — [2]Institute for Quantum Information, RWTH Aachen University, D-52056 Aachen, Germany — [3]IQMT, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [4]PHI, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [5]Physics Institute 1, Stuttgart University, 70569 Stuttgart, Germany

The low connectivity in superconducting systems has become a crucial bottleneck for scaling up superconducting QPU and implementing error correction. Building on our previous theory of multi-mode couplers, we propose a coupler and QPU design with superconducting qubits that support native all-to-all connectivity and long distance couplings. In our design, each module consists of a central multi-mode coupler with qubits around it. The central coupler provides all-to-all coupling within the module. Between the modules, central couplers are coupled via a bus coupler. The central couplers and the bus coupler together provide long-distance coupling among qubits in different modules. We give theory analysis and numerical simulations for such a QPU design. We believe this gives a feasible path for scaling up superconducting qubits.

QI 8.2 Tue 14:15 BEY/0137

Accelerated CZ gates on Tunable Fluxonium architecture — •Aneesh Anand Kamat[1,2], Dimitrios Georgiadis[1,3], Francisco Cárdenas-López[1], and Felix Motzoi[1,3] — [1]Peter Grünberg Institute, Quantum Control (PGI-8), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Institute for Quantum Information, RWTH Aachen University, 52056 Aachen, Germany — [3]Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

Fluxonium qubits offer superior coherence for large-scale superconducting processors, but their protected nature complicates standard entangling schemes due to smaller matrix elements. The Fluxonium-Transmon-Fluxonium (FTF) architecture leverages a flux-tunable Transmon coupler to mediate interaction, enabling stronger effective couplings for fast gates. We analyze the error budget for a flux-controlled CZ gate in the FTF architecture by characterizing the dominant leakage channels for experimentally realized systems, and developing the strategies to remove them using quantum optimal control.

QI 8.3 Tue 14:30 BEY/0137

Realising Superconducting Qubit Architectures using Scalable Flip-Chip Integration — •Anirban Bhattacharjee[1,2], Lea Richard[1,2], Julius Feigl[1,2], Ivan Tsitsilin[1,2,3], Niklas Bruckmoser[1,2], Johannes Schirk[1,2], João Romeiro[1,2], David Bunch[1,2], Leon Koch[1,2,3], Haiyang Hu[1,2], Lasse Södergren[1,2], Christian Schneider[1,2], Max Werninghaus[1,2], and Stefan Filipp[1,2] — [1]Technical University of Munich, School of Natural Sciences, Physics Department, Garching, Germany — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [3]Peak Quantum GmbH, Garching, Germany

Flip-chip integration technologies have emerged as a promising approach to scale superconducting qubits. This enables flexible signal routing and minimizes crosstalk. Separating the qubit chip from the control chip, consisting of microwave signal lines, allows tackling fabrication challenges independently. In this work, we use high quality indium bumps for inter chip bonding and polymer spacers to achieve precise control of inter chip spacing and alignment. We demonstrate qubits exhibiting average relaxation times of $T_1 = 102 \pm 13\mu s$ and microwave resonators with quality factors of $Q_{int} \geq 10^6$, demonstrating that our techniques do not degrade the resonator or qubit performance. We also report our ongoing work in realizing high fidelity two-qubit gates using a tunable coupler architecture, an essential step towards scaling up superconducting quantum processors using flip-chip technologies.

QI 8.4 Tue 14:45 BEY/0137

Inherent crosstalk in superconducting circuits — •Balázs Gulácsi and Guido Burkard — University of Konstanz, Konstanz, Germany

Crosstalk refers to unwanted qubit addressing. This is particularly detrimental for scaling quantum information systems because unintended interactions limit overall performance. For superconducting qubits, tunable couplings and frequency tunability achieved through externally applied magnetic fluxes enable high-fidelity entangling gates; however, they also introduce crosstalk through flux linkage. In this work, we are investigating the impact of time-dependent external-flux-aware circuit quantization on superconducting qubit couplings. We find that non-trivial couplings emerge between capacitively linked qubits when the magnetic flux threading one qubit's loop varies in time, in a manner analogous to Faraday's law of induction. These effects influence the performance of parametrically activated two-qubit gates and enable flux noise to propagate even to fixed-frequency transmons.

QI 8.5 Tue 15:00 BEY/0137

Ultrafast Single Qubit Gates through Multi-Photon Transition Removal — •Yuan Gao[1,2], Asier Galicia[1,2], José Da Costa Jesus[3,4], Yebin Liu[1], Yorgo Haddad[1,2], Dmitriy Volkov[1,2], Jéferson Guimarães[1,2], Harsh Bhardwaj[1,2], Markus Jerger[1], Marc Neis[1,2], Boxi Li[3], Francisco Cárdenas-López[3], Felix Motzoi[3,4], Pavel Bushev[1], and Rami Barends[1,2] — [1]Institute for Functional Quantum System (PGI-13), Forschungszentrum Jülich, Jülich, Germany — [2]Department of Physics, RWTH Aachen University, Aachen, Germany — [3]Institute for Quantum Control (PGI-8), Forschungszentrum Jülich, Jülich, Germany — [4]Institute for Theoretical Physics, University of Cologne, Cologne, Germany

Qubits typically have multilevel structures making them prone to unwanted transitions from fast gates. Previous works focus on suppressing leakage by mitigating the first to second excited state transition, overlooking multi-photon transitions, and achieving faster gates with further reductions in leakage has remained elusive. Here, we demonstrate single qubit gates with a total leakage error consistently below 2.0×10^{-5}, and obtain fidelities above 99.98% for pulse durations down to 6.8 ns for both X and $X/2$ gates. This is achieved by removing direct transitions beyond nearest-neighbor levels using a double recursive implementation of the Derivative Removal by Adiabatic Gate (DRAG) method, which we name the R2D method. We also introduce an approach for amplifying leakage error that can precisely quantify leakage rates below 10^{-6}. The presented approaches can be readily applied to other qubit types as well.

QI 8.6 Tue 15:15 BEY/0137

Analytical blueprint for 99.999% single-qubit gate fidelities via multi-photon error suppression on present hardware — •José Diogo Da Costa Jesus[1,2], Boxi Li[1,2], Francisco Cárdenas-López[1], and Felix Motzoi[1,2] — [1]Forschungszentrum Jülich — [2]University of Cologne

To attain high-fidelity single-qubit gates on a quantum processor, precise control of the quantum system is required. Nevertheless, such operations suffer from a plethora of errors arising from residual couplings to higher levels, resulting in leakage and phase errors that limit gate accuracy and make this task significantly challenging. Here, we demonstrate that single-qubit gate errors on the order of 10^(-5) can be achieved by introducing simple control methods based on multi-derivative pulse shaping, termed R1D and R2D, which correct the leading sources of error and enable gate infidelities below 10^(-5) for a 7ns pi-rotation in a superconducting ladder system. Moreover, we show that for a gate duration below ten nanoseconds, modeling the ladder as a three-level system does not provide an adequate description, because multi-photon transitions involving the third excited state become a major source of error. Based on this formalism, we also obtain analytical expressions for the drive amplitude and drive detuning allowing further error suppression and simplifying the calibration process. These results demonstrate that analytical pulse-shaping techniques can substantially improve single-qubit gate performance.

QI 9: Decoherence and Open Systems I

Time: Tuesday 14:00–15:30 Location: BEY/0245

QI 9.1 Tue 14:00 BEY/0245

Asymptotic Exceptional Steady States in Dissipative Dynamics — •Yu-Min Hu[1] and Jan Carl Budich[1,2] — [1]Max Planck Institute for the Physics of Complex Systems, Nöthnitzer Str. 38, 01187 Dresden, Germany — [2]Institute of Theoretical Physics, Technische Universität Dresden and Würzburg-Dresden Cluster of Excellence ct.qmat, 01062 Dresden, Germany

Spectral degeneracies in Liouvillian generators of dissipative dynamics generically occur as exceptional points, where the corresponding non-Hermitian operator becomes non-diagonalizable. Steady states, i.e., zero-modes of Liouvillians, are considered a fundamental exception to this rule since a no-go theorem excludes non-diagonalizable degeneracies there. Here, we demonstrate that the crucial issue of diverging timescales in dissipative state preparation is largely tantamount to an asymptotic approach towards the forbidden scenario of an exceptional steady state in the thermodynamic limit. With case studies ranging from NP-complete satisfiability problems encoded in a quantum master equation to the dissipative preparation of a symmetry-protected topological phase, we reveal the close relation between the computational complexity of the problem at hand and the finite-size scaling towards the exceptional steady state, exemplifying both exponential and polynomial scaling. Formally treating the weight W of quantum jumps in the Lindblad master equation as a parameter, we show that exceptional steady states at the physical value W=1 may be understood as a critical point hallmarking the onset of dynamical instability.

QI 9.2 Tue 14:15 BEY/0245

Dissipation as a resource: non-Markovian pathways to autonomous steady-state entanglement in photonic platforms — •Karol Kawa[1], Katarzyna Roszak[1], Radim Filip[2], and Tomáš Novotný[3] — [1]FZU – Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic — [2]Palacký University Olomouc, Olomouc, Czech Republic — [3]Charles University, Prague, Czech Republic

Decoherence is usually cast as the nemesis of entanglement in open quantum systems. Here we overturn that narrative and show that environmental engineering can, by itself, generate and stabilize entanglement. We analyze two bosonic modes, each coupled to an independent, uncorrelated thermal bath, and explore two complementary routes toward autonomous entanglement: (i) direct mode*mode coupling and~(ii) dissipation-induced single-mode squeezing followed by passive linear optics. Going beyond previous Markov-limit studies that dismissed the possibility of steady-state entanglement by neglecting anomalous coupling terms, we perform a full non-equilibrium treatment that embraces non-Markovian noise and counter-rotating interactions. Logarithmic negativity reveals a robust, sizable entanglement in both scenarios. Our results depict an experimentally realistic blueprint compatible with contemporary photonic circuitry to transform unavoidable dissipation into a functional resource. By revealing how tailored system-bath couplings autonomously drive quantum correlations, this work enriches the toolbox of reservoir engineering and advances the quest for scalable, self-contained quantum technologies.

QI 9.3 Tue 14:30 BEY/0245

Emergent decoherent histories from first principles — •Philipp Strasberg — Instituto de Fisica de Cantabria (IFCA), Santander, Spain

I overview recent progress about the emergence of decoherent histories from first principles, i.e., without the use of ensembles or approximations to the Schroedinger dynamics —akin to approaches in pure state statistical mechanics. After briefly reviewing the importance of decoherent histories to understand a unitarily evolving quantum Universe, I show that generic (non-integrable) many-body systems are characterized by an exponential suppression of interference effects (as a function of the particle number of the system) whereas integrable systems are characterized by a much weaker form of decoherence. I conclude with an outlook about how (long) (de/re)coherent histories shape the structure of the Multiverse, a hitherto unappreciated phenomenon.

QI 9.4 Tue 14:45 BEY/0245

Random matrix perspective on probabilistic error cancellation — •Leonhard Moske[1], David Luitz[1], Pedro Ribeiro[2], Tomaž Prosen[3], Sergiy Denysov[4], and Karol Zyczkowski[5,6] — [1]Institute of Physics, University of Bonn, Germany — [2]CeFEMA-LaPMET, Departamento de Fisica, Instituto Superior Tecnico, Universidade de Lisboa, Portugal — [3]Faculty of Mathematics and Physics, University of Ljubljana, Slovenia — [4]Department of Computer Science, OsloMet, Oslo Metropolitan University, Norway — [5]Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University, Poland — [6]Center for Theoretical Physics, Polish Academy of Sciences, Poland

Probabilistic error cancellation is an attempt to reverse the effect of dissipative noise channels on quantum computers by applying unphysical channels after the execution of a quantum algorithm on noisy hardware. We investigate on general grounds the properties of such unphysical quantum channels by considering a random matrix ensemble modeling noisy quantum algorithms. We show that the complex spectra of denoiser channels inherit their structure from random Lindbladians. Additional structure imposed by the locality of noise channels of the quantum computer emerges in terms of a hierarchy of timescales.

QI 9.5 Tue 15:00 BEY/0245

Quantum Memory in Strongly Coupled Systems via Time-Evolving Matrix Product Operators — •Ilja List, Konrad Mickiewicz, Matteo Garbellini, Charlotte Bäcker, and Walter Strunz — Dresden University of Technology, Dresden, Germany

The steady exchange of information and energy between system and environment in open quantum systems introduces noise and dissipation into the dynamics. In the interest of modelling realistic quantum systems, it is crucial to investigate systems strongly coupled to the environment. In such non-Markovian quantum dynamics, the origin of memory effects requires a strict classification as classical or quantum. Using the paradigmatic spin-boson model, we examine numerically the behavior of open quantum systems via local quantum memory criteria based on process tensors [1]. To this end, we use the recently introduced method uniTEMPO [2] to construct the process tensors. We focus on the long-range multi-time correlations of non-Markovian open quantum systems for in-

creasing coupling strength, and investigate the detection of quantum memory near the quantum phase transition.

[1] C. Bäcker, V. Link, and W. T. Strunz. Phys. Rev. Res. 5bfc-znkj (2025)
[2] V. Link, H.-H. Tu, and W. T. Strunz, Phys. Rev. Lett. 132, 200403 (2024)

QI 9.6 Tue 15:15 BEY/0245

Signatures of correlated noise in cavity QED — •Nadine Lenke and Guido Burkard — Department of Physics, University of Konstanu, 78457 Konstanz, Germany

Noise effects limit the performance of quantum computation drastically. While the effects of noise are examined in various publications a detailed theoretical description of the influence of noise correlations is missing. In this work we examine the effects of noise correlations in cavity QED. Our underlying system consists of two qubits, which are coupled to the same cavity but not directly to each other. Both qubits are affected by longitudinal noise impacting their energy separation. The effects from noise correlations are indirectly examined with the transmission through the cavity. We compare the influences of white noise and quasi-static noise in the transient regime by applying input-output theory. We find that after averaging over many measurements, the noise correlation spectral density $S_{12}(\omega)$ can be extracted from the cavity transmission amplitude A. We compare its dependence on $S_{12}(\omega)$ for the two noise models. We conclude that in both cases a higher noise correlation spectral density leads to a decreasing A. In the quasi-static noise case the reduction of the cavity transmission amplitude is weaker. We find that in special parameter settings and for certain initial conditions it is possible to extract the noise correlation spectral density for general types of noise from the second derivative of A with respect to the sensitivities to the noise on the two qubits. The recreation of $S_{12}(\omega)$ can be achieved by writing this quantity as a sum of convolutions and by applying the convolution theorem.

QI 10: Quantum Information: Concepts and Methods I

Time: Wednesday 9:30–12:45 Location: BEY/0137

QI 10.1 Wed 9:30 BEY/0137

Deciding finiteness of Hamiltonian algebras I — •David Edward Bruschi, Tim Christoph Heib, and Robert Zeier — Forschungszentrum Jülich, Jülich, Germany

The ability to exactly obtain the dynamics of a physical system is a core goal of most areas of modern physics. Full knowledge of the state of a system at all times would be of greatest advantage for a myriad of tasks of current interest, such as quantum simulation, computing, and control. Quantum dynamics are characterized by the non-commutativity of operators in the Hamiltonian, which in turn implies that analytical solution are, in general, impossible to obtain. A standard way to approach this problem is to use of ad-hoc solutions or numerical techniques. While this allows for a better understanding of the physical processes of interest, such understanding remains only partial, and the question of how to obtain full control over the dynamics remains open.

We introduce a novel approach to determine the dimensionality of a Hamiltonian Lie algebra of interacting bosonic systems by appropriately classifying the space of its generating terms, thereby dividing the space of arbitrary linear Hermitian operators into classes with a meaningful physical interpretation. A first main result on the constraints that must be fulfilled by Hamiltonians without drift in order for the Hamiltonian Lie algebra to be finite-dimensional is obtained. Extension of this work to the classification of such algebras for one self-interacting bosonic mode is also provided. Our work has important implications for theoretical (quantum) physics as well as the theory Lie algebras.

QI 10.2 Wed 9:45 BEY/0137

Deciding finiteness of bosonic dynamics II — •Tim Heib — Institute for Quantum Computing Analytics (PGI-12), Forschungszentrum Jülich, 52425 Jülich, Germany — Theoretical Physics, Universität des Saarlandes, 66123 Saarbrücken, Germany

Determining the exact dynamics of a given system is paramount in most areas of physics, especially in quantum mechanics. A well-known method for systematically solving these dynamics by factorizing the time-evolution operator into a finite product of exponentials is the Wei-Norman method.

Recently, a new approach has been proposed to investigate the classes of Hamiltonians for which this method is applicable. This involves analyzing the dimensionality of Hamiltonian Lie algebras by appropriately characterizing their generating terms. In our work, we generalize previous results by significantly extending their applicability to a broader class of physically relevant bosonic Hamiltonians. We reduce the complexity of verifying finiteness conditions from quadratic to linear, and we also introduce a visual algorithm to implement the corresponding procedure. Furthermore, we identify a universal Lie algebraic structure encompassing all finite-dimensional algebras within this framework. Our contributions represent a substantial step toward a comprehensive classification of Hamiltonian Lie algebras, with potential impact for practical applications in quantum technologies.

QI 10.3 Wed 10:00 BEY/0137

Identification of unital channels without mixed-unitary representation — •Charlotte Bäcker and Walter Strunz — Dresden University of Technology, Dresden, Germany

Unital quantum channels are characterized by their property of leaving the maximally mixed state invariant. Among these channels are mixed-unitary channels, which can be represented as a probabilistic mixture of unitary operations. For qubits (d = 2), any unital channel is also mixed-unitary, however this does not hold for d > 2. A well-known, open NP-hard problem is to distinguish between these two classes of channels in higher-dimensional quantum dynamics. This question is relevant not only from a theoretical perspective but also for applications in quantum technology (e.g., error correction). In this talk, we will present a new method to identify non-mixed-unitary channels using tools from quantum memory theory. After introducing the relevant concepts, we will demonstrate how this method allows for a more sensitive characterization, illustrated by specific examples.

QI 10.4 Wed 10:15 BEY/0137

Understanding Quantum Reservoir Computing through the lens of Krylov Complexity — •Saud Cindrak, Lina Jaurigue, and Kathy Lüdge — Technische Universität Ilmenau, Ilmenau, Deutschland

Recent years have seen growing interest in using information-theoretic and dynamical measures to characterize quantum systems. Krylov complexity, in particular, quantifies how an operator or state spreads within a Krylov basis and distinguishes integrable from chaotic dynamics.

Here we show that time-evolved states and operators generate the same Krylov space, leading to a natural formulation of time-dependent Krylov spaces. Instead of relying on Krylov complexity, we introduce an effective phase-space dimension on the Krylov space that does not inherently assign larger complexity to states deeper in the Krylov chain. We term this measure Krylov observability (for operators) and Krylov expressivity (for states).

We then compare Krylov observability with the data generalizability of a quantum reservoir computer, quantified by its information processing capacity (IPC), and find that the two exhibit almost identical behavior. Lastly, we introduce a quantum Zeno time for operators and use it to further clarify the behavior of Krylov observability up to the Heisenberg time obtained from level statistics.

[1] S. Čindrak, L. Jaurigue, K.Lüdge, Phys. Rev. Res. 7, L042039
[2] S. Čindrak, L. Jaurigue, K.Lüdge, Phys. Rev. Res. 7, 043190
[3] S. Čindrak, L. Jaurigue, K.Lüdge, J. High Energ. Phys 2024, 83

QI 10.5 Wed 10:30 BEY/0137

Characterizing Criteria of Non-Markovian Dynamics and Quantum Memory — •Nick Maryshchak, Charlotte Bäcker, and Walter Strunz — Dresden University of Technology, Dresden, Germany

The occurrence of non-Markovianity in the dynamics of open quantum systems gives rise to the classification of memory phenomena. While in classical dynamics, non-Markovian processes are well defined, there is no unique quantum analogue. Several concepts of quantum non-Markovianity have been proposed, based for example on divisibility of the quantum map or on distinguishability of quantum states. We examine the fraction of non-Markovian dynamics in regard to different criteria in the state space of time-discrete dynamics. A growing debate is whether these memory effects are of truly quantum origin. In the subclass of non-Markovian dynamics, we examine different proposed witnesses for quantum memory and their relation among themselves.

QI 10.6 Wed 10:45 BEY/0137

Use of Neural Networks to Reconstruct Information on NV-Center Spin Registers — •Alessia Camuti Borani[1], Matthias Müller[2], and Tommaso Calarco[1,2,3] — [1]Università di Bologna — [2]Forschungszentrum Jülich — [3]Universität zu Köln

The presentation will focus on the use of Neural Networks to reconstruct information about spin states in NV-center platforms from computational-basis measurement outcomes. Neural Networks can in fact serve as a more efficient alternative to standard reconstruction protocols, thanks to their ability to detect patterns in data.

The quantum platform we simulate consists of the electronic spin of a Nitrogen-Vacancy (NV) defect in diamond, used for initialization and readout, together with the surrounding nuclear carbon spins, which serve as the actual qubits.

In the first part of the talk, we will discuss results on full-state tomography of spin states in NV-center registers using Neural Networks. We will compare the

performance obtained when feeding the network with Pauli-basis measurement outcomes to that of a randomized protocol, in which randomly selected gates are applied prior to measurement. In the second part of the talk, we will instead present results on the reconstruction of observables of NV-center systems, rather than full density matrices.

30min. break

QI 10.7 Wed 11:30 BEY/0137

Entanglement quantification with randomized measurements is maximally difficult — Julian Eisfeld and •Nikolai Wyderka — Institut für Theoretische Physik III, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf, Germany

The certification of quantum systems is essential for emerging quantum technologies, particularly in quantum communication, networks, and distributed computing, where maintaining a common reference frame across distant nodes poses significant challenges. Reference frame independent approaches, such as randomized measurement schemes, offer a promising route by reducing experimental demands while granting access to basis-independent quantities, including entanglement. However, the efficiency of such schemes in measuring local invariants has remained unclear.

In this contribution, we determine the minimal number of measurement settings required to access all two-qubit invariants using randomized measurement schemes. We further demonstrate that entanglement certification necessarily involves the most demanding invariants, establishing it as a maximally difficult task. Our results reveal a fundamental hierarchy among invariants, with direct implications for experimental feasibility and theoretical understanding of quantum certification. Finally, we extend our analysis beyond bipartite systems by applying it to the Kempe invariant in three-qubit systems, providing a first step toward uncovering similar hierarchies in higher dimensions.

QI 10.8 Wed 11:45 BEY/0137

The three kinds of three-qubit entanglement — •Szilárd Szalay — Wigner Research Centre for Physics, Budapest, Hungary

We construct an important missing piece in the entanglement theory of pure three-qubit states, which is a polynomial measure of W entanglement, working in parallel to the three-tangle, which is a polynomial measure of GHZ entanglement, and to the bipartite concurrence, which is a polynomial measure of bipartite entanglement. We also show that these entanglement measures are ordered, the bipartite measure is larger than the W measure, which is larger than the GHZ measure. It is meaningful then to consider these three types of three-qubit entanglement, which are also ordered, bipartite is weaker than W, which is weaker than GHZ, in parallel to the order of the three equivalence classes of entangled three-qubit states.

QI 10.9 Wed 12:00 BEY/0137

Gaussian fermionic embezzlement of entanglement — •Alessia Kera, Lauritz van Luijk, Alexander Stottmeister, and Henrik Wilming — Institute for Theoretical Physics, Leibniz University Hanover, Hanover, Germany

Embezzlement of entanglement allows to extract arbitrary entangled states from a suitable embezzling state using only local operations while perturbing the resource state arbitrarily little. A natural family of embezzling states is given by ground states of non-interacting, critical fermions in one spatial dimension. This raises the question of whether the embezzlement operations can be restricted to Gaussian operations whenever one only wishes to extract Gaussian entangled states.

In our work we showed that this is indeed the case and proved that the embezzling property is in fact a generic property of fermionic Gaussian states. Our results provide a fine-grained understanding of embezzlement of entanglement for fermionic Gaussian states in the finite-size regime and thereby bridge finite-size systems to abstract characterizations based on the classification of von Neumann algebras. To prove our results, we established novel bounds relating the distance of covariances to the trace-distance of Gaussian states, which may be of independent interest.

QI 10.10 Wed 12:15 BEY/0137

The relative entropy of magic and its nonadditivity — •Carolin Deckers, Justus Neumann, Hermann Kampermann, and Dagmar Bruss — Institut für Theoretische Physik III, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf, Germany

The resource theory of magic is a theoretical framework that quantifies the non-stabilizer quantum resource ”magic”, which is crucial for universal quantum computation. To quantify the amount of magic in states or operations, measures such as the relative entropy of magic have been introduced. The relative entropy of magic is a subadditive measure. Previous results [R. Rubboli, R. Takagi, and M. Tomamichel, Quantum 8, 1492 (2024)] have shown that this measure is additive for a special class of states. We show that for n-qubit product states, the relative entropy of magic is not additive if the states do not belong to that special class and fulfill an additional condition.

QI 10.11 Wed 12:30 BEY/0137

Characterizing covariance matrix and entanglement with finite Fourier transformed Observables — •Dimpi Thakuria[1], Konrad Szymański[2], Shuheng Liu[1], and Giuseppe Vitagliano[1] — [1]Atominstitut, Technische Universität Wien, Stadionallee 2, 1020 Vienna, Austria — [2]Research Center for Quantum Information, Slovenská Akadémia Vied, Dúbravská cesta 9, 84511 Bratislava, Slovakia

In Quantum physics, a covariance matrix provides us a means to certify a physically valid quantum system (through its positive semi-definiteness). It constrains the allowed quantum states and fully characterizes the Gaussian states. In continuous variable systems the covariance matrix is known to capture key properties like entanglement, squeezing, the purity of the states etc.. In this work we explore these concepts in the context of the discrete phase-space observables in finite-dimension, focusing on canonical position/momentum observables linked by finite Fourier transforms. Our approach is complementary to the typical way of using finite-dimensional Heisenberg-Weyl framework (especially discrete-displacement operators) for studying such systems. We characterize the allowed states via characterization of the invariants : the trace and the determinant of the covariance matrix. We also study the structure of the allowed covariance matrix transformations in the discrete phase-space, as well as the underlying Hilbert space. Our insights help us to discuss applications like entanglement detection in finite-dimensional systems, akin to covariance matrix criteria in continuous-variable systems.

QI 11: Implementations IV

Time: Wednesday 9:30–12:45 Location: BEY/0245

Invited Talk QI 11.1 Wed 9:30 BEY/0245

Nb-trilayer Josephson junction based parametric amplifiers for microwave frequency signals — •Lukas Grünhaupt — Physikalisch-Technische Bundesanstalt, Braunschweig, Germany

Parametric amplifiers have become a widely-used tool in cryogenic setups processing faint microwave signals. Such signals, with powers as low as femtowatts, are used, e.g., to read out solid state qubits or are hypothesized as signatures of dark matter. A large variety of superconducting parametric amplifiers exists, which can be broadly divided into two groups: devices based on resonators with typical bandwidth on the order of a few MHz and traveling-wave parametric amplifiers (TWPAs) providing bandwidths larger than 1 GHz. In addition to their bandwidth, dynamic range and added noise are the main parameters engineered in such devices, leading to a plethora of parametric amplifier implementations. At PTB we are exploring a range of superconducting parametric amplifiers harnessing the nonlinearity provided by Nb-trilayer Josephson junctions or by the kinetic inductance of granular aluminium thin films. In this talk I will discuss our recent results on rf-SQUID TWPAs [1] and present our implementation of dimer Josephson junction array amplifiers.

[1] V. Gaydamachenko & C. Kissling, L. Grünhaupt, Phys. Rev. Appl. 23, 064053 (2025)

QI 11.2 Wed 10:00 BEY/0245

Double-pumped Bogoliubov parametric amplifier using a superconducting Bose-Hubbard dimer — •Najmeh Etehadi Abari[1], Nicolas Zapata[1], Ioan Pop[1,2], and Anja Metelmann[1,3] — [1]Institute for Quantum Materials and Technology, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]Physics Institute 1, Stuttgart University, 70569, Stuttgart, Germany — [3]Institut de Sciences et d'Ingénierie Supramoléculaires,(ISIS, UMR7006), University of Strasbourg and CNRS, 67000 Strasbourg, France

Quantum limited standing-wave amplifiers in superconducting circuits are key tools for quantum-device readout, relying on Josephson junction or high kinetic inductance nonlinearities to convert pump energy into signal gain[1,2]. However, their performance is typically limited by operation near dynamic instability, restricting bandwidth. We discuss a class of standing-wave parametric amplifiers known as Bogoliubov amplifiers [3], which leverage double-pump drives to operate far from the instability region, thereby overcoming the intrinsic gain-bandwidth limitation. We demonstrate this concept on a Bose-Hubbard dimer formed by two coupled Kerr resonators [4], showing that double-pump driving enables tunable gain, bandwidth, and noise performance. This establishes Bogoliubov amplifiers as a promising platform for scalable qubit readout and precision quantum measurements. [1] P. Winkel, et al., Phys. Rev. Appl. 13.2

(2020). [2] D. J. Parker, et al., Phys. Rev. Appl. 17.3 (2022). [3] A. Metelmann, et al., arXiv:2208.00024 (2022). [4] N. Zapata, et al., Phys. Rev. Lett. 133. 26 (2024).

QI 11.3 Wed 10:15 BEY/0245

Universal Pulses for Superconducting Qudit Ladder Gates — Boxi Li[1,2], Francisco Cárdenas-López[1], Andrian Lupascu[3], and •Felix Motzoi[1,2] — [1]Forschungzentrum Jülich, Institute of Quantum Control — [2]Universität zu Köln — [3]University of Waterloo, Institute for Quantum Computing

In this work (PRX Quantum 6, 03035), we present a universal pulse construction for generating rapid, high-fidelity unitary rotations between adjacent qudit levels, thereby providing a prescription for any gate in SU(d). Control errors in these operations are effectively analyzed within a four-level subspace, including two leakage levels with approximately opposite detuning. By identifying the optimal degrees of freedom, we derive concise analytical pulse schemes that suppress multiple control errors and outperform existing methods. Remarkably, our approach achieves consistent coherent error scaling across all levels, approaching the quantum speed limit independently of parameter variations between levels. Numerical validation on transmon circuits demonstrates significant improvements in gate fidelity for various qudit sizes aiming for 10^-4 error. This method provides a scalable solution for improving qudit control and can be broadly applied to other quantum systems with ladder structures or operations involving multiple ancillary levels.

QI 11.4 Wed 10:30 BEY/0245

Superconducting Gralmonium Qubit Resilient to High Magnetic Fields — •Janic Beck[1], Simon Günzler[1], Dennis Rieger[1], Nicolas Gossling[1], Nicolas Zapata[1], Mitchell Field[1], Simon Geisert[1], Andreas Bacher[1], Judith Hohmann[1], Martin Spiecker[1], Wolfgang Wernsdorfer[1], and Ioan Pop[1,2] — [1]PHI, Karlsruhe Institute of Technology, 76131 Karlsruhe, Germany — [2]PI 1, Stuttgart University, 70569 Stuttgart, Germany

Superconducting qubits can be used as information engines to probe and manipulate microscopic degrees of freedom (DOF), whether intentionally designed or naturally occurring in their environment. In the case of magnetically susceptible DOF, the external magnetic field used to polarize them presents a challenge for superconductors and Josephson junctions. Here we demonstrate the operation of a granular aluminum nanojunction fluxonium qubit (Gralmonium), resilient to in-plane magnetic fields beyond one Tesla. By employing a gradiometric fluxonium design, we enhance the qubit's insensitivity to global magnetic flux fluctuations. The energy relaxation (T1 = 8 μs) and coherence (T2E = 2.5 μs) are unaffected by the magnetic field and we observe only minor changes in the qubit spectrum, caused by percent level gap suppression. The gradiometric gralmonium's field resilience highlights its potential for hybrid quantum architectures that combine superconducting qubits with spin systems.

QI 11.5 Wed 10:45 BEY/0245

Spin Environment of a Superconducting Qubit in High Magnetic Fields — •Simon Günzler[1], Janic Beck[1], Dennis Rieger[1], Nicolas Gosling[1], Nicolas Zapata[1], Mitchell Field[1], Simon Geisert[1], Andreas Bacher[1], Judith K. Hohmann[1], Martin Spiecker[1], Wolfgang Wernsdorfer[1], and Ioan M. Pop[1,2] — [1]Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Stuttgart University, Stuttgart, Germany

We leverage the magnetic field resilience of a granular aluminum nanojunction fluxonium qubit (Gralmonium) with a gradiometric design to uncover a paramagnetic spin-1/2 ensemble, which is the dominant Gralmonium loss mechanism when the electron spin resonance matches the qubit. We also report a suppression of fast flux noise measured in Spin-Echo experiments in magnetic fields exceeding 0.4 Tesla, which suggests the freezing of surface spins. In addition to these environments, by employing an active state stabilization sequence of the qubit, we hyperpolarize long-lived two-level systems (TLS), previously speculated to also be of magnetic origin. Surprisingly, the coupling to this TLS environment remains unaffected by magnetic fields, leaving the question of their origin open. These results demonstrate the gradiometric Gralmonium's potential for hybrid quantum architectures combining superconducting qubits with spins.

30min. break

QI 11.6 Wed 11:30 BEY/0245

High-Coherence Superconducting Qubits on Wafer-Scale — •Julius Feigl[1,2], Niklas Bruckmoser[1,2], Leon M. Koch[1,2,3], David Bunch[1,2], Léa Richard[1,2], Christian Gnandt[1,2], Ivan Tsitsilin[1,2,3], Anirban Bhattacharjee[1,2], Haiyang Hu[1,2], Vera P. Bader[1,2], Lasse Södergren[1,2], and Stefan Filipp[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, Garching, Germany — [2]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [3]Peak Quantum GmbH, Garching, Germany

Scaling superconducting quantum processors requires fabrication processes that maintain high qubit coherence across increasingly complex multi-qubit chips. While substantial progress has been achieved for isolated, single-qubit devices, preserving these coherence levels in multi-qubit architectures remains challenging due to added fabrication steps and potential loss mechanisms. In particular, as system performance is frequently limited by the least coherent qubit, understanding coherence variations across a wafer is crucial. Therefore, we present coherence measurements from twelve transmon qubits across two chips fabricated on a 100 mm wafer. The qubits exhibit an average relaxation time of $T_1 = 236 \pm 14$ μs, with the lowest device having a relaxation time of 111 ± 30 μs. We further examine the influence of fabrication processes required for large-scale integration, such as air bridges and indium bumps, on coherence. These lead to a reduction in coherence time, providing insight into the impact of additional processing required for large-scale superconducting quantum processors.

QI 11.7 Wed 11:45 BEY/0245

A charge-basis tomographic protocol for superconducting qubits — •Elena Lupo[1], Daniel Long[2], Daniel Dahan[3], Konstantin Yavilberg[3], Malcolm R. Connolly[2], Eytan Grosfeld[3], and Eran Ginossar[4] — [1]Forschungszentrum Jülich, 52428 Jülich, Germany — [2]Imperial College London, SW7 2AZ London, UK — [3]Ben-Gurion University of the Negev, 84105 Beer-Sheva, Israel — [4]University of Surrey, GU2 7XH Guildford, UK

The use of accurate models and parameters in superconducting circuits is essential for the understanding and control of quantum states. While conventional spectroscopic techniques allow the extraction of excited-state populations, transition frequencies, and decay rates, information about quantum coherence can only be obtained through phase-sensitive methods such as quantum state tomography, which is usually performed in the system's energy basis. Here we introduce a complementary tomographic protocol for the reconstruction of the ground state of a superconducting circuit with a generic Josephson junction potential [1]. The state reconstruction is done in the basis of its relative charge across the junction - a representation that can provide new insights into the quantum circuit and can assist in validating its Hamiltonian model. The method combines the flux-tuning of a split Josephson junction and adiabatic evolution to achieve the desired density matrix reconstruction of the circuit's ground state. Further possible applications of this method include the study of hybrid superconductor-semiconductor junctions [2]. [1] Lupo et al, arXiv: 2502.07748; [2] Dahan et al, arXiv: 2502.07684.

QI 11.8 Wed 12:00 BEY/0245

Magnetic-Field and Temperature Limits of a Kinetic-Inductance Traveling-Wave Parametric Amplifier — Lucas M. Janssen[1], Farzad Faramarzi[2], Henry G. LeDuc[2], Sahil Patel[3,2], Gianluigi Catelani[4,5], Peter K. Day[2], Yoichi Ando[1], and •Dickel Christian[1] — [1]Physics Institute II, University of Cologne, Germany — [2]Jet Propulsion Laboratory, Caltech, USA — [3]Department of Applied Physics and Materials Science, Caltech, USA — [4]JARA Institute for Quantum Information (PGI-11), Forschungszentrum Jülich, Germany — [5]Quantum Research Center, TII, Abu Dhabi, UAE

Kinetic-inductance traveling-wave parametric amplifiers (KI-TWPAs) offer broadband near-quantum-limited amplification with high saturation power. In this work [1], we study how magnetic field and temperature affect the performance of a KI-TWPA based on a thin-NbTiN inverse microstrip with a Nb ground plane. This KI-TWPA can provide substantial signal-to-noise ratio improvement (ΔSNR) up to in-plane magnetic fields of 0.35 T and out-of-plane fields of 50 mT, considerably higher than what has been demonstrated with TWPAs based on Josephson junctions [2]. We also find that the gain does not degrade when the temperature is raised to 3 K (limited by the Nb ground plane) while ΔSNR decreases with temperature consistently with expectation. The operability of KI-TWPAs in high magnetic fields opens the door to a wide range of applications in spin qubits, spin ensembles, topological qubits, low-power NMR, and the search for axion dark matter. [1] Janssen et al., PR Appl. 2024 [2] Janssen et al., arXiv:2509.15043

QI 11.9 Wed 12:15 BEY/0245

Toward Chemically Resilient Superconducting Qubit Fabrication — •Niklas Bruckmoser[1,2], Leon M. Koch[1,2,3], Thomas Brenninger[2], Ivan Tsitsilin[1,2,3], Amanda Scoles[1,2], David Bunch[1,2], Julius Feigl[1,2], Lea Richard[1,2], Christian Gnandt[1,2], Christian M.F. Schneider[1,2], Vera P. Bader[1,2], Haiyang Hu[1,2], Lasse Södergren[1,2], and Stefan Filipp[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, Garching, Germany — [2]Walther-Meißner-Institut, BAdW, Germany — [3]Peak Quantum GmbH, Germany

As superconducting quantum processors scale up, there is an increasing need for fabrication methods that combine low loss with high yield. One promising strategy is the implementation of subtractive processes that also withstand aggressive interface cleaning, particularly by replacing aluminum with chemically resilient materials. In this talk, we demonstrate a fully subtractive process for niobium-based air bridges that are used as interconnects as well as vacuum-gap capacitors. Rigorous surface cleaning allows us to achieve mean internal quality factors of coplanar waveguide resonators exceeding $Q_{\text{int}} = 7.9\times10^6$ in the single-photon limit, with no detectable added loss from air bridges. By integrating large

vacuum-gap capacitors into transmon qubits, we observe median lifetimes above $T_1 = 50\ \mu s$.

Building on this platform, we share our first exploratory efforts toward the implementation of chemically resilient Josephson junctions. At this early stage, we focus on challenges and discuss pathways to achieve a scalable, high-yield, and low-loss fabrication process.

QI 11.10 Wed 12:30 BEY/0245

TiN superconducting resonators: influence of sputter conditions on Qi(T) and TLS-based loss modeling — •Benedikt Schoof[1], Moritz Singer[1], Harsh Gupta[1], Simon Lang[2], and Marc Tornow[1,2] — [1]TUM CIT, 85748 Garching, Germany — [2]EMFT, 80686 Munich, Germany

We investigate how reactive sputter conditions affect the internal quality factor as a function of temperature (Qi(T)) of TiN coplanar-waveguide resonators. TiN films were grown on high-ohmic silicon (100) under varied substrate temperature (RT to 500 C), pressure (2 mbar to 18 mbar) and N2/Ar gas flow ratio (0.0 to 1.0). Electrical characterization yielded resistivity values in the range of 100 microOhm cm to 100 milliOhm cm and Tc values from 0.5 K to 5.1 K, which together with XPS, XRD and ToF-SIMS data were correlated with the Qi(T) data extracted from CPW resonators fabricated from these films. We find that films sputtered at elevated substrate temperature exhibit higher Qi (0.8e6) in the single-photon regime at 100 mK and are well described by a standard additive loss model with a single two-level-system (TLS) component. In contrast, room-temperature sputtered films require two distinct TLS contributions to reproduce the full Qi(T) dependence, indicating multiple dielectric defect populations or enhanced interfacial disorder introduced during low-temperature growth. Tc shows only a weak correlation with Qi, confirming that superconducting transition metrics alone do not capture the relevant microwave loss mechanisms. Our results provide quantitative guidance for optimizing TiN resonators for superconducting-qubit applications.

QI 12: Quantum Foundations

Time: Wednesday 15:00–18:00 Location: BEY/0137

QI 12.1 Wed 15:00 BEY/0137

On the Dynamics of Local Hidden-Variable Models — •Nick von Selzam[1,2] and Florian Marquardt[1,2] — [1]Max Planck Institute for the Science of Light, Erlangen — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg

Bell nonlocality is an intriguing property of quantum mechanics with far reaching consequences for information processing, philosophy and our fundamental understanding of nature. However, nonlocality is a statement about static correlations only. It does not take into account dynamics, i.e. time evolution of those correlations. Consider a dynamic situation where the correlations remain local for all times. Then at each moment in time there exists a local hidden-variable (LHV) model reproducing the momentary correlations. Can the time evolution of the correlations then be captured by evolving the hidden variables? In this light, we define dynamical LHV models and motivate and discuss a wide range of physical and mathematical assumptions. Based on a simple counter example we conjecture that such LHV dynamics does in general not exist. This is further substantiated by a rigorous no-go theorem. Our results suggest a new type of dynamical nonlocality expressed by the quantum time evolution of local correlations.

QI 12.2 Wed 15:15 BEY/0137

Today's Experiments Suffice to Verify the Quantum Essence of Gravity — •Martin Plávala — Institut für Theoretische Physik, Leibniz Universität Hannover, 30167 Hannover, Germany

The gravity-mediated entanglement experiments employ concepts from quantum information to argue that if gravitational interaction creates entanglement between two systems, then gravity cannot be described by a classical system. However, the proposed experiments remain beyond out current technological capability, with optimistic projections placing the experiment outside of short-term future. Here we leverage quantum information techniques to argue that current matter-wave interferometers are sufficient to indirectly prove that gravitational interaction creates entanglement between two systems. Specifically, we prove that if we experimentally verify the Schrödinger equation for a single delocalized system interacting gravitationally with an external mass, then the time evolution of two delocalized systems will lead to gravity-mediated entanglement. Our findings indicate that the experimental verification of the quantum essence of gravity is on the horizon.

QI 12.3 Wed 15:30 BEY/0137

Paradox-free classical non-causality and unambiguous nonlocality without entanglement are equivalent — Hippolyte Dourdent[1], Kyrylo Simonov[2], •Andreas Leitherer[1], Emanuel-Cristian Boghiu[2], Ravi Kunjwal[3], Saronath Halder[4], Remigiusz Augusiak[4], and Antonio Acín[1,5] — [1]ICFO-Institut de Ciències Fotòniques — [2]Fakultät für Mathematik, Universität Wien — [3]Aix-Marseille University, CNRS, LIS — [4]Center for Theoretical Physics, Polish Academy of Sciences — [5]ICREA - Institució Catalana de Recerca i Estudis Avançats

Definite causal order is an intuitive assumption which can, however, be violated without introducing paradoxes such as the grandfather antinomy. Interestingly, it is not necessary to invoke quantum or more exotic physics: process functions generalize classical deterministic communication by relaxing the assumption of a fixed causal structure between local operations. Previous work demonstrated that for three-parties, non-causal process functions can distinguish qubit product bases that cannot be realized by local operations and classical communication - a phenomenon known as quantum nonlocality without entanglement (QNLWE). We significantly elevate this result for any dimension and any number of parties, establishing an equivalence between the unique fixed-point condition characterizing process functions and a simple "unambiguity" condition, requiring that local parties perform local disjoint operations. We refine previous characterizations of process functions and demonstrate how to construct non-causal process functions from unambiguous QNLWE product bases and vice versa.

QI 12.4 Wed 15:45 BEY/0137

Generalised Quantum Dynamics under Operational Constraints — •Joel Huber and Matthias Kleinmann — Universität Siegen

Generalised phase space theories can be considered to study potential deviations from quantum time evolution given by the Schrödinger equation. In the phase space formulation, quantum dynamics is governed by the Moyal bracket. We consider generalisations thereof and impose operational conditions – such as probability positivity – to characterise consistent dynamics. We show how (generalised) quantum dynamics impacts the momentum and position distributions in the presence of a cubic potential, and argue that this effect is experimentally accessible. The consistency of a proposed evolution depends critically on both the bracket structure and the underlying state space. We analyse scenarios where the state space contains Gaussian states or the first excited state of the harmonic oscillator. In the case of ideal preparation of these states, phase space dynamics is strongly constrained and quantum dynamics is found to be the only consistent time-reversible evolution, at least to the order that can be probed in a cubic potential.

QI 12.5 Wed 16:00 BEY/0137

Phase space tableau simulation for quantum computation — •Selman Ipek[1], Cihan Okay[2], Atak Talay Yücel[3], Cagdas Ozdemir[4], and Farzad Shahi[2] — [1]Institut Für Theoretische Physik, Leibniz Universität Hannover — [2]Department of Mathematics, Bilkent University — [3]Department of Computer Engineering, Bilkent University — [4]Department of Physics, Bilkent University

We introduce a novel tableau-based classical simulation method for quantum computation, formulated within the phase space framework of the extended stabilizer theory of closed non-contextual operators. This method enables the efficient classical simulation of a broader class of quantum circuits beyond the stabilizer formalism. We implement the simulator and benchmark its performance on basic quantum algorithms, including the hidden shift and Deutsch-Jozsa algorithms.

QI 12.6 Wed 16:15 BEY/0137

Witnessing nonstabilizerness with Bell inequalities — Rafael Macêdo[1,2], •Patrick Andriolo[2,3,4], Santiago Zamora[1,2], Davide Poderini[2,5], and Rafael Chaves[2,6] — [1]Departamento de Física Teórica e Experimental, Universidade Federal do Rio Grande do Norte, 59078-970 Natal-RN, Brazil — [2]International Institute of Physics, Federal University of Rio Grande do Norte, 59078-970, Natal, Brazil — [3]Physics Institute, University of São Paulo, Rua do Matão, 1371, São Paulo, Brazil — [4]Atominstitut, Technische Universität Wien, Stadionallee 2, 1020 Vienna, Austria — [5]Università degli Studi di Pavia, Dipartimento di Fisica, QUIT Group, via Bassi 6, 27100 Pavia, Italy — [6]School of Science and Technology, Federal University of Rio Grande do Norte, 59078-970 Natal, Brazil

Non-stabilizerness is a fundamental resource for quantum computation, enabling quantum algorithms to surpass classical capabilities. Despite its importance, characterizing this resource remains challenging due to the intricate geometry of stabilizer polytopes and the difficulty of simulating non-stabilizer states. In this work, through device-independent considerations, we reveal an unexpected connection between non-stabilizerness and Bell inequalities. Although certain stabilizer states can already achieve maximal violations of specific Bell inequalities, we demonstrate that appropriately constructed Bell inequalities can nevertheless serve as witnesses of non-stabilizerness, revealing when a state

lies beyond the stabilizer set. This uncovers a novel relationship between the device-independent framework and quantum computation. Phys. Rev. A 112, L050401.

30min. break

QI 12.7 Wed 17:00 BEY/0137

Beyond Mermin: Multipartite Bell Inequalities with Many Measurement Settings — •Fynn Otto[1], Junxiang Huang[2], Carlos de Gois[1,3,4], Xiao Yuan[2], and Otfried Gühne[1] — [1]Universität Siegen, Siegen, Germany — [2]Peking University, Beijing, China — [3]Inria de Saclay, Palaiseau, France — [4]École polytechnique, Palaiseau, France

Nonlocal correlations in multipartite quantum systems are typically probed through Bell inequalities with only a few measurement settings, limiting the sensitivity of existing tests. Here we introduce a generalization of the Mermin inequality to an arbitrarily large number of measurement settings per party. This family of inequalities is maximally violated by Greenberger-Horne-Zeilinger states and substantially lowers the noise thresholds required to certify nonlocality and nonlocality depth. We further derive Bell inequalities capable of detecting genuine multipartite entanglement in broad classes of graph states. Finally, we discuss prospects for experimental implementations of these inequalities in state-of-the-art quantum platforms. Together, these advances expand the toolbox for probing the structure of quantum correlations and strengthen practical routes toward certifying entanglement in complex quantum systems.

QI 12.8 Wed 17:15 BEY/0137

A Causal-Modelling Reconstruction of Quantum Mechanics That Comes With its Own Interpretation — •Joppe Widstam — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

We reconstruct quantum mechanics from intuitive causal-modelling principles for time-symmetric physics. In this reconstruction, the quantum state is a mere convenient mathematical object for agents able to control the initial conditions and who are able to choose what observable to measure.

QI 12.9 Wed 17:30 BEY/0137

The Quantum Rashomon Effect: A Strengthened Frauchiger-Renner Argument — •Jochen Szangolies — Deutsches Zentrum für Luft- und Raumfahrt, Köln

The Frauchiger-Renner argument aims to show that 'quantum theory cannot consistently describe the use of itself': in many-party settings where agents are themselves subject to quantum experiments, agents may make predictions that contradict observations. Here, we introduce a simplified setting using only three agents, that is independent of the initial quantum state, thus eliminating in particular any need for entanglement, and furthermore does not need to invoke any final measurement and resulting collapse. Nevertheless, the predictions and observations made by the agents cannot be integrated into a single, consistent account. We propose that the existence of this sort of Rashomon effect, i.e. the impossibility of uniting different perspectives, is due to failing to account for the limits put on the information available about any given system as encapsulated in the notion of an epistemic horizon.

QI 12.10 Wed 17:45 BEY/0137

Multiple solutions of the classical shooting problem: consistent histories and decoherence — •Julian Rettenberger-Zweck and Juan-Diego Urbina — Institut für theoretische Physik, Universität Regensburg, Regensburg, Germany

The *consistent histories* approach to quantum mechanics [1] provides a framework for defining whether a sequence of events occurring at different times—a *history*—exhibits emergent classical behavior. Specifically, a set of histories is called consistent if the off-diagonal elements of the decoherence functional, which quantify the interference between histories, vanish in an appropriate limit, leaving only the (properly normalized) classical probabilities on the diagonal [2]. The semiclassical (Van Vleck–Gutzwiller) propagator [3] consists of a coherent sum over all classical paths—or, in the language of consistent histories, all classical histories satisfying the specified boundary conditions—which enables a direct calculation of the decoherence functional. In this way, we explicitly evaluate the decoherence functional for two simple systems: the particle on a circle and the particle in a box, confirming the suppression of interference between distinct classical histories as well as the effect of decoherence within a Caldeira–Leggett approach [4].

[1] R. B. Griffiths, *J. Stat. Phys.* 36, 219 (1984).
[2] H. F. Dowker and J. J. Halliwell, *Phys. Rev. D* 46, 1580 (1992).
[3] M. C. Gutzwiller, *Chaos in Classical and Quantum Mechanics*, Springer, New York (1990).
[4] A. O. Caldeira and A. J. Leggett, *Physica A* 121, 587 (1983).

QI 13: Quantum Control

Time: Wednesday 15:00–18:00 Location: BEY/0245

QI 13.1 Wed 15:00 BEY/0245

A Statistical-Physics Approach to Quantum Control Landscape Exploration — •Malte Krug and Jürgen Stockburger — Institute for Complex Quantum Systems, Ulm, Germany

Conventional approaches to quantum optimal control rely on local optimizers that return a single high-fidelity pulse but offer little insight into the global structure of the cost landscape. A new method is presented, motivated by a statistical-physics inspired approach to stochastic control theory [1], that maps the quantum optimal control problem to an exploration of a high-dimensional landscape using ideas from protein-folding methods [2]. Instead of a single pulse, the method generates a distribution of control trajectories, represented by a Markov chain whose stationary distribution reflects the dominant regions of the cost landscape. This ensemble captures globally competitive pulses, reveals the diversity of near-optimal solutions, and allows for characterization of the local landscape through soft and stiff directions around optimal pulses. Moreover, the sampled trajectories provide high-quality initial guesses for conventional optimization methods, strongly biased toward the most promising regions of the landscape.

[1] Kappen, H. J.,*Phys. Rev. Lett.* 95, 200201 (2005).
[2] Trebst, S. & Troyer, M., in: *Computer Simulations in Condensed Matter Systems*, eds. Ferrario, M., Ciccotti, G. & Binder, K., Springer (2006).

QI 13.2 Wed 15:15 BEY/0245

Closed-Loop Control with Tailored Benchmarking Protocols — •Matthias Müller — Forschungszentrum Jülich

Quantum technology is a fast-emerging field with both scientific and technological importance. The performance relies on unique features like superposition and entanglement and depends on sophisticated mechanisms of control to perform the desired tasks. Quantum Optimal Control (QOC) has proven to be a powerful tool to accomplish this task. I will give a brief overview on the CRAB algorithm for QOC [1] and the optimal-control software QuOCS [2], and then talk about recent work on closed-loop control [3,4,5] for one- and two-qubit gates.

[1] M. M. Müller et al., Rep. Prog. Phys. 85 076001 (2022) [2] M. Rossignolo et al. Comp. Phys. Comm. 291, 108782 (2023) [3] N. Oshnik et al., Phys. Rev. A 106, 013107 (2022) [4] P. Vetter et al., npj Quantum Information 10 (1), 96 (2024) [5] A. Marcomini et al., in preparation (2025)

QI 13.3 Wed 15:30 BEY/0245

Efficient pulse-sequence optimization method for quantum control under realistic hardware constraints — Marco Dall'Ara[1,2], Florentin Reiter[1], Thomas Wellens[1], Martin Koppenhöfer[1], and •Walter Hahn[1] — [1]Fraunhofer Institute for Applied Solid State Physics IAF, Freiburg, Germany — [2]Dipartimento di Fisica e Astronomia G. Galilei & Padua Quantum Technologies Research Center, Università degli Studi di Padova, Padova, Italy

We propose a simple yet efficient pulse-sequence optimization method for controlling quantum systems. The ansatz leads to an efficient exploration of the unitary space without over-parameterization, even when the pulse amplitudes are restricted to a few discrete values suitable for quantum devices. Bandwidth and power limitations of experimental settings can be straightforwardly included with only minor computational overhead. We numerically validate the method by applying it to (i) unitary synthesis of a three-qubit gate and (ii) ground-state preparation on a globally-driven Rydberg-atom platform, and (iii) state transfer in an Ising spin chain. For all problems considered, our method approaches an information-theoretic lower bound on the number of parameters and exhibits advantages when compared to commonly used quantum control algorithms.

QI 13.4 Wed 15:45 BEY/0245

Optimal Control for Open Quantum System in Circuit Quantum Electrodynamics — •Francisco Cardenas-Lopez[1] and Xi Chen[2] — [1]Forschungszentrum Jülich GmbH, Peter Grünberg Institute, Quantum Control (PGI-8), 52425 Jülich, Germany — [2]Instituto de Ciencia de Materiales de Madrid (CSIC), Cantoblanco, E-28049 Madrid, Spain

We propose a quantum optimal control framework based on the Pontryagin Maximum Principle to design energy- and time-efficient pulses for open quantum systems. By formulating the Langevin equation of a dissipative LC circuit as

a linear control problem, we derive optimized pulses with exponential scaling in energy cost, outperforming conventional shortcut-to-adiabaticity methods such as counter-diabatic driving. When applied to a resonator dispersively coupled to a qubit, these optimized pulses achieve an excellent signal-to-noise ratio comparable to longitudinal coupling schemes across varying critical photon numbers. Our results provide a significant step toward efficient control in dissipative open systems and improved qubit readout in circuit quantum electrodynamics.

QI 13.5 Wed 16:00 BEY/0245

Learning to Steer Quantum Mmany-Body Dynamics with Tree Optimization — Jixing Zhang[1], Bo Peng[2], Yang Wang[1], •Cheuk Kit Cheung[1], Guodong Bian[3], Andrew Edmonds[4], Matthew Markham[4], Zhe Zhao[2], Durga Dasari[1], Ruoming Peng[1], Ye Wei[2], and Jörg Wrachtrup[1] — [1]3rd Institute of Physics, University of Stuttgart, Allmandring 13, Stuttgart, 70569, Germany — [2]Department of Data Science, City University of Hong Kong, Hong Kong, China — [3]School of Chemistry, University of Birmingham, B15 2TT, Edgbaston Birmingham, UK — [4]Element Six Global Innovation Centre, Fermi Avenue, Harwell Oxford, Didcot, Oxfordshire OX11 0QR, United Kingdom

Achieving practical quantum technologies requires high-quality control over complex quantum systems, but progress is hindered by exponentially growing state spaces and experimental challenges. We present an AI framework that learns to design optimized pulse sequences for many-body spin control, offering a powerful alternative to conventional theory-driven methods. The framework combines tree search, neural network filtering, and numerical simulation guidance to navigate highly nonlinear optimization landscapes using minimal resources. It identifies high-performing, non-intuitive sequences that established methods struggle to find. Experiments in a diamond spin ensemble show the best AI-designed sequences achieved spin coherence times exceeding 200 microseconds, a 100% improvement over state-of-the-art baselines. This work highlights AI's potential to steer complex many-body dynamics, marking a decisive shift toward data-driven sequence design.

QI 13.6 Wed 16:15 BEY/0245

Efficient analytical gradient evaluation for locally-interacting large multi-qubit platforms — •Alessandro Ciani[1], Ashutosh Mishra[1,2], Elena Lupo[1], and Frank Wilhelm-Mauch[1,2] — [1]Forschungszentrum Jülich, Jülich, Germany — [2]Universität des Saarlandes, Saarbrücken, Germany

We present a general framework for the computation of derivatives of time-ordered propagators in quantum optimal control, for both closed and open quantum systems, with respect to any general pulse parameterization, by deriving the formal solution from first principles. We obtain a series expansion for the gradients of the propagator, and utilize locality constraints to efficiently compute the derivatives. Further, we demonstrate that such a method can be used to efficiently compute gradients in large multi-qubit platforms, without running necessarily into the problem of storing the whole quantum state, whose size grows exponentially with the number of qubits. Our approach, can be viewed in terms of the recently introduced Pauli propagation framework applied to the computation of gradients in optimal control tasks. Finally, we show that our method is capable of accurately estimating the gradients, with much reduced memory and runtime compared to direct numerical evaluation.

30min. break

QI 13.7 Wed 17:00 BEY/0245

Analytical flux-tuned iSWAP pulse suppressing leakage channels — •Dimitrios Georgiadis[1,2], Boxi Li[1], Francisco Cardenas Lopez[1], and Felix Motzoi[1,2] — [1]Forschungszentrum Jülich GmbH, Peter Grünberg Institute, Quantum Control (PGI-8), 52425 Jülich, Germany — [2]Institute for Theoretical Physics, University of Cologne, Zülpicher Straße 77, 50937 Cologne, Germany

Achieving fast, high-fidelity qubit gates remains one of the major challenges in quantum computing, and despite recent progress, enhancing the efficiency of superconducting two-qubit gates still presents complications. In this work we investigate optimal control methods in order to improve the fidelity of two qubit gates in a flux tunable architecture based on a tunable coupler. We emphasize the importance of suppression of various leakage channels and we demonstrate simulations with analytical optimal control methods, (DRAG) and (DRAG-like), on the external flux on the tunable coupler, achieving further improved fidelities for an iSWAP gate. Finally, we propose a generalized pulse-shaping approach for the external flux, leading to significant leakage suppression across different circuit parameters.

QI 13.8 Wed 17:15 BEY/0245

Autonomous reachability of quantum states on random graphs — •Konrad Szymański[1], Tomasz Andrzejewski[2], Yuri Minoguchi[2], and Phila Rembold[2] — [1]Research Center for Quantum Information, Bratislava, Slovakia — [2]Atominstitut, TU Wien, Vienna, Austria

We study a particle hopping on a graph under a Hamiltonian with fixed but tunable couplings (no time-dependent control). We ask: which states can be reached from a given initially localized state via such autonomous dynamics? The Hamiltonian is a linear combination of generators corresponding to graph edges, with weights chosen freely but held constant during evolution. We develop three criteria to determine whether a given state is reachable from another. The first is analytical: if a certain matrix constructed from expectation values of the two states is strictly positive definite, the target state is certified unreachable from the initial one. The remaining two rely on numerical optimization over overlaps in the Hamiltonian eigenspaces and Krylov subspace structure. Applying these tools to random graph ensembles, we characterize how the fraction of Haar-random pure states that are unreachable from a localized initial state depends on graph connectivity.

QI 13.9 Wed 17:30 BEY/0245

Coherent control in V-type system: Simulation insights using intense two-dimensional coherent spectroscopy — •Rishabh Tripathi, Krishna Maurya, and Rohan Singh — Indian Institute of Science Education and Research (IISER) Bhopal, Bhopal, India

Our study investigates coherent control in V-type three-level systems using high-intensity, ultrafast laser pulses, explored through two-dimensional coherent spectroscopy (2DCS). Employing numerical solutions of the optical Bloch equations, we analyze the response of a V-type system to Gaussian pulses of 10 fs and 120 fs. The research reveals that shorter pulses induce uniform Rabi oscillations, whereas longer pulses result in complex quantum interference and state-specific population dynamics. This distinction underscores the pivotal role of pulse duration and spectral properties in modulating quantum interactions. Our 2DCS simulations, utilizing phase-cycling methods, provide insight into the system's spectral response in both perturbative and non-perturbative regimes. These simulations reveal the manipulation of spectral peak amplitudes and phases by adjusting the pulse areas, demonstrating control over the system.

This work contributes to the understanding of light-matter interactions in quantum systems and highlights the potential of tailored laser pulses for advanced coherent control, with implications for atomic vapors, semiconductor nanostructures, and photonics research.

QI 13.10 Wed 17:45 BEY/0245

Applications of dynamical decoupling to qubit noise suppression — •Chun Kit Dennis Law[1], Francisco Andrés Cárdenas-López[2], and Felix Motzoi[3] — [1]Peter Grünberg Institute, Forschungszentrum Jülich, Institute of Quantum Control (PGI-8), D-52425 Jülich, Germany — [2]Peter Grünberg Institute, Forschungszentrum Jülich, Institute of Quantum Control (PGI-8), D-52425 Jülich, Germany — [3]Peter Grünberg Institute, Forschungszentrum Jülich, Institute of Quantum Control (PGI-8), D-52425 Jülich, Germany

Noises are one of the major sources of the high error rates in the operation of modern quantum devices. Dynamical decoupling are some of the earliest experimentally demonstrated and least resource-intensive methods to suppress errors. We construct a many-level quantum system and isolate the lowest two energy levels for information processing. Upon the introduction of noise, we investigate how effective the XY4 sequence is by studying the associated leakage and the fidelity concerning the lowest two energy levels. Time permitting, we also investigate the effects of modifying the pulse shape by DRAG (derivative removal by adiabatic gate), which has been successfully applied to superconducting qubits to reduce leakage and phase errors.

QI 14: Quantum Information Poster Session

Time: Wednesday 18:00–21:00 Location: P4

QI 14.1 Wed 18:00 P4

An Efficient Error Correction Protocol Variant for Field Tests of Continuous-Variable Quantum Key Distribution — Lukas Eisemann[1,2], •Stefan Richter[1,2], Hüseyin Vural[1,2], Ömer Bayraktar[1,2], Kevin Jaksch[1,2], and Christoph Marquardt[1,2] — [1]Chair of Optical Quantum Technologies, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7 / A3, Erlangen — [2]Max Planck Institute for the Science of Light, Staudtstr. 2, Erlangen

Continuous-variable quantum key distribution (CV-QKD) requires near-optimally efficient information reconciliation (IR) to achieve high secret key rates (SKR) and transmission distances. Here, we present a novel and improved variant of a recently introduced IR-protocol, which is based on multiple decoding attempts (MDA). We evaluate our method on simulated data sets and employ it in the IR step for our fiber-based discrete-modulated CV-QKD system, which we deployed during a large-scale public technology demonstration in Berlin. In

each instance, we observe meaningful key rate improvements over both the ubiquitous single decoding attempt protocol and the original MDA implementation, even at a fixed decoding complexity. We also discuss some of the practical challenges associated with CV-QKD deployments in real networks outside of a lab context, arguing that the adaptability of our method makes it well-suited to solve them, providing implementation benefits in the process.

QI 14.2 Wed 18:00 P4

Entanglement with a mode observable via a tunable interaction with a qubit — •Malgorzata Strzalka[1,2], Radim Filip[3], and Katarzyna Roszak[1] — [1]FZU - Institute of Physics of the Czech Academy of Sciences,. — [2]Faculty of Mathematics and Physics, Charles University. — [3]Department of Optics, Palacký University.

We propose a qubit-environment entanglement (QEE) detection scheme for time dependent pure dephasing Hamiltonians. We study the entanglement for a transmon qubit interacting with an environment of microwave cavity photons. The QEE detection schemes that were previously developed for interactions that lead to pure decoherence of the qubit are based on measurements and operations performed only on the qubit alone [1]. Yet they could not be used in the studied scenario because of inherent symmetries in the Hamiltonian. We show that it is possible to override this problem by using different Hamiltonias in the preparation and the measurement stage. We take advantage of the possibility of tuning of the qubit-environment coupling to detect entanglement. Qubit-oscillator entanglement is seen to play a essential role in developing bosonic quantum technology. We previously studied the evolution of QEE for the same system [2] and now we present how the developed detection scheme can signify this type of entanglement. The scheme can be also used for other systems, where the decoherence is predominantly pure dephasing.

[1] M. Strzalka and K. Roszak, Phys. Rev. A 104, 042411 (2021).

[2] M. Strzalka et al. Phys. Rev. A 109, 032412 (2024).

QI 14.3 Wed 18:00 P4

Non-perturbative approach to entanglement harvesting — •Fabian Ganzer, Mei Yu, and Walter Strunz — Institute for Theoretical Physics, TU Dresden

It has been shown that two localized quantum systems like qubits or atoms can harvest entanglement from a quantum vacuum field through local interactions [1]. This phenomenon is often interpreted as a buildup of quantum correlations that can be established faster than with the speed of light due to a vacuum field. To date, however, most investigations have relied on perturbative approaches, leaving the genuine non-perturbative dynamics largely unexplored. In this work, we study entanglement harvesting using the non-perturbative numerical uniTEMPO method [2], enabling us to access both the weak- and strong-coupling regimes. Our results demonstrate that reliable statements about entanglement harvesting require both, a non-perturbative method and a careful analysis of correlations, particularly quantum correlations.

[1] C. Sabín, J. J. García-Ripoll, E. Solano, and J. León, Dynamics of entanglement via propagating microwave photons, Phys. Rev. B 81, 184501 (2010)

[2] V. Link, H.-H. Tu and W. T. Strunz, Open quantum system dynamics from infinite tensor network contraction, Phys. Rev. Lett. 132, 200403 (2024)

QI 14.4 Wed 18:00 P4

Simulating and Utilizing Dissipative Non-Equilibrium Physics on NISQ Devices — •Rochus Lechler[1], Pascal Stadler[2], Jan Reiner[2], Dominik Maile[1], Michael Marthaler[2], and Joachim Ankerhold[1] — [1]Institute for Complex Quantum Systems, Ulm University, Ulm — [2]HQS Quantum Simulations GmbH, Karlsruhe

Driven dissipative quantum many-body systems hold a variety of interesting phenomena like dissipative quantum phase transitions and non-equilibrium steady states. Typically, the full theoretical understanding of these phenomena is hindered by complex dynamics in large Hilbert spaces. Within this context, quantum simulation is a promising alternative bridging the gap between theory and experiment. Our project aims at finding efficient ways to simulate dissipative and driven many-body systems on NISQ devices. To this end, we make use of a software package provided by HQS Quantum Simulations capable of simulating complex open quantum systems. The key idea of this approach is to view quantum hardware itself as being a driven dissipative many-body system. More specifically, we utilize the noise on the hardware to engineer the required decoherence processes for the system under study. Building up on recent theoretical advances we show how to reduce the resources needed for these simulations.

QI 14.5 Wed 18:00 P4

Entanglement generation in quantum networks driven by multi-mode squeezed radiation — •Miguel Angel Palomo Marcos[1,2], Franz Pöschl[1,2], and Peter Rabl[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, D-85748 Garching, Germany — [2]School of Natural Sciences, Technische Universität München, D-85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology, D-80799 Munich, Germany

The development of scalable and efficient entanglement generation schemes is of central importance for the practical realization of quantum computing. Conventional approaches suffer from cumulative gate errors and decoherence, which have motivated the search for more scalable and robust protocols. Here we propose and analyze a quantum network, where a set of distant qubits is illuminated by multi-mode squeezed radiation. The dissipative dynamics drives the system into a stationary entangled state. We discuss different phase space techniques to numerically simulate this system for a large number of qubits and photonic modes and characterize the resulting entanglement generation properties for different parameter regimes.

QI 14.6 Wed 18:00 P4

Non-Markovian bound-state formation in a giant atom with two coupling points — •Mei Yu[1], Stefan Nimmrichter[2], and Walter Strunz[1] — [1]TUD Dresden University of Technology, — [2]University of Siegen

Superconducting qubits coupled to meandering transmission lines or to surface acoustic waveguides can realize giant artificial atoms, whose interaction with the waveguide occurs at multiple, spatially separated coupling points. Such a geometry introduces well-controlled propagation delays between the coupling points and thereby enables strongly non-Markovian dynamics with memory effects beyond the atomic lifetime [1, 2]. In this work, we investigate the relaxation dynamics of a single giant atom coupled to a one-dimensional acoustic waveguide through two coupling points in the strong-coupling regime. We show that interference between the delayed feedback channels leads to the formation of a bound state embedded in the continuum of waveguide modes, which in turn results in partial population trapping within the giant atom.

[1] L. Guo, A. Grimsmo, A. F. Kockum, M. Pletyukhov, and G. Johansson, Giant acoustic atom: A single quantum system with a deterministic time delay, Phys. Rev. A 95, 053821 (2017).

[2] G. Andersson, B. Suri, L. Guo, T. Aref, and P. Delsing, Non-exponential decay of a giant artificial atom, Nature Physics 15, 1123 (2019).

QI 14.7 Wed 18:00 P4

Entanglement distillation of microwave entangled states — •Ivan Solomakhin[1,2], Simon Gandorfer[1,2], Maria-Teresa Handschuh[1,2], Jasmine Frijters[1,2], Wun Kwan Yam[1,2], Achim Marx[1,2], and Kirill G. Fedorov[1,2,3] — [1]Walther-Meißner- Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]School of Natural Sciences, Technische Universität München, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany

Quantum entanglement is a crucial resource in continuous-variable quantum protocols, such as quantum teleportation and quantum key distribution. However, as the communication distance and complexity increase, losses due to unavoidable imperfections along the signal path lead to the degradation of shared entanglement and diminish the protocol performance. This challenge motivates the development and optimization of entanglement distillation strategies. Here, we investigate experimental implementations of entanglement distillation based on photon-subtraction techniques in application to two-mode squeezed, path-entangled microwave states. We employ superconducting Josephson amplifiers for the generation of two-mode squeezed states. Photon subtraction is realized by using a single-photon microwave detector composed of a transmon qubit in a multimode cavity. We analyze the resulting improvement in entanglement and discuss its implications for quantum communication and quantum networks in the microwave regime.

QI 14.8 Wed 18:00 P4

Noise mitigation in microwave quantum key distribution using single-photon detection — •Jasmine Frijters[1,2], Ivan Solomakhin[1,2], Simon Gandorfer[1,2], Wun Kwan Yam[1,2], Maria-Teresa Handschuh[1,2], Achim Marx[1], and Kirill G. Fedorov[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology (MCQST), 80799 Munich, Germany

Quantum key distribution (QKD) is a cryptographic protocol that allows for the unconditionally secure exchange of secret keys between two parties. While QKD implementations in the optical domain are rapidly developing toward practical applications, we analyse a continuous-variable microwave QKD protocol that utilizes single-photon detection to increase the secure transmission distance in both direct and reverse reconciliation schemes. In view of current experimental capabilities for microwave QKD, we predict an increase of up to 80% in secure transmission distance and estimate a key distribution of more than 300 m.

QI 14.9 Wed 18:00 P4

Bounds on quantum conference key agreement in networks with bipartite links — •Justus Neumann, Anton Trushechkin, Hermann Kampermann, and Dagmar Bruss — Heinrich Heine Universität Düsseldorf

Quantum conference key agreement allows several users to establish a shared secret key. A common approach is to use multipartite entangled states like Greenberger-Horne-Zeilinger states, but these are difficult to create in real networks. We instead consider a more practical setting where only two-party entan-

gled states are available between network nodes, and users can only perform local measurements followed by classical communication, without quantum memory. We study the general conference key agreement problem and derive a fundamental upper bound on the achievable key rate. We prove that, in any network composed only of bipartite sources, one cannot outperform a simple strategy: perform ordinary two-party quantum key distribution between one user and each of the others, and then merge the pairwise keys into a common conference key. This shows that complex multipartite strategies offer no rate advantage in such networks.

QI 14.10 Wed 18:00 P4

Entanglement of Electron and Nuclear Spins in Diamond — •Magnus J. R. Platena, Marius M. Strassner, Tim C. Duka, and Martin S. Brandt — Walter Schottky Institut, TU München, Am Coulombwall 4, 85748 Garching

Entanglement is one of the most surprising and counterintuitive phenomena of quantum physics. Nitrogen-vacancy (NV) centers in diamond provide a platform for studying this phenomenon at room temperature, a unique advantage of this solid-state system. The goal of this work is to demonstrate and quantify the entanglement of electron spins and ^{15}N nuclear spins in ensembles of NV centers via optically detected magnetic resonance. In a first step, we characterize isotopically engineered diamonds as a function of ^{15}N concentration, electron irradiation, and annealing and reproduce the published dependence of T_2 and T_2^* on nitrogen concentration. With the help of electron nuclear double resonance, we entangle the two spins and quantify the entanglement via quantum state tomography and application of the Peres criterion.

QI 14.11 Wed 18:00 P4

Differential magnetometry with partially flipped Dicke states — •Iagoba Apellaniz[1,2], Manuel Gessner[3], and Géza Tóth[1,2,4,5,6] — [1]Department of Theoretical Physics, University of the Basque Country UPV/EHU, P. O. Box 644, ES-48080 Bilbao, Spain — [2]EHU Quantum Center, University of the Basque Country UPV/EHU, P.O. Box 644, E-48080 Bilbao, Spain — [3]Departament de Física Teòrica, IFIC, Universitat de València, CSIC, Carrer del Dr. Moliner 50, 46100 Burjassot (València), Spain — [4]Donostia International Physics Center DIPC, Paseo Manuel de Lardizabal 4, San Sebastián, E-20018, Spain — [5]IKERBASQUE, Basque Foundation for Science, E-48009 Bilbao, Spain — [6]HUN-REN Wigner Research Centre for Physics, P.O. Box 49, H-1525 Budapest, Hungary

Dicke states on two ensembles can be sensitive to magnetic gradients by locally rotating the spins on one well. We determine bounds for the precision for gradient metrology in the three orthogonal directions as a function of the sensitivities of the homogenous field. The resulting partially flipped Dicke state saturates these bounds. Exploiting entanglement between the two ensembles, this state achieves roughly twice the precision attainable by the best bipartite separable state, which is a product of local Dicke states. For small ensembles, we explicitly identify measurement operators saturating the quantum Cramér-Rao bound, while for larger ensembles, we propose simpler schemes. The gradient is estimated from second moments of local angular momentum operators. Our results demonstrate how metrological properties of Dicke states can be exploited for quantum-enhanced estimation.

QI 14.12 Wed 18:00 P4

Calculation of Binding Energies for a Total of 25 Nuclei Between 2 and 12 nucleon Nuclei Using the Quantum Computer VQE Algorithm — •Taylan BAŞKAN and Ahmet Hakan YILMAZ — Faculty of Sciences, Department of Physics, Karadeniz Technical University, Trabzon, 61080 Turkey

In this study, the binding energies of the first 25 nuclear nuclei were calculated using a quantum computer simulator provided by IBM. These 25 nuclei include nuclei with a nucleon number of 12 and their isotopes, from hydrogen to oxygen. The VQE (variational quantum eigensolver) algorithm was used in the calculation process. The Hamiltonian designed for this purpose was designed to cover all nuclei. This developed a basic approach encompassing light nuclei and generated a model for estimating binding energies. The binding energies of the nuclei were obtained with an average deviation of 17% from known experimental values. For the VQE algorithm, a pre-written Hamiltonian was mapped to the quantum computer and determined by selecting ansatz and minimizing eigenvalues.

QI 14.13 Wed 18:00 P4

Quantum error mitigation on a bosonic quantum processing unit — •Corvin Lenz[1], Tanay Roy[2], Yao Lu[2], and Peter Orth[1] — [1]Theoretische Physik, Universität des Saarlandes, 66123 Saarbrücken, Germany — [2]Superconducting Quantum Materials and Systems Division, Fermi National Accelerator Laboratory, Batavia, IL 60510, USA

Bosonic processing units offer a scalable platform for continuous-variable quantum computation, but their interaction with noisy ancillary systems introduces significant errors that must be mitigated for reliable performance.

In this work, we simulate a bosonic qudit dispersively coupled to a two-level transmon, controlled via pulse-based external drives. Using process tomography on a synthesized, universal gate set, we characterize gate-dependent error channels arising from transmon-induced noise. We then apply probabilistic error cancellation (PEC) as an error mitigation technique, which reduces the impact of noise without relying on full fault-tolerant schemes.

Our results demonstrate a substantial improvement in individual gate performances, highlighting the effectiveness of PEC for error mitigation.

QI 14.14 Wed 18:00 P4

Efficient Spin-Adapted QPE Initial State Preparation — •Hampus Brunander[1,2] and Werner Dobrautz[1,2,3,4] — [1]Center for Advanced Systems Understanding, 02826 Görlitz, Germany — [2]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [3]Center for Scalable Data Analytics and Artificial Intelligence Dresden/Leipzig, 01069 Dresden, Germany — [4]Technical University Dresden, 01069 Dresden, Germany

The performance of quantum algorithms for strongly correlated electronic systems hinges on the overlap between the initial trial wavefunction and the ground state. However, a critical trade-off exists: the circuit cost of state preparation must not outweigh the algorithmic advantage. We address this by identifying regimes where problem-specific preparations yield high overlaps with minimal circuit depth. By adapting classical spin-group approaches, we utilize Localized Orbitals (LOs) to identify the optimal spin-coupling ordering. This chemically motivated approach constructs a dominant spin-adapted state that maximizes overlap while ensuring a compact, hardware-efficient implementation. We demonstrate that this strategy significantly improves fidelity for challenging systems, such as the stretched nitrogen dimer and iron-sulfur clusters.

QI 14.15 Wed 18:00 P4

Superconducting Digital-Analog Circuits for Quantum Approximate Optimization — •Siyu Wang and Mohammad H. Ansari — Forschungszentrum Juelich, 52425 Juelich, Germany

Digital-analog quantum algorithms such as the digital-analog Quantum Approximate Optimization Algorithm (DA-QAOA) offer a scalable approach to quantum optimization by combining digital gate-based control with native analog evolution. In this work, we aim to explore a quantum processor architecture that supports DA-QAOA using the multi-mode superconducting resonator as the analog interaction resource.

The structure leverages the finite-mode resonator to enable effective ZZ-type interactions between different pairs of qubits without requiring tunable couplers. Single-qubit gates are applied digitally via dedicated drive lines, enabling a clear separation between analog and digital layers. This approach naturally realizes qubit interactions, thus eliminating the need for SWAP operations that are typically required in digital only architectures with limited connectivity, thereby reducing the circuit depth. The goal is to identify a layout and interaction scheme that preserves the essential properties of DA-QAOA while remaining fabrication-friendly and scalable to larger systems.

Our findings provide a design framework for implementing variational quantum algorithms in NISQ hardware using fewer resources.

QI 14.16 Wed 18:00 P4

Mitigating Noise in Quantum-Classical Electronic Band Structure Calculations — •Vojtěch Vašina[1,2] and Martin Friák[1] — [1]Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic — [2]Brno University of Technology, Institute of Material Sciences and Engineering

Computational materials science is currently facing a significant scalability issue. Simulating large condensed matter systems requires immense computational resources because the computational complexity grows exponentially as the size of the system increases. Quantum computers are emerging as a possible solution to overcome this problem because they theoretically offer up to an exponential speedup for certain problems. Current Noisy Intermediate-Scale Quantum (NISQ) computers are too noisy to provide results that are sufficiently accurate so classical and quantum algorithms are combined into so-called quantum-classical hybrid algorithms to overcome high levels of noise. In our study, we focused on computing the electronic band structure of diamond as this problem is well known and can be accurately solved on classical computers allowing us to compare those results to results obtained from the Variational Quantum Deflation (VQD) algorithm. We specifically investigate different error suppression and error mitigation techniques because the fidelity of results sensitively depends on them. The quantum parts of the VQD algorithm were executed on real quantum computers provided by IBM.

QI 14.17 Wed 18:00 P4

Effects of geometry on the error threshold of the toric code — •Daniel Lessing, Calvin Kraemer, Jan Alexander Koziol, Anja Langheld, and Kai Phillip Schmidt — Department Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen, Germany

The Random-Bond Ising Model can serve as a theoretical model for determining the error threshold of the toric code. This threshold is the maximum physical error rate tolerable for fault-tolerant quantum computation. We employ Monte Carlo Integration combined with finite-size scaling to map the RBIM's

phase boundary for different temperatures and antiferromagnetic bond concentrations, which correspond to the different error rates in the toric code. The intersection of this phase boundary with the Nishimori line directly defines the critical error threshold for the toric code. Our investigation determines how this critical error threshold is influenced by varying the underlying geometry of the lattice.

QI 14.18 Wed 18:00 P4

Effect of Long-range Crosstalk Errors on the Surface Code — •Solomon Birhanu Samuel[1] and Janos Karoly Asboth[1,2,3] — [1]Department of Theoretical Physics, Institute of Physics, Budapest University of Technology and Economics, Muegyetem rkp. 3., H-1111 Budapest, Hungary — [2]HUN-REN Wigner Research Centre for Physics, H-1525 Budapest, P.O. Box 49., Hungary — [3]HUN-REN-BME-BCE Quantum Technology Research Group, Muegyetem rkp. 3., H-1111 Budapest, Hungary

Crosstalk errors (due to unintended interactions between qubits and coupling between different circuit elements) pose a challenge to quantum error correction. They are often assumed to only affect nearest or next-nearest neighbor qubits[1], but experiments on some superconducting quantum processors[2] show that they can occur between more distant qubits as well. In this work, we study the effect of longer-range crosstalk errors on the surface code using numerical models (Clifford simulation) with realistic parameters of superconducting chips. We use Pauli error models to simulate the effect of the crosstalk both on the threshold and the logical error rate below threshold.

[1] Zhou, Zeyuan, Andrew Ji, and Yongshan Ding. "Surface Code Error Correction with Crosstalk Noise." arXiv preprint arXiv:2503.04642 (2025).

[2] Kosen, Sandoko, et al. "Signal crosstalk in a flip-chip quantum processor." PRX Quantum 5.3 (2024): 030350.

QI 14.19 Wed 18:00 P4

Hybrid Quantum-Classical Walks with Applications to Machine Learning — •Adrián Marín Boyero[1], Daniel Manzano Diosdado[1], and Carlos Cano Gutiérrez[2] — [1]Department of Electromagnetism and Condensed Matter Physics, Avenida de la Fuente Nueva, 18071 Granada, University of Granada, Granada, Spain — [2]Institute Carlos I for Theoretical and Computational Physics, Avenida de la Fuente Nueva, 18071 Granada, University of Granada, Granada, Spain

Complex systems can often be described as networks, where nodes represent elements and edges represent interactions. Classical Random Walks (CRWs) are widely used for machine learning tasks on such structures. In this work, we introduce a Hybrid Quantum-Classical Walk (HQCW) model based on a modified Lindblad equation. This framework interpolates between quantum coherence and classical jumps through a parameter $\alpha \in [0, 1]$, generating node-visit trajectories whose statistics recover the Lindblad dynamics. The trajectories are generated with a Monte Carlo method known as Quantum Jumps, which reproduces the statistics of the underlying open system evolution. We use these trajectories for Graph Representation Learning and show that HQCWs break node ranking degeneracies, correctly recover communities, and separate node clusters in synthetic networks, even at low embedding dimension d. Performance peaks in a near-classical regime ($\alpha \approx 0.8$), capturing the global graph structure effectively. Our results highlight HQCWs as a scalable quantum-inspired tool for network analysis and machine learning.

QI 14.20 Wed 18:00 P4

GRAPE with feedback: the method and the Python package — •Pavlo Bilous[1] and Florian Marquardt[1,2] — [1]Max Planck Institute for the Science of Light, Staudtstr. 2, 91058 Erlangen, Germany — [2]Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany

Quantum control with feedback is an essential component of modern quantum technology applications. While open-loop control tasks are usually solved using gradient methods like GRadient Ascent Pulse Engineering (GRAPE), it was until recently not clear how feedback from measurements in the control process can be integrated in these methods. Here, we discuss the "Feedback GRAPE" method introduced recently in Ref. [1] where feedback is combined with GRAPE using machine learning techniques. Given the potential use of "Feedback GRAPE" for the community, we developed an efficient GPU-accelerated Python package implementing the approach. Here we discuss our codes and showcase them on three main closed-loop tasks: state preparation with feedback, state purification and state stabilization. Using the presented examples as the starting point, the users can conveniently apply our package for their problem at hand.

[1] R. Porotti, V. Peano, and F. Marquardt, PRX Quantum 4, 030305 (2023).

QI 14.21 Wed 18:00 P4

Characterization of spin-relaxation dynamics of rare earth ions in $CaWO_4$ — •Sebastian Dominguez-Calderon[1,2], Georg Mair[1,2], Arjun Bhasker[1,2], Robert Pant[1,2], Hans Huebl[1,2,3], and Nadezhda Kukharchyk[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, D-85748 Garching, Germany — [2]School of Natural Sciences, Technische Universität München, D-85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology, D-80799 Munich, Germany

Rare-earth spin ensembles doped into bulk crystals, such as $CaWO_4$, are promising candidates for quantum memory devices operating at microwave frequencies and compatible to superconducting quantum technologies. To further improve this technology, it is of pivotal importance to understand the mechanisms which affect information lifetimes. In the present work, we investigate spin interactions in ensembles of rare-earth (RE) ions in $CaWO_4$ via superconducting coplanar waveguides at millikelvin temperatures. Using spatially separated transmission lines, as well as pump-probe detection schemes, we aim to understand the ensemble's spin diffusion, suspected to be dominated by spin-spin as well as spin-phonon interactions. Characterization of the diffusion will give insights into different relaxation channels for RE:$CaWO_4$ that would aid the design of future quantum memory devices.

QI 14.22 Wed 18:00 P4

Qubit analogues in exciton-polariton condensates with optical manipulation — •Roman Lebs[1], Jan Wingenbach[1,2], Hendrik Rose[2], and Stefan Schumacher[1,2] — [1]Physics Department and CeOPP, Paderborn University, Germany — [2]PhoQS, Paderborn University, Germany

Exciton-polariton condensates provide a promising platform for quantum information processing, offering long coherence times, robust information storage and operation up to room temperature. Here we build upon earlier demonstrations of vortex-based information encoding (Ma et al., Nat. Commun. 11, 897, 2020), split ring qubit analogues (Xue et al., Phys. Rev. Research 3, 013099, 2021), and recent progress toward polaritonic qubit prototypes in annular traps (Barrat et al., Science Advances 10, eado4042, 2024), investigating a polariton condensate as a fully optically controllable qubit analogue. The condensate dynamics are modelled using the nonlinear Gross-Pitaevskii equation and numerically solved with PHOENIX, a highly optimized CUDA accelerated solver for two-dimensional nonlinear Schrödinger equations (Wingenbach et al., Comput. Phys. Commun. 315, 109689, 2025), which enables efficient and high-resolution simulations. We show that all points of the Bloch sphere can be reached by encoding the $|0\rangle$ and $|1\rangle$ states as localized spatial profiles with distinct phases. A simple pump geometry, combining a ring pump and a Gaussian pump applied on the ring, allows precise control of trajectories on the Bloch sphere. We also outline how this scheme can be extended toward coupled condensates in multi qubit architectures.

QI 14.23 Wed 18:00 P4

Si/SiGe interfaces for scalable qubit devices - a depth resolved HAXPES study — •Nathalie Niederbudde[1], Andreas Fuhrberg[1], Denny Dütz[2], Andrej Gloskovskii[3], Christoph Schlueter[3], Lars R. Schreiber[2], and Martina Müller[1] — [1]Universität Konstanz — [2]RWTH Aachen University — [3]DESY, Hamburg, Germany

An ongoing challenge in quantum physics research is optimizing the performance of silicon-based spin qubits. These devices use the intrinsic spin of electrons as logic states. The electron location is electrostatically controlled by biased gate pattern on top of the device. A common spin qubit platform compatible with industrial processes is based on SiGe/Si/SiGe heterostructures, where the electron is trapped in the strained Si layer. To achieve reliable control of the trapping potential, defects occurring mainly at the Si-capping layer and the amorphous gate-oxide must be explored, studied and minimized.

This study investigates an Al_2O_3/Si/SiGe-qubit structure using hard X-ray photoelectron spectroscopy (HAXPES) with synchrotron radiation of 2.8 & 6 keV at beamline P22, DESY. The influence of thermal annealing typical for device fabrication on the Si capping layer is analysed. Si oxide formation is observed independently of annealing, with a thicker oxide layer forming in the annealed sample and an additional shift in binding energies. Additional oxidation states are found close to the Si/Al_2O_3 interface. Although the entire Si layer is thought to be oxidized, no Ge oxide was detected. This study improves our understanding of the influence of qubit preparation processes.

QI 14.24 Wed 18:00 P4

Industrially fabricated and isotopically enriched Si/SiGe Quantum Dots for coherent spin qubit control — •Dominic Barthlott[1], Viktor Adam[1], Daniel Sitter[1], Daniel Schroller[1], Clement Godfrin[2], and Wolfgang Wernsdorfer[1] — [1]Physikalisches Institut (PHI), Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany — [2]Interuniversity Microelectronics Centre (imec), Leuven, Belgium

Spin qubits represent a promising quantum-computing platform due to their combination of long coherence times and compatibility with established, industry-supported semiconductor fabrication techniques. Enrichment with ^{28}Si isotopes can increase the coherence time of the qubit by reducing the amount of naturally occurring ^{29}Si which has a non-zero nuclear spin. Hence, we are investigating this effect by comparing enriched to non-enriched samples fabricated using industry-level processes. The devices consist of two quantum dots and one single-electron transistor (SET) which is used for charge sensing, thereby detecting electron tunnel events in the quantum dots. By adjusting the gate voltages,

the system can be tuned to its ground-state charge configuration, allowing individual electrons to be loaded into each quantum dot. After this initialization, two individual qubits are defined and can be coherently driven. Their performance is concluded by carrying out standard benchmark protocols, including T_1 relaxation measurements or Ramsey and Hahn-echo sequences for T_2 determination.

QI 14.25 Wed 18:00 P4

Induced quantum dot microscopy of germanium and graphene quantum devices — •Patrick Raif[1,2], Aurèle Kamber[1], Luca Forrer[1,2], Christian Olsen[1], Martino Poggio[1,2], Andrea Hofmann[1,2], and Floris Braakman[1,2] — [1]Department of Physics, Basel, Switzerland — [2]Swiss Nanoscience Institute, Basel, Switzerland

Quantum dots are fundamental building blocks for semiconductor-based qubits [1], which are a promising platform for quantum computation due to the high compatibility with currently existing manufacturing technology and the potential for scaling up. In recent years, planar Ge/SiGe heterostructures have been established as a leading material for such devices, in particular for the implementation of spin qubits [2].

However, even the highest quality qubit devices show significant variations of important parameters like coherence times, pinch-off voltages, tunnel barrier heights, Landé g-factors, spin-orbit lengths, and valley splittings. These variations represent a serious obstacle for scaling up as they necessitate tuning of the individual quantum dots.

To map out the spatial variations we will apply newly developed scanning probe microscopy techniques using cantilevers that are patterned with multiple gates via electron-beam lithography [3] by inducing quantum dots in a quantum well underneath the cantilever.

[1] G. Burkard, et al., *Rev. Mod. Phys.* **95**, 025003 (2023). [2] G. Scappucci, et al., *Nat. Rev. Mat.* **6**, 926-943 (2021). [3] L. Forrer, et al., *AIP Advances* **13**, 035208 (2023).

QI 14.26 Wed 18:00 P4

Exploration of exotic dielectric barrier materials for quantum computing — •Leqi Zhou[1], Thomas J. Smart[1], Christine Falter[1,2], Josua Thieme[1,2], Joscha Domnick[1], Benjamin Bennemann[1,2], Detlev Grützmacher[1], Peter Schüffelgen[1], and Alexander Pawlis[1,2] — [1]Peter Gruenberg Institute, Forschungszentrum Juelich GmbH, Juelich, Germany — [2]JARA-Fundamentals of Future Information Technology, Juelich-Aachen Research Alliance, Aachen, Germany

A majority of the modern research performed on superconducting quantum systems uses Al2O3 as the dielectric barrier material of interest. However, there has been renewed interest in alternatives to Al2O3 as a barrier material, due to the formation of two-level systems (TLSs) which can impede device performance. Within this work, we explore the deposition of alternative dielectric materials, such as AlN and TiO2. These films, grown via different epitaxy techniques are then electrically characterized to determine their resistive and capacitive properties. By optimizing the growth processes, based on these electrical measurements, we aim to implement these alternative dielectric materials into Josephson Junctions to test their suitability for future quantum computing systems.

QI 14.27 Wed 18:00 P4

Low-overhead Liouvillian Learning of Superconducting Qubit Arrays via Simultaneous Weak Measurements — •Markus Sifft, Armin Ghorbanietemad, and Daniel Hägele — Ruhr University Bochum, Faculty of Physics and Astronomy, Germany

Building on quantum polyspectra for higher-order noise analysis [1,2], we present a low-overhead protocol to reconstruct the Liouvillian of an open system from continuous weak multi-detector measurements of qubits. From a parameterized Liouvillian and measurement operators, we use closed-form expressions for multi-channel polyspectra up to fourth order, which compactly encode coherent dynamics and dissipation. Fitting theory to measured spectra allows us to extract key Hamiltonian and dissipative parameters of superconducting-qubit processors, including qubit frequencies, coherent couplings, crosstalk, drive leakage, and effective temperatures, even with background noise and in the ultra-weak measurement regime. A Fisher-information-based figure of merit quantifies identifiability and optimizes drive frequencies, amplitudes, measurement strengths, and operating temperature. The framework scales to many detectors and qubits, yields error bars and measurement-time estimates, and, compared to standard pulsed characterization, enables spectroscopy-style characterization from a single continuous experiment. All ingredients are implemented in our open-source QuantumCatch [3] and SignalSnap [4] libraries. [1] Hägele, Phys. Rev. B 98, 205143 (2018) [2] M. Sifft et al., arXiv:2505.01231 (2025) [3] github.com/markussifft/quantumcatch [4] github.com/ArminGEtemad/SignalSnap-PyTorch

QI 14.28 Wed 18:00 P4

Making entanglement witnesses robust to measurement errors — •Elisa Monchietti and Otfried Gühne — Naturwissenschaftlich-Technische Fakultät, Universität Siegen, Walter-Flex-Straße 3, 57068 Siegen, Germany

In recent years, a variety of methods have been developed to characterise quantum entanglement, among which entanglement witnesses are one of the most widely studied tools. A major limitation of these operators, however, is their high sensitivity to measurement imperfections, which can lead to false positives in the detection of entangled states. In realistic experimental scenarios, even with advanced error-mitigation techniques, measurement errors arising from device imperfections and external noise cannot be completely eliminated. In this work, we aim to characterise quantum correlations in a more realistic framework by explicitly accounting for imprecise measurements. To this end, we investigate correction terms that can be incorporated to compensate for the effects of measurement misalignment and device imperfections. In particular, we study the existence and construction of entanglement witnesses for multiqubit systems that remain robust against misalignment errors.

QI 15: Quantum Information: Concepts and Methods II

Time: Thursday 9:30–12:30 Location: BEY/0137

QI 15.1 Thu 9:30 BEY/0137

Quantum dynmics induced by Pauli strings — •Roberto Gargiulo[1,2] and Robert Zeier[1] — [1]Forschungszentrum Jülich GmbH, Peter Grünberg Institute, Quantum Control (PGI-8), 52425 Jülich, Germany — [2]University of Cologne, Institute for theoretical physics (THP), 50937 Cologne, Germany

General quantum dynamics in qubit systems are described by independently controlled Hamiltonians consisting of sums of Pauli strings (i.e. tensor products of Pauli operators). We consider the case where each independently controlled Hamiltonian is given by a single Pauli string. We provide a unified description of the resulting dynamics relying on inherent symmetries and generated Lie algebras. This allows us to describe dynamical properties in terms of simple invariants and to detail possible free-fermionic mappings. We expand and extend recent work [1-3] which enables us to re-interpret them in a general framework. Our description addresses various questions of controllability, computational power, and many-body properties, especially in the context of Heisenberg picture and operator subspaces.

[1] Chapman et al. Quantum 4, 278 (2020)
[2] Kökcü et al., arXiv:2409.19797
[3] Aguilar et al. arXiv:2408.00081

QI 15.2 Thu 9:45 BEY/0137

Robust certification of non-projective measurements — •Raphael Brinster[1], Peter Tirler[2], Shishir Khandelwal[3], Michael Meth[2], Hermann Kampermann[1], Dagmar Bruss[1], Rainer Blatt[2,4], Martin Ringbauer[2], Armin Tavakoli[3], and Nikolai Wyderka[1] — [1]Institut für Theoretische Physik III, Heinrich-Heine-Universität Düsseldorf — [2]Institut für Experimentalphysik, Universität Innsbruck — [3]Physics Department and NanoLund, Lund University, — [4]Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, Innsbruck

Determining the conditions under which the most general class of quantum measurements (positive operator-valued measures (POVMs)), outperform projective measurements remains a challenging and largely unresolved problem. Of particular interest are projectively simulable POVMs which offer no advantage over projective schemes, as they can be realized through probabilistic mixtures of projective measurements. Characterizing the boundary between simulable and non-simulable POVMs is, however, a difficult task, and existing tools either fail to scale efficiently, provide limited experimental feasibility or work only for specific POVMs. Here, we introduce a general method to certify non-simulability of a POVM by constructing non-simulability witnesses and demonstrate how to make them robust against state preparation errors in experiments.

QI 15.3 Thu 10:00 BEY/0137

Entanglement detection close to Dicke states with many-body correlations — •Géza Tóth[1,2,3,4], Martin Quensen[5,6], Mareike Hetzel[5,6], Luis Santos[5], Augusto Smerzi[7,8,9], Luca Pezzè[7,8,9], and Carsten Klempt[5,6] — [1]Theoretical Physics and EHU Quantum Center, University of the Basque Country UPV/EHU, 48080 Bilbao, Spain — [2]Donostia International Physics Center (DIPC), 20018 San Sebastián, Spain — [3]IKERBASQUE, Basque Foundation for Science, 48009 Bilbao, Spain — [4]HUN-REN Wigner Research Centre for Physics, 1525 Budapest, Hungary — [5]Institut für Quantenoptik, Leibniz Universität Hannover, 30167 Hannover, Germany — [6]Institut für Satellitengeodäsie und Inertialsensorik (DLR-SI), Deutsches Zentrum für Luft- und Raumfahrt e.V.

(DLR), 30167 Hannover, Germany — [7]Instituto Nazionale di Ottica, Consiglio Nazionale delle Ricerche (INO-CNR), 50125 Firenze, Italy — [8]European Laboratory for Nonlinear Spectroscopy (LENS), 50019 Sesto Fiorentino, Italy — [9]Quantum Science and Technologies in Arcetri (QSTAR), 50125 Firenze, Italy

We will review methods for detecting multipartite entanglement in an ensemble of spin-1/2 atoms with collective measurements. We will introduce entanglement criteria based on the measurement of many-body correlations, such as the parity. Interestingly, such criteria can detect a larger entanglement depth in some practical situations than previous methods. In an experimental application, our criteria require a single-particle resolution in measuring the particle number.

QI 15.4 Thu 10:15 BEY/0137

Higher-dimensional information lattice: Quantum state characterization through inclusion-exclusion local information — •Claudia Artiaco — Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

The information lattice provides a universal characterization of quantum many-body states through local information. Local information quantifies the total amount of correlations in a region on a given scale that cannot be found in any smaller subregion. This framework allows us to define the intrinsic correlation length scales of many-body states. Moreover, within the information lattice, the total information in a system becomes akin to a hydrodynamic quantity with well-defined local densities and local currents, which allow us to characterize quench dynamics and develop efficient approximate methods for the time evolution of large-scale many-body systems.

However, the original information lattice is strictly valid only for one-dimensional states, and its key properties, such as locality and the conservation of local information under unitary dynamics, do not easily extend to higher dimensions. In this talk, I will discuss these challenges and introduce a higher-dimensional generalization of the information lattice based on the inclusion-exclusion principle. I will show how this approach enables the characterization of two-dimensional states in different universality classes, including Anderson localized states, gapped states with critical boundaries, and ground states of the toric code in various geometries. I will further demonstrate how topological features can be interpreted in terms of inclusion-exclusion local information.

QI 15.5 Thu 10:30 BEY/0137

Remote quantum certification from prepare-measure correlations: theory and experiment — •Albert Rico[1], Javier Fernandez[2], Anna Sanpera[2], Some Sankar[2], and Adam Valles[2] — [1]University of Siegen — [2]Universitat Autonoma de Barcelona

For the practical implementation of quantum protocols, it is essencial to verify the presence of quantumness from classically observable data, under realistic assumptions. In a recent work, we demonstrated how this can be done in theory and experiment from the correlations between the inputs and outputs of a prepare-measure quantum setup, under the assumption that our quantum devices are limited in operational dimension and memory. Our contributions are: (1) we derive an inequality for the classical dimension needed to reproduce anti-correlated probability distributions; (2) we show that this inequality can be saturated, and this event displays quadratic quantum advantage with respect to classical siulation; (3) we prove that there is a unique strategy saturating the inequality, and thus find a method to self-test SIC-POVMs; (4) we engineer a certification protocol with low experimental error; and (5) we perform this method experimentally with orbital angular momentum with noise tolerance, thus certifying quantumness in practice. In this talk we will summarize the main ingredients of prepare-measure setup under consideration, sketch the results presented, and explain their implications in practical remote quantum certification for distant communication protocols.

QI 15.6 Thu 10:45 BEY/0137

Computable measures of fermionic non-Gaussianity — Poetri Sonya Tarabunga[1,2], Bernhard Jobst[1,2], Sheng-Hsuan Lin[3], Marc Langer[1,2], •Raúl Morral-Yepes[1,2], Barbara Kraus[1,2], and Frank Pollmann[1,2] — [1]Technical University of Munich, TUM School of Natural Sciences, Physics Department, 85748 Garching, Germany — [2]Munich Center for Quantum Science and Technology (MCQST), Schellingstr. 4, 80799 München, Germany — [3]Quantinuum, Leopoldstrasse 180, 80804 Munich, Germany

Quantum many-body states generally cannot be efficiently simulated on classical computers. However, certain classes of states with special structure admit efficient representations and simulations. Among these, fermionic Gaussian states are fully characterized by their two-point correlation functions. In this work, we investigate two measures of fermionic non-Gaussianity, which quantify how close a given state is to being Gaussian: the occupation number entropy, defined in terms of the eigenvalues of the correlation matrix, and the natural orbital Rényi entropy, given by the participation entropy in the basis that diagonalizes the correlation matrix. We present efficient methods to compute these quantities and analyze their connection to classical simulability and the complexity of state preparation. Additionally, we prove the monotonicity of these measures under specific conditions. Finally, we demonstrate their behavior in several models.

30min. break

Invited Talk QI 15.7 Thu 11:30 BEY/0137

Robust shadow tomography: from quantum simulation to high-energy physics — •Hai-Chau Nguyen — University of Siegen, Siegen, Germany

Starting with a brief introduction to shadow tomography, we show that it can be reformulated in terms of generalised measurements. On the one hand, this allows for taking into account the measurement errors in the implementation of shadow tomography in a canonical way. On the other hand, the symmetry of a shadow tomography protocol can be investigated in parallel with the symmetry of its associated generalised measurement, revealing its robustness against even complex measurement noise. We then show that measurement errors in shadow tomography can be efficiently mitigated even when they are correlated. This can be achieved by effectively symmetrising the shadow tomography protocol through simple controlled randomised (qu)bit flips, which provides a simple and robust protocol in comparison to those that are more demanding, such as protocols based on sampling Clifford gates. While the theory of shadow tomography and its technical developments were motivated by applications in quantum simulators, we emphasise its more general conceptual implications. In particular, we demonstrate a natural application of shadow tomography in the characterisation of relativistic spin-spin correlations of output particles in high-energy physics experiments. As a concrete example, we discuss how shadow tomography can shed light on conceptual aspects of the recent experiments demonstrating top-quark entanglement at ATLAS and CMS.

QI 15.8 Thu 12:00 BEY/0137

Detection of many-body entanglement partitions in a quantum computer — Albert Rico[1,2], Dmitry Grinko[3,4,5], •Robin Krebs[6], and Lin Htoo Zaw[7] — [1]Quantum information Group, Autonomous University of Barcleona, Spain — [2]Theoretische Quantenoptik, Universität Siegen, Germany — [3]QuSoft, Amsterdam, Netherlands — [4]Institute for Logic, Language and Computation, University of Amsterdam, Netherlands — [5]Korteweg-de Vries Institute for Mathematics, University of Amsterdam, Netherlands — [6]Quantum Computing, Technische Universität Darmstadt, Germany — [7]Centre for Quantum Technologies, National University of Singapore, Singapore

We present a method to detect entanglement partitions of multipartite quantum systems, by exploiting their inherent symmetries. Structures like genuinely multipartite entanglement, m-separability and entanglement depth are detected as special cases. This formulation enables us to characterize all the entanglement partitions of all three- and four-partite states and witnesses with unitary and permutation symmetry. In particular, we find and parametrize a complete set of bound entangled states therein. For larger systems, we provide a large family of analytical witnesses detecting many-body states of arbitrary size where none of the parties is separable from the rest. This method relies on weak Schur sampling with projective measurements, and thus can be implemented in a quantum computer. Beyond physics, our results apply to mathematics: we establish new inequalities between matrix immanants, and characterize the set of such inequalities for matrices of size three and four.

QI 15.9 Thu 12:15 BEY/0137

k-body correlations of graph states — •Mengying Hu[1,2], Elisa Monchietti[2], Ismaël Septembre[2], Kenneth Goodenough[2], Raphaël Mothe[2], and Otfried Gühne[2] — [1]School of Mathematical Sciences, Hebei Normal University, Shijiazhuang 050024, China — [2]Naturwissenschaftlich-Technische Fakultät, Universität Siegen, Germany

Graph states play a key role in quantum information processing tasks, for instance quantum computing and quantum error correction. Understanding their intrinsic structure is fundamental for assessing their usefulness in computational or informational tasks. In particular, graph states are stabilizer states, meaning they can be uniquely defined by the group of local Pauli operators stabilizing them. Here, we study the groups that arise after deleting certain subsets of qubits from the stabilizer group, which we use to capture the k-body correlations of graph states, and we use these correlations as invariants to distinguish graph states up to local unitaries.

QI 16: Quantum Software

Time: Thursday 9:30–12:45 Location: BEY/0245

Invited Talk QI 16.1 Thu 9:30 BEY/0245

Measurement-free universal fault-tolerant quantum computation — •Friederike Butt[1,2], Ivan Pogorelov[3], Alex Steiner[3], Marcel Meyer[3], Thomas Monz[3,4], Markus Müller[1,2], and Robert Freund[3] — [1]Institute for Theoretical Nanoelectronics (PGI-2), Forschungszentrum Jülich — [2]Institute for Quantum Information, RWTH Aachen University — [3]Universität Innsbruck, Institut für Experimentalphysik, Innsbruck — [4]Alpine Quantum Technologies GmbH, Innsbruck

The ability to perform quantum error correction (QEC) and robust gate operations on encoded qubits opens the door to demonstrations of quantum algorithms. Contemporary QEC schemes typically require mid-circuit measurements with feed-forward control, which are challenging for qubit control, often slow, and susceptible to relatively high error rates. I will present protocols and the experimental realization of a universal toolbox of fault-tolerant logical operations without mid-circuit measurements on a trapped-ion quantum processor. This includes modular logical state teleportation between two four-qubit error-detecting codes without measurements during algorithm execution, as well as a fault-tolerant universal gate set on an eight-qubit error-detecting code hosting three logical qubits, based on state injection, which can be executed by coherent gate operations only. This toolbox can then be used to realize Grover's quantum search algorithm fault-tolerantly on three logical qubits encoded in eight physical qubits, with the implementation displaying clear identification of the desired solution states.

QI 16.2 Thu 10:00 BEY/0245

A Framework for Spectator Error Mitigation in Surface-Code Hamiltonian Modeling — •Xuexin Xu[1], Mohammad H. Ansari[1], and John M. Martinis[2] — [1]PGI-2, Forschungszentrum Juelich, Juelich, 52428, Germany — [2]Qolab, Madison, Wisconsin, 53706, USA

Realistic surface-code architectures rely on precisely engineered single and two-qubit gates across large-scale quantum lattices. Yet subtle whispers from spectator qubits those surrounding but not directly involved in a target operation can disturb intended surface-code Hamiltonian and degrade logical fidelity. We analyze the origin and effects of spectator-induced errors in lattices and propose a mitigation scheme based on the inherent symmetry of spectator qubits. Through numerical simulations and perturbative analysis, we show that our method gently suppresses parasitic effects while boosting the performance of intended two-qubit gates. This approach offers a scalable and systematic path to enhance gate fidelity and tame crosstalk, bringing surface-code quantum processors closer to practical, reliable operation.

QI 16.3 Thu 10:15 BEY/0245

Handling Quantum Errors under Realistic Noise Models of Trapped Ion Quantum Devices — •Niko Trittschanke[1,2], Daniel Borcherding[2], and Robert Raussendorf[1,3] — [1]Institut für Theoretische Physik, Leibniz Universität Hannover — [2]QUDORA Technologies GmbH — [3]Stewart Blusson Quantum Matter Institute, University of British Columbia

Quantum computers are poised to grant an advantage over classical computers for some specific problems. These applications will require fully fault-tolerant quantum computers in order to produce significant results. However, due to the overhead of gates and qubits required by quantum error correction, fault-tolerant computation is out of scope for current devices. This necessitates the development of lightweight yet effective strategies to handle errors in noisy quantum devices. We investigate a $[[2m, 2m-2, 2]]$ error-detection code based on the 'Iceberg code' by applying it to realistic quantum simulations of the Schwinger model. Using an accurate noise model for the two-qubit entangling gate based on the upcoming trapped ion architecture of QUDORA, we simulate the dynamics of the particle number density on a noisy emulator. We demonstrate that the Iceberg code is able to substantially reduce the errors in this simulation, if correctly tuned. To that end, we propose a workflow to optimize the Iceberg code by selecting an optimal number of stabilizer measurements for a given problem. These results show that noisy intermediate-scale quantum computing can extensively be improved by carefully choosing low-overhead error-handling methods.

QI 16.4 Thu 10:30 BEY/0245

Probabilistic error cancellation for single-mode Gottesman-Kitaev-Preskillev-Preskill codes — Alessandro Ciani[1] and •Victoria Wadewitz[1,2] — [1]Institute for Quantum Computing Analytics (PGI-12), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Theoretical Physics, Universität des Saarlandes, 66123 Saarbrücken, Germany

To solve practical problems on a quantum computer, fault-tolerant quantum error correction schemes are necessary to overcome noise from imperfections in physical components. The Gottesman-Kitaev-Preskill (GKP) code achieves this by encoding finite-dimensional logical space within the continuous variables of bosonic modes, offering a pathway to scalable, fault-tolerant quantum computing. However, it is not feasible to eliminate errors entirely, so they must be mitigated. In this work, we study a quantum error mitigation method known as probabilistic error cancellation (PEC) in the context of GKP codes. We compare Steane-type and teleportation-based GKP error correction, and calculate sampling overheads for square and hexagonal GKP codes. The PEC sampling probabilities are derived using a stabilizer subsystem decomposition for GKP codes. Considering noise from finite squeezing of the data and the two ancilla modes, as well as other contributions like pure loss and Gaussian random displacement, we examine the relationship between the overhead and the noise. Our results cover single- and two-GKP-qubit Clifford gates. Preliminary analysis suggests that, when combined with error mitigation techniques, teleportation-based GKP error correction outperforms Steane-type GKP error correction.

QI 16.5 Thu 10:45 BEY/0245

Real-time adaptive quantum error correction by model-free multi-agent learning — •Manuel Guatto[1,2], Francesco Preti[1], Michael Schilling[1,2], Tommaso Calarco[1,2,3], Francisco Cardenas-Lopez[1], and Felix Motzoi[1,2] — [1]Forschungszentrum Jülich GmbH, Peter Grünberg Institute, Quantum Control (PGI-8), 52425 Jülich, Germany — [2]Institute for Theoretical Physics, University of Cologne, D-50937 Cologne, Germany — [3]Dipartimento di Fisica e Astronomia, Università di Bologna, 40127 Bologna, Italy

Can Quantum Error Correction (QEC) adapt in real time to changing noise? We show that it can. We introduce a two-level reinforcement-learning framework that learns QEC from scratch and adapts it on the fly. At the first level, a model-free multi-agent RL system automatically discovers full QEC cycles*encoding, stabilizer measurements, and recovery*using only orthogonality constraints and no prior knowledge of the device. Using the stabilizer formalism, we demonstrate that it can generate new QEC codes tailored to multi-level quantum architectures. At the second level, we present BRAVE (Bandit Retraining for Adaptive Variational Error correction), an efficient algorithm that continuously retunes the variational layer to track time-dependent noise with minimal retraining. Combined, these methods yield more than an order-of-magnitude improvement in logical fidelity under time-varying bit- and phase-flip noise compared to standard QEC schemes.

30min. break

QI 16.6 Thu 11:30 BEY/0245

Continuous vs. Pauli Noise: Impact on Small-Scale Quantum Codes — •Yunos El Kaderi[1,2], Andreas Honecker[1], and Iryna Andriyanova[2] — [1]LPTM CNRS UMR 8089, CY Cergy Paris University, France — [2]ETIS CNRS UMR 8051, CY Cergy Paris University, France

Noise remains the main limit to reliable quantum computation. Standard Pauli models treat faults as discrete events, but real devices exhibit small, coherent shifts in gate rotations that accumulate over time [1,2]. These shifts follow directional patterns linked to axis and angle drift, which are well described by von Mises–Fisher statistics [3].

We study a continuous coherent-noise model built from these rotational laws and apply it to memory circuits based on the $[[5, 1, 3]]$ and $[[7, 1, 3]]$ stabilizer codes. We compare its logical performance with that of a matched-entropy Pauli channel, so both models share the same binary-symmetric uncertainty at readout. This isolates how the *shape* of noise, not only its strength, affects logical error rates.

We also introduce an approximate method that propagates small coherent errors through Clifford circuits without full Monte Carlo.

[1] S. Sheldon *et al.*, Phys. Rev. A 93, 012301 (2016)
[2] E. Huang *et al.*, Phys. Rev. A 99, 022313 (2019)
[3] G. Ragazzi *et al.*, Phys. Rev. A 110, 052425 (2024)

QI 16.7 Thu 11:45 BEY/0245

Encoding Numerical Data for Generative Quantum Machine Learning — •Michael Krebsbach[1], Hagen-Henrik Kowalski[2], Florentin Reiter[1], Ali Abedi[2], and Thomas Wellens[1] — [1]Fraunhofer IAF, Tullastraße 72, 79108 Freiburg — [2]Bundesdruckerei GmbH, Kommandantenstraße 18, 10969 Berlin

Generative quantum machine learning has the potential to model probability distributions that are out of reach for their classical counterparts. Due to the binary nature of samples drawn from a quantum computer, many of the generative models described in the literature focus on binary data. The transition from binary to real-world data, which is typically numerical, necessitates an additional encoding step that can obscure structure in the data and hinder effective learning.

In this talk, we present our investigation into binary encodings and their effect on the training process of generative quantum machine learning algorithms. We identify situations in which the conventional approach is limited, and propose strategies that circumvent these limitations at essentially no additional cost. We

test these strategies on a range of datasets and provide numerical evidence that they provide an average-case improvement over the conventional approach.

QI 16.8 Thu 12:00 BEY/0245

Machine Learning methods for Entanglement Detection in High Dimensional Systems — •Yasmin Bougammoura[1], Martin Plávala[1], Fabio Anselmi[2], and Fabio Benatti[2] — [1]Institute of Theoretical Physics - Leibniz University Hannover, Germany — [2]University of Trieste, Italy

A universal approach to entanglement detection can be cast as a semidefinite program (SDP), but this formulation becomes computationally inefficient as the dimension of the system grows. Since entanglement detection for systems of dimension $d \geq 6$ is already an NP-hard task, this motivates the search for practical numerical strategies. Although current machine learning models reach high accuracy values, they do not provide robust and verifiable separability criteria. We propose two simple approaches: i. using automatic differentiation to approximate a given quantum state, and ii. training an artificial neural network to construct a certifiable entanglement witness W for a given entangled quantum state. The former efficiently approximates separable states; the latter achieves an improvement of two orders of magnitude in the dimension of the optimisation problem, which increases exponentially with the number of qubits. In terms of computational resources, the neural network model runs on a local machine with 16 GB RAM for a system of 8 qubits, whereas the SDP formulation is limited to a system of only 4 qubits.

QI 16.9 Thu 12:15 BEY/0245

Reducing the cost of gate-set tomography of superconducting quantum processors — •Martin Koppenhöfer, Michael Krebsbach, and Thomas Wellens — Fraunhofer-Institut für Angewandte Festkörperphysik IAF, Tullastraße 72, 79108 Freiburg, Deutschland

Gate errors remain one of the biggest obstacles on the road towards scalable quantum processors. Obtaining a precise understanding of these errors and of their origin is a necessary step for hardware improvements and error mitigation. In principle, gate-set tomography protocols allow one to obtain a detailed, self-consistent picture of quantum processors including state-preparation and measurement steps. However, a drawback of these protocols is that they become computationally very costly when multi-qubit gates are analyzed, leading to a very large set of germ circuits as well as an exponential growth of the initial states that need to be prepared and measurements that need to be performed.

In this talk, we present a modified approach to gate-set tomography that exploits different gate fidelities for single- and two-qubit gates to reduce the number of germ circuits and fiducial states. For two-qubit gate-set tomography, this approach reduces the number of required experiments by more than an order of magnitude and thus speeds up gate-set tomography protocols. We demonstrate this new technique on a superconducting quantum processor.

QI 16.10 Thu 12:30 BEY/0245

Detecting genuine multipartite entanglement in multi-qubit devices with restricted measurements — •Nicky Kai Hong Li[1,2], Xi Dai[3,4], Manuel Muñoz-Arias[5], Kevin Reuer[3,4], Marcus Huber[1,2], and Nicolai Friis[1] — [1]Atominstitut, Technische Universität Wien, Stadionallee 2, 1020 Vienna, Austria — [2]Institute for Quantum Optics and Quantum Information (IQOQI), Austrian Academy of Sciences, Boltzmanngasse 3, 1090 Vienna, Austria — [3]Department of Physics, ETH Zurich, CH-8093 Zurich, Switzerland — [4]Quantum Center, ETH Zurich, CH-8093 Zurich, Switzerland — [5]Institut Quantique and Département de Physique, Université de Sherbrooke, Sherbrooke J1K 2R1 QC, Canada

Detecting genuine multipartite entanglement (GME) is a state-characterization task that benchmarks coherence and experimental control in quantum systems. Existing GME tests often require joint measurements on many qubits, posing experimental challenges for systems like time-bin qubits and microwave photons from superconducting circuits. Here we introduce GME and k-inseparability criteria applicable to any state, which only require measuring $O(n^2)$ out of 2^n $\leqslant m$-body stabilizers of n-qubit target graph states, with m at most twice the graph's maximum degree. For cluster or ring-graph states, only constant-weight stabilizers are needed. Using SDP, we further reduce both the number and weight of required stabilizers. Analytical and numerical results show that our criteria are noise-robust and can infer state infidelity from certified k-inseparability in microwave photonic graph states generated under realistic conditions.

QI 17: Decoherence and Open Systems II

Time: Thursday 15:00–17:30 Location: BEY/0137

QI 17.1 Thu 15:00 BEY/0137

A mathematical justification to apply the secular approximation to the Redfield equation — •Niklas Jung[1,2], Francesco Rosati[1,2], Gabriel Rath[1,2], Frank Wilhelm[1,2], and Peter Schuhmacher[3] — [1]Theoretical Physics, Saarland University, Campus, 66123 Saarbruecken, Germany — [2]Institute for Quantum Computing Analytics (PGI-12), Forschungszentrum Juelich, 52425 Juelich, Germany — [3]Department of High Performance Computing, Institute of Software Technology, German Aerospace Center (DLR), Rathausallee 12, 53757 Sankt Augustin, Germany

In this work, we prove that the solutions of the master equation obtained by applying the secular approximation are also obtained by an approximation of the same order as the one performed to obtain the Redfield equation. We hereby provide a mathematical justification for the secular approximation. We show that the result of applying the secular approximation is obtained naturally by applying a self-consistency argument. This shows that the resulting master equation is also in the same equivalence class of approximations as the Redfield master equation.

QI 17.2 Thu 15:15 BEY/0137

Quantum Zeno effect versus adiabatic quantum computing and quantum annealing — Naser Ahmadiniaz[1], Dennis Kraft[1], Gernot Schaller[1], and •Ralf Schuetzhold[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden, Germany — [2]Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

For the adiabatic version of Grover's quantum search algorithm as proposed by Roland and Cerf, we study the impact of decoherence caused by a rather general coupling to some environment. For quite generic conditions, we find that the quantum Zeno effect poses strong limitations on the performance (quantum speed-up) since the environment effectively measures the state of the system permanently and thereby inhibits or slows down quantum transitions. Generalizing our results, we find that analogous restrictions should apply universally to adiabatic quantum algorithms and quantum annealing schemes which are based on isolated Landau-Zener type transitions at avoided level crossings (similar to first-order phase transitions). As a possible resort, more gradual changes of the quantum state (as in second-order phase transitions) or suitable error-correcting schemes such as the spin-echo method may alleviate this problem.
https://doi.org/10.48550/arXiv.2509.04057

QI 17.3 Thu 15:30 BEY/0137

Cat state preparation and stabilization in open quantum systems — •Suocheng Zhao[1], Sofia Qvarfort[2,3], and Anja Metelmann[1,4,5] — [1]IQMT, KIT, 76344 Eggenstein-Leopoldshafen, Germany — [2]Nordita, KTH Royal Institute of Technology and Stockholm University, SE-106 91 Stockholm, Sweden — [3]Department of Physics, Stockholm University, AlbaNova University Center, SE-106 91 Stockholm, Sweden — [4]TKM, KIT, 76131 Karlsruhe, Germany — [5]ISIS, University of Strasbourg and CNRS

Cat states are a valuable resource for quantum metrology applications, promising to enable sensitivity down to the Heisenberg limit. Moreover, Schrödinger cat states, based on a coherent superposition of coherent states, show robustness against the bit-flip error making them a promising candidate for bosonic quantum codes. Despite these advantages, cat states are generally difficult to generate, and their practical usefulness is fundamentally challenged by environmental noise, which degrades both their preparation and subsequent performance. In this talk, I present three complementary strategies for mitigating the impact of noise, illustrated through the preparation and protection of cat states: (1) accelerating state preparation to outrun noise accumulation using self- and cross-Kerr interactions, as well as quantum optimal control, (2) squeezing the cat states to enhance their intrinsic robustness against noise, and (3) engineering tailored dissipative processes that drive the system toward cat states, and counteract noise to extend their lifetime. Together, these approaches pave the way for deploying cat states in practical quantum technologies.

QI 17.4 Thu 15:45 BEY/0137

Exact Floquet dynamics of strongly damped driven quantum systems — •Konrad Mickiewicz[1], Valentin Link[2], and Walter T. Strunz[1] — [1]Institut für Theoretische Physik, Technische Universität Dresden, D-01062, Dresden, Germany — [2]Institut für Physik und Astronomie, Technische Universität Berlin, D-10623, Berlin, Germany

We introduce an approach for efficiently simulating strongly damped, periodically driven quantum systems [1] using a translationally invariant matrix product operator representation of the influence functional [2]. This allows us to construct a numerically exact Floquet propagator that captures non-Markovian open system dynamics, serving as a dissipative analogue to the Floquet Hamiltonian of isolated periodically driven systems. We apply our method to investigate deviations from equilibrium in spin-boson models by studying the asymptotic reservoir heating. Additionally, we demonstrate that local driving of two

qubits can stabilize a transient, environmentally induced buildup of entanglement. Our approach enables a direct analysis of both stationary and transient dynamics in strongly damped, driven quantum systems within a consistent theoretical and computational framework. [1] K. Mickiewicz, V. Link, and W. T. Strunz, arXiv:2511.08754 (2025) [2] V. Link, H.-H. Tu, and W. T. Strunz, Phys. Rev. Lett. 132, 200403 (2024)

QI 17.5 Thu 16:00 BEY/0137

Exceptional Points and Optimized Encoding under Continuous Measurement — •Yves Rottstaedt[1], Andrei Pavlov[2], Alexander Shnirman[2], Yuval Gefen[3], and Bernd Rosenow[1] — [1]Universität Leipzig, Leipzig, Germany — [2]Karlsruhe Institut für Technologie, Karlsruhe, Germany — [3]Weizmann Institute of Science, Rechovot, Israel

We study a system of three qubits subject to blind continuous stabilizer measurements and stochastic bit-flip errors. The resulting open-system dynamics are governed by a non-Hermitian Liouvillian superoperator, which exhibits an exceptional point (EP) at a specific critical error rate: two eigenvalues coalesce and their eigenmodes merge into a single vector, forming a nontrivial Jordan chain. Motivated by this structure, we construct a logical-qubit basis directly from the Liouvillian eigenmodes, thereby incorporating both measurement-induced dissipation and error processes into the encoded subspace. By analyzing the Jordan chain at the EP, we identify dynamical features that enhance logical-state stability over short and intermediate times. We then optimize the logical basis to reproduce these EP-induced properties for arbitrary error rates, effectively extending the favorable dynamical behavior beyond the singular point.

QI 17.6 Thu 16:15 BEY/0137

Closed-Form approximation of Kraus operators for GKSL dynamics in the weak-noise regime — •Shahrukh Chishti[1,2], Francisco Cardenas-Lopez[1], and Felix Motzoi[1,2] — [1]Forschungszentrum Juelich GmbH, Peter Gruenberg Institute, Quantum Control (PGI-8), 52425 Juelich, Germany — [2]Institute for Theoretical Physics, University of Cologne, D-50937 Cologne, Germany

Quantum system interacts unavoidably with the surrounding environment leading to decoherence and thermalization. The dynamics of an open quantum system is equivalently represented with the GKSL equation or the Kraus operators that includes the effects of the environment. For a general noise channel, it is difficult to obtain the Kraus operators from the Lindbladian and vice-versa. We derive a closed-form approximation of the Kraus operators for the GKSL dynamics by employing two approximations; first, weak noise limit of the dynamical map and then discretizing this map via a Riemann summation. Further, this technique could be extended to higher orders in evolution and time-dependent Hamiltonians. These results provide insight into the interaction between noise and coherent dynamics.

30min. break

QI 17.7 Thu 17:00 BEY/0137

Non-perturbative switching rates in bistable open quantum systems: from driven Kerr oscillators to dissipative cat qubits — •Leon Carde[1], Ronan Gautier[1], Nicolas Didier[1], Alexandru Petrescu[2], Joachim Cohen[1], and Alexander McDonald[3] — [1]Alice&Bob, Paris, France — [2]Mines ParisTech, Paris, France — [3]University of Sherbrooke, Sherbrooke, Canada

In this work, we use path integral techniques to predict the switching rate in a single-mode bistable open quantum system. While analytical expressions are well-known to be accessible for systems subject to Gaussian noise obeying classical detailed balance, we generalize this approach to a class of quantum systems, those which satisfy the recently-introduced notion of hidden time-reversal symmetry. .In particular, in the context of quantum computing, we obtain analytical estimates of bit-flip error rates in cat-qubit architectures. We confirm these findings by comparing our results to numerically exact diagonalization of the Linbladian. Our results provide a path towards exploring switching phenomena in multistable open quantum systems

QI 17.8 Thu 17:15 BEY/0137

Conserved quantities enable the quantum Mpemba effect in weakly open systems — •Iris Ulcakar[1,2], Gianluca Lagnese[1], Rustem Sharipov[2], and Zala Lenarcic[1] — [1]"Jozef Stefan" Institute, Ljubljana, Slovenia — [2]Faculty of Mathematics and Physics, University of Ljubljana, Slovenia

Observation of the quantum Mpemba effect has spurred much interest in its enabling conditions and its relation to the classical counterpart. Here, we consider weakly open many-body quantum systems initialized in different thermal states and examine when the initially farther state relaxes to the (non-equilibrium) steady state faster. We claim that the number of conserved quantities in the unitary part plays a crucial role: the Mpemba effect is possible only when the Hamiltonian commutes with other extensive operators or is integrable. The reason lies in the dynamical evolution happening in spaces of different dimensions. When energy is the only approximately conserved quantity, dissipation pushes the dynamics within a single-parameter manifold of different thermal states. In contrast, for Hamiltonians with several conserved quantities, the dynamics drift in the multi-dimensional space of generalized Gibbs ensembles, whose distance to the steady state is less trivial. We provide numerical results for large system sizes using tensor networks and free-fermion techniques, thereby supporting our claim.

QI 18: Quantum Communication

Time: Thursday 15:00–18:00 Location: BEY/0245

Invited Talk QI 18.1 Thu 15:00 BEY/0245

Multipartite Quantum states from guided-wave structures — •Virginia D'Auria[1], Adrien Bensemhoun[1], Silvia Cassina[2], Carlos Gonzalez-Arciniegas[3], Mohamed Fauzi Melalkia[1], Giuseppe Patera[4], Jonathan Faugier-Tovar[5], Quentin Wilmar[5], Ségolène Olivier[5], Alessandro Zavatta[6], Anthony Martin[1], Jean Etesse[1], Laurent Labonté[1], and Sébastien Tanzilli[1] — [1]University Côte d'Azur, Institut of Physics of Nice, Nice, FR — [2]University of Insubria, Como, IT — [3]University of Virginia, Charlottesville, VA, US — [4]University of Lille, Lille, FR — [5]CEA-LETI, Grenoble, FR — [6]Istituto Nationale di Ottica, Florence, IT

Our experimental work demonstrates multipartite quantum correlation in bright frequency combs out of a microresonator integrated on silicon nitride operating above its oscillation threshold. Multipartite features, going beyond so far reported two-mode correlation, naturally arise due to a cascade of non-linear optical processes, making a single-color laser pump sufficient to initiate their generation. Our results show the transition from two-mode to multipartite correlation.

QI 18.2 Thu 15:30 BEY/0245

Microwave quantum communication over thermal quantum networks — •Wun Kwan Yam[1,2], Simon Gandorfer[1,2], Maria-Teresa Handschuh[1,2], Achim Marx[1], Rudolf Gross[1,2,3], and Kirill G. Fedorov[1,2,3] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology, 80799 Munich, Germany

Quantum communication in the microwave regime is set to play an important role in distributed quantum computing and hybrid quantum networks. In a step towards practical quantum networks, we demonstrate quantum teleportation of microwave coherent states over a thermal quantum network composed of two spatially-separated dilution refrigerators, achieving teleportation fidelities of 72.3 % at channel temperatures of 1 K and 59.9 % at 4 K. Furthermore, we theoretically analyze quantum communication of discrete-variable qubit states using a continuous-variable two-mode squeezing resource state, paving the way towards hybrid quantum communication protocols. Our results show the experimental feasibility of distributed superconducting architectures and motivate further investigations of noisy quantum networks in various frequency regimes.

QI 18.3 Thu 15:45 BEY/0245

Entanglement distribution in hybrid-variable microwave networks — •Simon Gandorfer[1,2], Ivan Solomakhin[1,2], Maria-Teresa Handschuh[1,2], Joan Agustí[1,2], Achim Marx[1], Peter Rabl[1,2,3], Rudolf Gross[1,2,3], and Kirill G. Fedorov[1,2,3] — [1]Walther-Meißner- Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany — [2]School of Natural Sciences, Technische Universität München, 85748 Garching, Germany — [3]Munich Center for Quantum Science and Technology, 80799 Munich, Germany

Distributing entanglement between distant nodes of a large-scale quantum network is a fundamentally important milestone for quantum information processing. In particular, quantum entanglement is crucial for quantum teleportation protocols or logical quantum gates with remote qubits. In our experiment, we investigate remote entanglement of discrete-variable qubits by using contiunuos-variable entangled signals. The latter is represented by the two-mode squeezed microwaves generated with Josephson parametric circuits, while the former are given by superconducting transmons in 3D cavities. We observe a build-up of entanglement between the qubits due to their interaction with the common, quantum-correlated, reservoir. The corresponding entanglement conversion between continuous- and discrete-variables allows for promising and robust, hybrid-variable, quantum microwave networks. Finally, we discuss possible extensions and applications of our findings for distributed quantum computing architectures.

QI 18.4 Thu 16:00 BEY/0245

Quantum Key Distribution without Hidden Message Transmission — •Yien Liang, Anton Trushechkin, Hermann Kampermann, and Dagmar Bruss — Institut für Theoretische Physik III, Heinrich-Heine-Universität Düsseldorf, Universitätsstraße 1, 40225 Düsseldorf, Germany

Steganography is the practice of hiding secret information within irrelevant information. A way to hide information within a valid digital signature is to take advantage of the random number required by a digital signature protocol, the adversary can maliciously choose a number that hides information instead of randomly choosing one. Such steganography technique is called subliminal channel [1]. A quantum key distribution (QKD) protocol involves communicating a large set of random random numbers, which can be used to establish a subliminal channel. The participants of a QKD protocol can intentionally hide information within the public announcement which is undetectable by any third party. Malicious QKD devices could also use a subliminal channel as a covert channel [2] to leak information to a third party. In our contribution, we propose a modified QKD protocol which is information-theoretic secure against eavesdropping and provable (more-than-one-bit-)subliminal-channel-free. We also generalize our results to quantum conference key agreement protocols.

[1] Simmons G J. Advances in cryptology: proceedings of crypto 83. Boston, MA: Springer US, 1984: 51-67. [2] Curty M, Lo H K. npj Quantum Information, 2019, 5(1): 14.

QI 18.5 Thu 16:15 BEY/0245

Verified delegated quantum computation requires techniques beyond cut-and-choose — •Fabian Wiesner and Anna Pappa — Technische Universität Berlin, Einsteinufer 17, 10587 Berlin, Germany

Delegated quantum computation enables a client with limited quantum capabilities to outsource computations to a more powerful quantum server while preserving correctness and privacy. Verification is crucial in this setting to ensure that the untrusted quantum server performs the computation honestly and returns correct results. A common verification method is the quantum cut-and-choose technique. Inspired by classical verification methods for two-party computation, the client uses the majority of the delegated rounds to test the server's honesty, while keeping the remaining ones for the actual computation. Combining this technique with other methods, such as quantum error correction, could help achieve negligible cheating probabilities for the server; however, such methods can impose significant overheads, making implementations unfeasible for the near-term future. In this work, we investigate whether cut-and-choose can yield efficient and secure verifiable quantum computation without additional costly techniques. We find that verifiable delegated quantum computation protocols relying solely on cut-and-choose techniques cannot be secure and efficient at the same time.

30min. break

QI 18.6 Thu 17:00 BEY/0245

Deployed BBM92 quantum key distribution using frequency-converted entangled photons emitted by a quantum dot — •Benjamin Breiholz[1], Michal Vyvlecka[1], Raphael Joos[1], Aurélien Marmasse[1], Ilenia Neureuther[1], Timo Schnieber[1], Anna Frederike Köhler[1], Tim Strobel[1], Tobias Bauer[2], Marlon Schäfer[2], Nand Lal Sharma[3], Caspar Hofmann[3], Simone Luca Portalupi[1], Christoph Becher[2], and Peter Michler[1] — [1]Institut für Halbleiteroptik und Funktionelle Grenzflächen, Center for Integrated Quantum Science and Technology (IQST) and SCoPE, 70569 Stuttgart, Germany — [2]Fachrichtung Physik, 66123 Saarbrücken, Germany — [3]Institute for Integrative Nanosciences, 01069 Dresden, Germany

We implemented an entanglement-based BBM92 quantum key distribution (QKD) protocol over approximately 700 m across the university campus buildings using the existing deployed fiber network. The entangled-photon pair at wavelength of 780 nm was emitted by an epitaxially grown droplet-etched GaAs quantum dot (QD) embedded in a dielectric antenna. The QD was excited via two-photon excitation using a pulsed laser that emits 10 ps pulses at 779 nm with a 380 MHz repetition rate. To minimize losses in silica fibers, we employed bidirectional, polarization-conserving quantum frequency conversion to shift the QD emission to a telecom wavelength. We achieved stable QKD operation for more than 10 hours, with a raw key rate exceeding 200 Hz and a quantum bit error rate below 4.5 %. After error correction and privacy amplification, we distilled a secure key at a rate of 100 Hz.

QI 18.7 Thu 17:15 BEY/0245

GHz-clocked Single-photon Quantum Key Distribution in the Telecom C-band — •Koray Kaymazlar[1], Mareike Lach[1], Robert B. Behrends[1], Lucas Rickert[1], Martin von Helversen[1], Jochen Kaupp[2], Yorick Raum[2], Tobias Huber Loyola[2,3], Sven Höfling[2], Andreas Pfenning[2], and Tobias Heindel[4] — [1]Institute of Physics and Astronomy, Technische Univeristät Berlin — [2]Technische Physik, Physikalisches Institut and Würzburg-Dresden Cluster of Excellence — [3]Karlsruher Institut für Technologie, Institute of Photonics and Quantum Electronics — [4]Department for Quantum Technology, Univeristät Münster

High speed operation is one of the most desired properties for implementations of quantum key distribution (QKD). This requires however the generation and state-preparation of photonic qubits at high speed. Here, we report on a QKD system based on the BB84 protocol that operates at GHz clock-rates using a highly Purcell-enhanced single-photons source emitting in the telecom C-band. We use a laser with a repetition rate of 2.5 GHz to pump the quantum dot source and prepare the polarization states fot the protocol using a customized fiber-based electro-optic modulator (EOM) controlled by an arbitrary waveform generator (AWG) using the trigger output of the pump laser as common clock. Our results show that our system performs the BB84 protocol succesfully with a quantum bit error ratio (QBER) around 5 % at these unprecendeted high clock-rates.

QI 18.8 Thu 17:30 BEY/0245

Multiplexed multipartite quantum repeater rates in the stationary regime — •Anton Trushechkin, Julia Kunzelmann, Nikolai Wyderka, Hermann Kampermann, and Dagmar Bruss — Heinrich Heine University Düsseldorf, Faculty of Mathematics and Natural Sciences, Institute for Theoretical Physics III, Universitätsstr. 1, Düsseldorf 40225

We consider a multipartite quantum repeater creating GHZ states between several parties from bipartite entanglement links. Each bipartite link is characterised by a success probability, i.e., probability of successful establishment of bipartite entanglement per round. We are interested in GHZ generation rate in such repeater on long times, i.e., in the stationary regime. On an abstract level, the mathematical description is also equivalent to the usual bipartite quantum repeater chain between two parties and the corresponding bipartite entanglement generation rate. We also consider the case of memory multiplexing and study its effect on the generation rate. We derive closed-form expressions for the stationary generation rate depending on the number of parties (or the segments in a chain of bipartite repeaters) and the multiplexing number.

QI 18.9 Thu 17:45 BEY/0245

Anonymous and private parameter estimation in networks of quantum sensors — Jarn De Jong[1], Santiago Scheiner[2], Naomi R. Solomons[2], •Ziad Chaoui[1], Damian Markham[2], and Anna Pappa[1] — [1]Technische Universität Berlin, Einsteinufer 19, 10587 Berlin, Germany — [2]LIP6, CNRS, Sorbonne Université, 4 place Jussieu, F-75005 Paris, France

Anonymity and privacy are two key properties of modern communication networks. In quantum networks, distributed quantum sensing has emerged as a powerful use case, with applications to clock synchronization, detecting gravitational effects, and more. In this work, we develop a new protocol that, for the first time, combines the different cryptographic properties of anonymity and privacy for the task of distributed parameter estimation. That is, we present a protocol that allows a selected subset of network participants to anonymously collaborate in estimating the average of their private parameters. Crucially, this is achieved without disclosing either the individual parameter values or the identities of the participants, neither to each other nor to the broader network.

QI 19: Members' Assembly

Time: Thursday 18:00–19:00 Location: BEY/0245

All members of the Quantum Information Division are invited to participate.

QI 20: Metrology and Sensing

Time: Friday 9:30–12:00 Location: BEY/0137

QI 20.1 Fri 9:30 BEY/0137

Nitrogen Vacancy center based gradiometry: Towards unshielded magnetic biosensing applications — •Magnus Benke, Jixing Zhang, Michael Kübler, Yihua Wang, and Jörg Wrachtrup — 3rd Physics Insitute, University of Stuttgart, Stuttgart

Magnetometers based on Nitrogen Vacancy (NV) centers in diamond offer high sensitivities and spatial resolution, as well as a broad dynamic range. These properties allow for unshielded measurements by combining two or more sensors into a gradiometric array to suppress common-mode noise. In this work we present a DC-broadband gradiometer, comprised of two magnetometers using a CW-ODMR (Continuous-Wave Optically Detected Magnetic Resonance) measurement scheme. With this array we were able to effectively reduce an artificial background signal by 45 times without attenuating an applied test signal. For further detailed analysis of the noise floor, we equipped the sensors with flux concentrators to identify the different noise contributions in the signal.

QI 20.2 Fri 9:45 BEY/0137

Model-free error mitigation in NV center magnetometry — •Dennis Herb[1], Miriam Resch[1], Mirko Rossini[1], Joachim Ankerhold[1,2], and Dominik Maile[1] — [1]Institute for Complex Quantum Systems, Ulm University, Germany — [2]Center for Integrated Quantum Science and Technology (IQST), Ulm-Stuttgart, Germany

Quantum sensing is an emerging field with the potential to outperform classical methods in both precision and spatial resolution. However, the sensitivity of the underlying quantum platform also makes them highly susceptible to their environmental noise. To address this issue, techniques from the field of quantum error mitigation have been used to improve measurement results from noisy device signals via post-processing. We present a novel mitigation technique for quantum sensors to efficiently reverse the effects of any noise source that can be described by a completely positive trace preserving map. The method neither requires tomography of the final density matrix after the sensing protocol nor an underlying noise-model. It leverages the knowledge acquired by a pre-characterization step of the device to automatically adapt to the complexity of the dissipative evolution and to indicate which sensing times τ are best suited for the most accurate results. This method represents a further step toward perfecting a new family of sensors with the smallest scale of resolution, enabling measurements at the molecular scale.

QI 20.3 Fri 10:00 BEY/0137

Part 1: Optically Addressable Molecular Spins at 2D surfaces — •Yan Tung Kong, XuanKai Zhou, Cheuk Kit Cheung, Ruoming Peng, and Jörg Wrachtrup — 3. Physikalisches Institut, University of Stuttgart, 70569 Stuttgart, Germany

Optically addressable surface spins constitute a long-sought goal in quantum sensing, offering a pathway to probe quantum phenomena with atomic-scale precision. Here, we introduce a novel architecture in which pentacene spin molecules are anchored onto two-dimensional hexagonal boron nitride (hBN) and self-align with the underlying lattice. This configuration yields robust optically detected magnetic resonance (ODMR) signals from 4 K to room temperature. We further demonstrate ensemble spin sensing of Fe3GaTe2 (FGT), as well as controlled positioning of Pc molecules. This work represents the first demonstration of a surface molecular spin sensor that integrates long coherence, optical addressability, and interfacial functionality, thereby enabling quantum sensing capabilities beyond those of conventional solid-state spin systems.

QI 20.4 Fri 10:15 BEY/0137

Part 2: Optically Addressable Molecular Spins at 2D surfaces — •Xuankai Zhou[1], Yan-Tung Kong[1], Cheuk Kit Cheung[1], Ruoming Peng[1], and Jörg Wrachtrup[1,2] — [1]3. Physikalisches Institut, University of Stuttgart, 70569 Stuttgart, Germany — [2]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany

Surface spins with coherent control hold the potential to quantum sensing revolution by nanoscale magnetic imaging. On the pentacene-hBN hybrid platform, we demonstrate distinguished coherence engineering alongside versatile functional sensing. By employing isotope purification and dynamical decoupling, the spin-coherence time is extended to $T_2 > 30$ μs and $T_{2,DD} > 300$ μs, already approaching the intrinsic triplet state lifetime limit. Meanwhile, it is also available for the platform to sense nearby proton nuclear signals and magnetic responses of two-dimensional magnets beneath hBN layer. This work represents the first demonstration of surface molecular spin sensor, integrating long coherence, optical addressability and interfacial functionality, thereby enabling quantum sensing beyond conventional solid-state spins.

QI 20.5 Fri 10:30 BEY/0137

Iterative optimization in quantum metrology and entanglement theory using semidefinite programming — Árpád Lukács[1,2,3], •Róbert Trényi[2,3,4,5], Tamás Vértesi[6], and Géza Tóth[3,4,2] — [1]Dept. of Math. Sci., Durh. Univ., UK — [2]HUN-REN Wigner RCP, Budapest, Hungary — [3]Dept. of Th. Phys., UPV/EHU, Bilbao, Spain — [4]EHU Quantum Center, UPV/EHU, Bilbao, Spain — [5]Dept. of Th. Phys., Univ. of Szeged, Hungary — [6]HUN-REN Inst. for Nucl. Research, Debrecen, Hungary

Metrological performance of a quantum state is measured by how much it can outperform all separable states in a metrological task. We present efficient optimization techniques to maximize this performance by searching for the optimal local Hamiltonian generating the unitary dynamics for a given bipartite initial state. We show that this is equivalent to maximizing the Quantum Fisher Information over a specific set of local Hamiltonians. This task is very difficult, as it involves maximizing a convex function over a convex set. We reformulate the problem in a bilinear way and optimize it using an iterative see-saw method, where each optimization step is solved via semidefinite programming. We further show that the same optimization framework can be adapted to problems in entanglement theory, such as identifying bound entangled states that maximally violate the Computable Cross Norm-Realignment criterion. Finally, we provide examples where two copies of a quantum state outperform a single copy, demonstrating metrological activation for certain small systems.

QI 20.6 Fri 10:45 BEY/0137

Localization and coherent control of 25 nuclear spins in Silicon Carbide — •Pierre Kuna[1], Erik Hesselmeier-Hüttman[1], Phillip Schillinger[1], Felix Gloistein[1], Viktor Ivády[2], Wolfgang Knolle[3], Jawad Ul-Hassan[4], Vadim Vorobyov[1], and Jörg Wrachtrup[1,5] — [1]3rd Institute of Physics, University of Stuttgart, Stuttgart, Germany — [2]Eötvös Loránd University, Hungary — [3]Department of Sensoric Surfaces and Functional Interfaces, Leibniz-Institute of Surface Engineering (IOM), Leipzig, Germany — [4]Department of Physics, Chemistry and Biology, Linköping University, Linköping, Sweden — [5]Max Planck Institute for solid state physics, Stuttgart, Germany

Nuclear spins coupled to optically addressable defects provide long-lived quantum memories[1] and scalable resources for quantum algorithms. For the V2 center in 4H-SiC, leveraging this potential requires precise knowledge of the surrounding nuclear-spin environment to refine DFT models and enable advanced multi-qubit algorithms[3,4].

We report ångström-level 3D localization of 25 naturally occurring 29Si and 13C spins around a single V2 center. Using correlation-spectroscopy SEDOR, Our work establishes a new state of the art in controlling nuclear spin cluster in 4H-SiC. By selecting multi-spin chains up to length four, we access and characterize new nuclear spins and reconstruct their couplings to the central electron and neighboring nuclei.

[1] M. Zhong, Nature 517, 177 (2015) [2] Abobeih, M.H., Nature 606, 884*889 (2022) [3] J. Randall*et al..Science374,1474-1478(2021)

30min. break

QI 20.7 Fri 11:30 BEY/0137

Charge sensing back-action on spin qubit readout using a micromagnet — •Sudipto Das[1], Domonkos Svastits[1,2], Aritra Sen[1], and Andras Palyi[1,3] — [1]Budapest University of Technology and Economics, Budapest, Hungary — [2]Qutility @ Faulhorn Labs, Budapest, Hungary — [3]HUN-REN-BME-BCE Quantum Technology Research Group, Budapest, Hungary

This work presents a theoretical framework for the charge-sensing readout of semiconductor spin qubits in double quantum dots. We explain the readout based on Pauli blockade spin-to-charge conversion and subsequent charge sensing via quantum point contact using the Qubit Measures Qubit model [1]. Our analysis focuses on n-type Silicon double quantum dots with micromagnets enabling resonant single-qubit control, explicitly accounting for the inhomogeneous micromagnet field and its modulation by charge-sensor shot noise.

Within this model, we quantify key readout errors-fidelity loss due to Zeeman-field modulation, mixedness of the post-measurement state, and leakage caused by perpendicular field fluctuations. We also incorporate the noise from charge sensors to understand its effect on readout. By studying their dependence on device parameters, including the orientation of the external magnetic field, we offer insights into readout performance optimization and readout sweet spots.

[1] D. Svastits, B. Hetényi, G. Széchenyi, J. Wootton, D. Loss, S. Bosco, and A. Pályi, Readout sweet spots for spin qubits with strong spin-orbit interaction, arXiv:2505.15878.

QI 20.8 Fri 11:45 BEY/0137

Quantitative inspection of quantum chips using SQUID-on-tip atomic force microscopy — •Daan B. Boltje[1], Jessalyn DeVine[1], Dalal Benali[1], Matthijs Rog[2], Tycho Blom[2], Milan P. Allan[3], Alessandro Bruno[4], Kaveh Lahabi[1,2], and Johannes Jobst[1] — [1]QuantaMap B.V., Leiden, The Netherlands. — [2]LION, Leiden University, The Netherlands. — [3]Faculty of Physics, LMU Munich, Germany. — [4]QuantWare B.V., Delft, The Netherlands.

The performance of quantum chips and the physics of quantum materials in general and are often dominated by local properties and or defects. Understanding those local properties requires microscopy that operates at cryogenic temperatures and that does not disturb the highly sensitive quantum effects it aims to reveal. In this talk, we will show measurements obtained with a tuning-fork, atomic force microscope (AFM) that integrates a nano-SQUID sensor on the tip. This design enables extremely short sensor-chip distances and robust height feedback in tapping-mode to prevent crashes, which would damage the SQUID sensor as well as the chip under study. It offers a non-invasive, purely electronic readout and magnetic sensitivity in and out-of plane. Frequency multiplexing permits simultaneous imaging of chip topography, magnetic fields, current flow and thermal dissipation on the nanoscale. We will show experiments from this novel microscope on magnetic and superconducting nanostructures of spin qubits and transmon quantum chips. We demonstrate how insights from this SQUID microscopy into material properties and local effects can be used to improve the quantum chips. [1] M. Rog et al. arXiv:2508.21575 (2025)

QI 21: Quantum Information: Concepts and Methods III

Time: Friday 9:30–12:45 Location: BEY/0245

Invited Talk QI 21.1 Fri 9:30 BEY/0245

Non-Hermitian topology and directional amplification — •Clara Wanjura — Max Planck Institute for the Science of Light, Staudtstraße 2, Erlangen

Topology has been a major research theme in condensed matter physics and is associated with a number of remarkable phenomena such as robust edge states. More recently, topology started to be investigated in systems experiencing gain and loss, sparking the field of non-Hermitian topology. However, for a long time, a clear observable signature of non-Hermitian topology had been lacking.

We recently closed this gap and showed that non-trivial, non-Hermitian topology is in one-to-one correspondence with the phenomenon of directional amplification in one-dimensional driven-dissipative systems, e.g., cavity arrays. Directional amplification allows to selectively amplify signals depending on their propagation direction and has attracted much attention as key resource for applications, such as quantum information processing. We experimentally demonstrated this connection between non-Hermitian topology and directional amplification in a cavity optomechanical system as well as realised a sensor based on non-Hermitian topology for which the sensitivity is exponentially enhanced with increasing system size.

Our work opens up new routes for the design of multimode robust directional amplifiers and novel topological sensors that can be integrated in scalable platforms such as superconducting circuits, cavity optomechanical systems, plasmonic waveguides and nanocavity arrays.

QI 21.2 Fri 10:00 BEY/0245

Graph-State Gates as Scrambling Primitives: Entanglement Growth and Complexity in Quantum Circuits — •Zahra Raissi[1], Himanshu Sahu[2], Mario Flory[3], and Aranya Bhattacharya[4] — [1]Paderborn University, Germany — [2]Perimeter Institute, Canada — [3]Jagiellonian University, Poland — [4]University of Bristol, UK

Understanding how quantum information spreads in many-body systems is central to quantum simulation, error correction, and quantum network design. In this work, we investigate structured random circuits built from graph-state gates, where small multi-qubit graph states are repeatedly embedded into a one-dimensional Clifford circuit at random locations. Each gate acts on a fixed number of qubits but carries an internal graph structure, allowing us to disentangle the role of local graph geometry from that of global circuit architecture.

Within this model, we use stabilizer methods to compute bipartite entanglement entropies, height functions, and light-cone diagnostics based on both Pauli spreading and out-of-time-order correlators (OTOCs). We find that the entanglement growth rate and saturation time are strongly correlated with two graph-theoretic features: a local light-cone capacity (degree and connectivity) and a cross-entanglement capacity (edge cuts/height). This reveals a hierarchy of graph-state gates according to their entangling and scrambling power. Our results provide a graph-theoretic design principle and a concrete ranking for selecting small graph blocks that optimize entanglement generation and operator spreading in Clifford quantum circuits.

QI 21.3 Fri 10:15 BEY/0245

Analysis of multi-detector quantum measurements via their cross-correlation polyspectra — •Armin Ghorbanietemad, Markus Sifft, and Daniel Hägele — Ruhr University Bochum, Faculty of Physics and Astronomy, Experimental Physics VI, Germany

Recent work has shown that higher-order spectra of continuous quantum measurement records provide characteristic fingerprints of stochastic system dynamics. These polyspectra capture essential features of measurement processes in platforms as diverse as nano-transport, single-photon emission from quantum dots, and spin-noise spectroscopy [1 - 3]. This makes them a more versatile analysis tool than traditional approaches such as full counting statistics or Langevin-based methods. The framework naturally incorporates measurement-induced damping, detector backaction, and the quantum Zeno effect. Key system parameters can be extracted by comparing experimental polyspectra with their analytical counterparts [2].

Here, we extend our single-detector theory to the case of multiple observables monitored simultaneously. We derive general expressions for spectra up to fourth order, apply the formalism to a coupled quantum system, and present a GPU-accelerated implementation that enables efficient computation of cross-correlation polyspectra from arbitrary Liouvillians.

[1] Hägele et al., PRB 98, 205143 (2018)
[2] Sifft et al., PRR 3, 033123 (2021)
[3] Sifft et al., PRA 109, 062210 (2024)

QI 21.4 Fri 10:30 BEY/0245

Characterizing genuine multipartite high-dimensional entanglement with the partition rank — •Sophia Denker[1], Ismaël Septembre[1], Robin Krebs[2], and Otfried Gühne[1] — [1]Universität Siegen, Siegen, Germany — [2]Technische Universität Darmstadt, Darmstadt, Germany

Entanglement is an important resource in quantum information as it has been demonstrated to bring advantages in several applications. In fact, these advantages are even higher when going to larger systems, i. e. increasing the number of particles or their local dimensions. However, with increasing system size also the characterization and quantification of quantum entanglement becomes more complex.

We introduce a new measure for the entanglement dimensionality of multiparticle states, based on the partition rank. The partition rank is given by the number of biseparable terms, needed to decompose a multipartite quantum state. Different from the Schmidt decomposition the terms appearing here are allowed to be separable with respect to different bipartitions, making this approach a truly multipartite quantification. We translate the problem of finding the closest state with a certain partition rank to the problem of finding the closest product state, which is known as the geometric measure of entanglement. This translation allows us to tackle this new problem with well-established methods. Along the way, we identify quantum states which are maximally entangled with respect to this measure and further show that our methods could make a contribution towards solving an open problem in mathematics, related to the partition rank.

QI 21.5 Fri 10:45 BEY/0245

Analyzing Classical vs Quantum Temporal Correlations in Discrete-Time Counting Processes — •Bita Olamaei, Pharnam Bakhshinezhad, and Giuseppe Vitagliano — Vienna Center for Quantum Science and Technology, Atominstitut, TU Wien, 1020 Vienna, Austria

We consider the problem of characterizing temporal sequences or outcomes arising from a quantum finite-state automaton process. This approach can be also seen as a relaxation of the original idea of Leggett and Garg of distinguishing classical from quantum temporal correlations based on macrorealist hidden-variable theories. The latter correspond essentially to automata with only one available state [1]. We focus on discrete-time counting processes and characterize the strength of temporal correlations via the probability of the "tick" event or via the Fano factor, that have been shown to have a nontrivial memory cost [2]. In particular, we look for the quantum d-state automaton model that can saturate the memory cost of the counting process, achieving either maximal probability of tick or maximal Fano factor, thereby characterizing the nature of the resource that, in particular, allows to surpass the performance of the analogous classical d-state automaton model.

[1]- C. Budroni and G. Vitagliano, Leggett-Garg macrorealism and temporal correlations, Phys. Rev. A. 107. 040101 (2023) [2]- C. Budroni, G. Vitagliano, and M. P. Woods, Ticking-clock performance enhanced by nonclassical temporal correlations, Phys. Rev. Res. 3, 033051 (2021)

30min. break

QI 21.6 Fri 11:30 BEY/0245

Measurement-induced transitions in fermionic systems — •Ihor Poboiko, Igor Gornyi, and Alexander D. Mirlin — Karlsruhe Institute of Technology, Karlsruhe, Germany

We develop a theory of measurement-induced phase transitions (MIPT) for d-dimensional lattice free fermions subject to random projective measurements of local site occupation numbers. In the limit of rare measurements, $\gamma \ll J$ (where γ is measurement rate per site and J is hopping constant), we derive a non-linear sigma model (NLSM) as an effective field theory of the problem. On the Gaussian level, valid in the limit $\gamma/J \to 0$, this model predicts "critical" (i.e. logarithmic enhancement of area law) behavior for the entanglement entropy. However, one-loop renormalization group analysis shows that for $d = 1$, the logarithmic growth saturates at a finite value $(J/\gamma)^2$ even for rare measurements, implying existence of a single area-law phase. The crossover between logarithmic growth and saturation, however, happens at an exponentially large scale, $\ln(l_{corr}) \sim J/\gamma$, thus making it easy to confuse with a transition in a finite-size system. Furthermore, utilizing ε-expansion, we demonstrate that the "critical" phase is stabilized for $d > 1$ with a transition to the area-law phase at a finite value of γ/J. The analytical calculations are supported by and are in excellent agreement with the extensive numerical simulations for $d = 1, 2$.

QI 21.7 Fri 11:45 BEY/0245

Efficient Entanglement Quantification with a Graph Neural Network — •Susanna Bräu, Martina Jung, and Martin Gärttner — Institut für Festkörpertheorie und Optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena

Entanglement is a fundamental feature of quantum mechanics, yet quantifying it - using measures such as entanglement entropy - generally requires reconstruction of the full quantum state. However, this is infeasible for larger systems, limiting the accessible system sizes. In this work, we predict quantum correlation measures for many-body spin systems from measurement snapshots with a supervised machine learning approach, avoiding full quantum state tomography. Our approach uses a permutation-invariant graph neural network (GNN), which scales linearly with the system size. To improve the scaling with the number of snapshots, we implemented a mini-set architecture, that divides the input into smaller subsets processed in parallel. This modified architecture enables entanglement prediction for larger data sets, potentially allowing for more accurate predictions than the traditional architecture without increasing the number of parameters in the network significantly. Furthermore, we aim to extend the approach from quantum many-body systems to continuous variable systems.

QI 21.8 Fri 12:00 BEY/0245

Chaotic melting of superconducting quantum chips: Quantum chaos in effective Hamiltonians — •Lucas Resch and Juan Diego Urbina — University of Regensburg

Superconducting qubits, in particular transmons, are at the forefront of quantum computing research [1]. Recent studies have revealed signatures of chaos near the ground state in these systems, challenging the conventional view that chaotic behavior emerges only at high energies [2]. In this work, we analyze spectral statistics, the inverse participation ratio, and the Lyapunov exponent to characterize this chaotic regime. Our results indicate that the observed chaotic features can be attributed to virtual interactions between computational states within an effective low-energy subspace and non-computational states outside it. This reinterpretation clarifies the origin of chaos in transmon-based architectures and provides a framework for understanding its implications for quantum control and device performance.

References

[1] J. M. Gambetta et al., *Building logical qubits in a superconducting quantum computing system,* npj Quantum Information 3, 2 (2017). [2] S. Börner et al., *Classical chaos in quantum computers,* Phys. Rev. Research 6, (2024).

QI 21.9 Fri 12:15 BEY/0245

Stabilizing Rényi entropy and entanglement distributions in unitary random circuits — Dominik Szombathy[1,2], Angelo Valli[1], Catalin Pascu Moca[3], Janos Asboth[1], Lorant Farkas[2], Tibor Rakovszky[1], and •Gergely Zarand[1] — [1]Budapest University of Technology and Economics, Budapest (Hungary) — [2]Nokia Bell Labs, Budapest (Hungary) — [3]University of Oradea, Oradea (Romania)

Entanglement and nonstabilizerness (or "magic") are instrumental in characterizing quantum complexity. While entanglement is related to the "quantumness" of a state, it is not exhaustive, as Clifford circuits generate highly entangled states but can be efficiently simulated classically. This lack of complexity is encoded in their peculiar spectral properties. Stabilizer Rényi entropy quantifies non-Clifford resources required to prepare a quantum state and is pivotal for achieving quantum advantage. These resources are related, yet their interplay is largely unexplored. We characterize entanglement and magic generation through their distributions, obtained by numerically sampling Clifford+T and Haar-random unitary circuits. For N qubits, the distributions are highly concentrated around typical values of entanglement (N/2 plus a quantum correction) and magic (N-2), which are not independent. However, we demonstrate that their fluctuations are asymptotically independent: both the covariance and mutual information of the joint entanglement-magic distribution vanish exponentially with system size.

Szombathy et al. PRR 7, 043080 (2025); PRR 7, 043072 (2025)

QI 21.10 Fri 12:30 BEY/0245

Quantitative bound entanglement in the Horodecki two-qutrit states — Gael Sentis[1] and •Jens Siewert[2,3] — [1]Grup d'Informació Quàntica, Universitat Autònoma de Barcelona, Barcelona, Spain — [2]University of the Basque Country and EHU Quantum Center, Bilbao, Spain — [3]Ikerbasque, Basque Foundation of Science, Bilbao, Spain

In 1999, Horodecki *et al.* [1] introduced a one-parameter family of two-qutrit states that has since become an archetypal example of entangled states with a positive partial transpose (PPT). PPT states are typically highly mixed, and their entanglement is widely regarded as rather weak. Yet the actual degree of this weakness has remained unclear. In Ref. [2], we provided a numerically exact solution for the linear entropy of the Horodecki two-qutrit PPT-entangled states. However, this result has limited practical relevance, as linear entropy is not commonly used in entanglement quantification, and no approximate analytical expression is known. In the present contribution, we investigate whether an exact formula for the concurrence of this emblematic family of states can be obtained.

[1] P. Horodecki, M. Horodecki, and R. Horodecki, Phys. Rev. Lett. **82**, 1056 (1999).

[2] G. Sentís, C. Eltschka, and J. Siewert, Phys. Rev. A **94**, 020302(R) (2016).

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Overview of Invited Talks and Sessions

(Lecture hall MER/0002; Poster P1)

Invited Talks

UP 2.4	Tue	10:15–10:45	MER/0002	**Klimakommunikation in der Schule? Mehr als nur darüber reden!** — •Michael Sach
UP 3.1	Tue	11:15–11:45	MER/0002	**Supporting the monitoring and tracking of carbon dioxide and methane emissions with satellites** — •Dominik Brunner, Gerrit Kuhlmann, Yasjka Meijer
UP 5.1	Tue	14:00–14:30	MER/0002	**A path to seamless modelling of the convective atmospheric boundary layer** — •Mirjana Sakradzija

Discussion on Sustainability on Monday during Lunch Break

PSV I	Mon	13:00–13:45	HSZ/AUDI	**Sustainability! And now? – Opportunities for young researchers** — •Roxana Scharpegge, Hiroki Sayama, Thomas Schubatzky, Birte Höcker, Uwe Riedel, John Plane, Pauleo Nimtz, Stefanie Falk

Invited Talks of the joint Symposium The Sustainability Challenge: A Decade of Transformation (SYSC)

See SYSC for the full program of the symposium.

SYSC 1.1	Mon	15:00–15:30	HSZ/AUDI	**Open-Endedness and Community-Based Approaches to Sustainability Challenges** — •Hiroki Sayama
SYSC 1.2	Mon	15:30–16:00	HSZ/AUDI	**Education as a Social Tipping Element: Evidence from Climate and Physics Education Research** — •Thomas Schubatzky
SYSC 1.3	Mon	16:00–16:30	HSZ/AUDI	**Mechanistic and Material Perspectives on Enzymatic Hydrolysis of Semicrystalline Polyesters** — •Birte Höcker
SYSC 1.4	Mon	16:45–17:15	HSZ/AUDI	**Decarbonization Options for Industry** — •Uwe Riedel
SYSC 1.5	Mon	17:15–17:45	HSZ/AUDI	**Impacts of Cosmic Dust and Space Debris in the Terrestrial Atmosphere** — •John Plane

Invited Talks of the Symposium Tipping Points in Socio-Economic and Climate Systems (SYTP)

See SYTP for the full program of the symposium.

SYTP 1.1	Thu	15:00–15:30	HSZ/AUDI	**Social Tipping in Heterogeneous and Polarized Populations** — •Sara Constantino, Sonke Ehret, Elke Weber, Sonja Vogt, Charles Efferson
SYTP 1.2	Thu	15:30–16:00	HSZ/AUDI	**Tipping points and regime shifts in coupled social-climate systems** — •Chris Bauch
SYTP 1.3	Thu	16:00–16:30	HSZ/AUDI	**How to tune Earth system models toward tipping?** — •Sebastian Bathiany, Niklas Boers
SYTP 1.4	Thu	16:45–17:15	HSZ/AUDI	**Algorithmic amplification and contextual sensitivity in political information exposure** — Iris Damião, Ana Vranic, Paulo Almeida, Lília Perfeito, •Joana Gonçalves de Sá
SYTP 1.5	Thu	17:15–17:45	HSZ/AUDI	**The complex interplay between democracy and platform power** — •Philipp Lorenz-Spreen

Sessions

UP 1.1–1.4	Mon	9:30–10:30	MER/0002	**Sustainability: Challenges and Solutions (joint session UP/CPP/SOE)**
UP 2.1–2.4	Tue	9:30–10:45	MER/0002	**Climate Communication**
UP 3.1–3.5	Tue	11:15–12:45	MER/0002	**Air Quality, Exposure and Atmospheric Dynamics**
UP 4	Tue	13:00–13:45	MER/0002	**Members' Assembly**
UP 5.1–5.5	Tue	14:00–15:30	MER/0002	**Modelling and Prediction Across Scales**
UP 6.1–6.6	Wed	9:30–11:00	MER/0002	**Upper Atmosphere, Polar Chemistry and Volcanic Aerosols**
UP 7.1–7.5	Wed	11:15–12:30	MER/0002	**Aquatic Systems: Limnology, Natural Waters, Wetlands and Soilmoisture**
UP 8.1–8.6	Wed	15:00–17:00	P1	**Poster**

Members' Assembly of the Environmental Physics Division

Tuesday 13:00–13:45 MER/0002

- Annual Report
- Upcoming Conferences and Events
- Awards and Appointments
- Miscellaneous

Sessions

– Invited Talks, Contributed Talks, and Posters –

UP 1: Sustainability: Challenges and Solutions (joint session UP/CPP/SOE)

Accompanying session to Symposium SYSC

Time: Monday 9:30–10:30 Location: MER/0002

UP 1.1 Mon 9:30 MER/0002

Making a university climate neutral: First experiences from implementing a Climate Protection Strategy at the University of Greifswald — •Christoph G. Hoffmann, Tiemo Timmermann, and Christian von Savigny — University of Greifswald, Greifswald, Germany

With a resolution of its Academic Senate, the University of Greifswald has in 2021 set the goal to achieve climate neutrality by the end of the decade.

While the aim of achieving climate neutrality within a few years is expectedly ambitious, a university as a bigger research institution has also a unique combination of knowledge to achieve it. This has already led to synergies from which particularly the teaching in the environmental subjects can benefit due to "home-made" practical experiences. This makes the whole University a living lab, in which the opportunities but also challenges of necessary transformations can be explored in an assessable setting.

Therefore, also the environmental physics group aims at contributing to and benefiting from this process. While our group is originally focused on basic atmospheric research, we cover a broader range of environmental physics topics in teaching, which overlap with the needs of the transformation process.

In this talk, we will give a short overview of the Climate Protection strategy of the University of Greifswald before we show some examples from our own work regarding the energy consumption of buildings.

UP 1.2 Mon 9:45 MER/0002

Life Cycle Assessment practices for PV technologies: systematic literature review — •Zeena Patel — Technische Universität Ilmenau

In response to the growing importance of sustainability in solar energy development, this study addresses critical gaps in the application of Life Cycle Assessment (LCA) to photovoltaic (PV) technologies. A systematic review of 48 recent LCA studies across first-, second-, and third-generation PV systems was conducted to evaluate current practices, identify methodological inconsistencies, and highlight emerging trends. Despite increasing research interest and technological diversification, substantial variability exists in the definition of functional units, system boundaries, and impact categories, which hinders comparability and reproducibility. The widespread reliance on secondary databases and the limited use of primary, site-specific data further constrains the accuracy of environmental impact assessments. Additionally, the underutilization of Life Cycle Costing (LCC) and inconsistent application of sensitivity analyses reveal significant gaps in comprehensive sustainability evaluation. To advance the field, this study proposes standardization of LCA methodologies, improved data transparency, and expansion of impact categories beyond global warming potential to include toxicity and resource depletion. These measures are essential for enhancing the robustness, reliability, and policy relevance of PV LCA studies, thereby supporting sustainable innovation and deployment in the solar energy sector.

UP 1.3 Mon 10:00 MER/0002

Electrochemical Modeling of SOFCs with Emphasis on Microkinetic and Anode Overpotential — •Iram Gul[1], Gabriela Soffiati[2], and Thiago Lopes[3] — [1]Research Center for Greenhouse Gas Innovation, University of São Paulo (USP), 05508-030, São Paulo * SP, Brazil — [2]Institute of Physics (IFUSP), University of São Paulo, Universidade, R. do Matão, 1371 - Butantã, São Paulo - SP, 05508-090 — [3]Research Center for Greenhouse Gas Innovation, University of São Paulo (USP), 05508-030, São Paulo * SP, Brazil

This study investigates Solid Oxide Fuel Cells (SOFCs) using a CO/H fuel mixture, focusing on thermodynamics, mass transport, and electrochemical kinetics. Thermodynamic properties such as heat capacity, enthalpy, entropy, and Gibbs free energy were analyzed across 600-800°C using MATLAB simulations. The Dusty Gas Model (DGM) revealed key mass transport behaviors in the anode, while Density Functional Theory (DFT) using VASP provided insights into surface reaction mechanisms. A microkinetic model examined the impact of anode overpotential on reaction kinetics and cell performance. Results show that higher temperatures improve mass transport and reduce Ohmic losses but slightly decrease the thermodynamic driving force. This multi-scale model enhances our understanding of SOFC behavior and offers a basis for improving fuel cell efficiency and material performance.

UP 1.4 Mon 10:15 MER/0002

Thermal stability of ceria-zirconia oxides(CeZrO4) nanoparticles using combustion synthesis for the CO oxidation and NOx reduction — •Hamza Mohamed — IMMM, UMRS 6283 CNRS, Le Mans Université, Bd O. Messiaen, 72085 Le Mans Cedex 09, France

The study presents a green synthesis approach for fabricating ceria-zirconia oxide nanoparticles (CeZrO4 NPs) using the solution combustion synthesis method. The synthesized CeZrO4 nanoparticles were characterized using various sophisticated instruments and methods to determine their detailed properties. The UV-Vis spectra showed a characteristic absorbance peak at 242 nm and a band gap (Eg) of 3.05 eV. Simultaneously, Fourier transform infrared spectra of CeZrO4 NPs displayed bands at 418 cm-1, 991 cm-1, 1382 cm-1, 1658 cm-1, 2306 cm-1, 3288 cm-1, and 3643 cm-1, which indicates the presence of phytochemicals that facilitate the reduction and stabilization of CeZrO4 NPs. The major peaks for cubic CeZrO4 NPs were obtained with a crystalline size of 9.6 nm by X-ray diffraction. The microscopic analyses revealed irregular, ovoid, and aggregated morphologies with sizes ranging from 3 to 10 nm. The XPS analysis revealed the existence of Ce3d, Zr3d, C1s, and O1s states with their corresponding atomic percentages. Therefore, this investigation focuses on synthesizing catalysts that demonstrate both thermal stability and high catalytic activity for the oxidation of CO and the reduction of NOx.

UP 2: Climate Communication

Climate communication, public engagement, education, and implementation of sustainability goals.

Time: Tuesday 9:30–10:45 Location: MER/0002

UP 2.1 Tue 9:30 MER/0002

Die AG Klima der DPG - Ziele und Projekte im Bereich Klimakommunikation — •Cedric Hossack — Mitglied des Vorstandes der AG Klima der DPG, Oberaudorf, Deutschland

Der anthropologische Einfluss auf das Erdsystem hat ein kritisches Ausmaß erreicht. Beinahe täglich werden wir mit Nachrichten über Starkregenfälle, Überschwemmungen, Sturmfluten oder Dürreperioden auf der ganzen Welt konfrontiert. Diese Ereignisse sind auf den Klimawandel zurückzuführen und betrifft die Menschen weltweit. Wie können die Menschen sensibilisiert werden und welchen Beitrag kann die Wissenschaft beim Thema Klimakommunikation leisten? Wer erklärt ihnen was da passiert und vor allem warum? Hier setzt Klimakommunikation an. Die Vermittlung von Fakten, der Austausch der Fachleute mit Politik und Gesellschaft.

Die Fakten und Risiken des Klimawandels für die menschliche Gemeinschaft sowie die sich daraus resultierende wissenschaftliche Verantwortung sind der Grund warum sich in der Deutschen Physikalischen Gesellschaft die Arbeitsgruppe Klima gegründet hat.

In diesem Vortrag werden die Ziele, Projekte und Resultate im ersten Jahr des Bestehens der Arbeitsgruppe Klima vorgestellt und was für die Zukunft geplant ist um das Thema Klima wieder in den Fokus des gesamtgesellschaftlichen Diskurses zu bringen.

UP 2.2 Tue 9:45 MER/0002

On the communication of climate research: Who wants to know about it, when and why? — •Mirjam Bourgett — Alfred-Wegener-Institut, Bremerhaven, Germany

Effective climate communication is crucial for translating scientific certainty into climate action, yet it presents unique challenges compared to communicating other scientific fields. This presentation explores the complex communication landscape of climate research.

A focus will be placed on the influence of media and how varying socio-ecological backgrounds shape the reception and perception of climate science. Who seeks climate information, when, and for what purpose? When does the reception of climate science appear to be political? We will also addresses the role of climate emotions and how scientific results trigger emotions. It is important to try to anticipate possible reactions of the public and provide different communication strategies as well as additional information on possible actions and processing strategies.

As an outloook we discuss a set of communication strategies for today's environment, emphasizing: 1) Direct Communication, bypassing traditional news filters; 2) Enrolling the power of climate science by linking it directly to essential planetary and human health outcomes; and 3) Target-Oriented Communication, where the message is adapted to the specific needs of the public. The presentation will conclude with concrete good practice examples to guide researchers in making their work more usable in achieving planetary health.

UP 2.3 Tue 10:00 MER/0002

From Climate Science to Collective Action: How Participatory Formats Shape Organizational Climate Engagement — •Clara Scheve and Thomas Wrona — Hamburg University of Technology, Hamburg, Germany

While climate science has established robust evidence on anthropogenic climate change, translating this knowledge into sustained organizational action remains a critical challenge. Our research investigates how science-based participatory formats function as socio-material devices that bridge climate science communication and organizational transformation. We study "Climate Fresk," a three-hour collaborative workshop format that translates IPCC-based climate science into 42 illustrated cards. Participants collectively reconstruct causal chains of climate change by arranging and connecting these cards, moving from cognitive understanding through emotional engagement to collective sensemaking. Implemented in large industrial organizations (e.g., aerospace, manufacturing, banking), Climate Fresk operates as more than a one-time educational intervention: through train-the-trainer structures, companies internalize the format, creating selfreinforcing "swarm effects" that enable sustained engagement. This work contributes to understanding how climate science communication can be designed not merely for awareness but for fostering collective agency and embedding climate action in organizational infrastructures. By examining how scientific knowledge is translated through participatory formats into organizational transformation, we offer evidence-based design principles for effective climate communication in organizations.

Invited Talk UP 2.4 Tue 10:15 MER/0002

Klimakommunikation in der Schule? Mehr als nur darüber reden! — •Michael Sach — Studienseminar für Gymnasien Bad Vilbel, Burggymnasium Friedberg, Uni Frankfurt

In diesem Kurzvortrag stelle ich einige Facetten der Klimabildung in Schulen mit speziellem Bezug zum Physikunterricht vor. Dabei beziehe ich mich auf alltägliche Unterrichtserfahrungen im Spannungsfeld curricularer Rahmenbedingungen und pädagogischer Herausforderungen der Klimakrise, auf das didaktische Konzept des Bildungsprogramms der LMU München (Klimawandel - verstehen und handeln), auf unterschiedliche Konzepte der BNE (Bildung für nachhaltige Entwicklung) sowie auf eine kritische Perspektive auf die Etablierung von Klimaschulen in Deutschland.

UP 3: Air Quality, Exposure and Atmospheric Dynamics

Remote sensing and transport modeling complemented by urban exposure, renewable energy-aerosol interactions, particle transport mechanics, and large-scale dynamics affecting aerosol transport.

Time: Tuesday 11:15–12:45 Location: MER/0002

Invited Talk UP 3.1 Tue 11:15 MER/0002

Supporting the monitoring and tracking of carbon dioxide and methane emissions with satellites — •Dominik Brunner[1], Gerrit Kuhlmann[1], and Yasjka Meijer[2] — [1]Empa, Dübendorf, Switzerland — [2]European Space Agency (ESA), Noordwijk, the Netherlands

Achieving the goals of the Paris Agreement to limit global warming to no more than 2°C above pre-industrial levels requires drastic cuts to emissions of carbon dioxide (CO2) and methane (CH4). The Enhanced Transparency Framework of the Paris Agreement requires all countries to provide transparent information on the implementation and achievement of their national mitigation objectives. The atmospheric community supports this process by providing independent emission monitoring based on atmospheric concentration measurements from ground and space. The European Copernicus CO2 Monitoring mission, CO2M, will be a constellation of three satellites to be launched from 2027, is designed to greatly enhance our capabilities to quantify CO2 and CH4 emissions from industrial sources, cities and countries. In this presentation, we will provide an overview of the CO2M mission, explain how CO2 and CH4 will be retrieved from spectral radiance measurements, and show its complementarity to other observations. We will present examples of how CO2M contributes to quantifying emissions, outline the atmospheric modelling frameworks that will assimilate its observations, and present a long-term perspective of how CO2M together with other observations will support policymakers in reaching the goals of the Paris Agreement.

UP 3.2 Tue 11:45 MER/0002

Stratification patterns of soil particle electric charge distribution boost wind-blown sand transport — •Danilo da Silva Borges, Sandesh Kamath, Gerhard Wurm, and Eric Josef Ribeiro Parteli — Faculty of Physics, University of Duisburg-Essen

Since the pioneering studies by Michael Faraday in the 19th century, it is known that wind-blown sand transport generates electric fields reaching various MV/m. Such fields are caused by contact electrification of sand particles during wind-blown transport, but their effect on the minimal threshold wind velocity (u_{ft}) required for wind-blown sand transport initiation remains controversial. Elucidating this effect is of utmost relevance for a broad range of fields, from desertification research to the geology of Mars. Here we show, by means of CFD–DEM simulations, that u_{ft} can be substantially affected not only by the presence of a particle charge distribution, but also by the spatial distribution of the charges within the granular soil. While a random spatial distribution of charges enhances u_{ft}, the presence of domains of like electric charges in the soil lowers the onset for sand transport. In a general fashion, our simulations suggest that the total electrostatic to gravitational potential energy ratio, C_0, is the most important control parameter, with u_{ft} increasing (decreasing) with the charge magnitude when C_0 is negative (positive). Our findings provide a theoretical framework for the interpretation of wind-tunnel and field data, and demonstrate that spatial charge patterns constitute a key parameter for wind-blown sand transport.

UP 3.3 Tue 12:00 MER/0002

Effective UV doses for the production of cutaneous vitamin D in Athens, Greece: assessing aerosol-related uncertainties in satellite-based retrievals — •Theodora Stavraka[1,2,5], Ilias Fountoulakis[1,5], Kostas Eleftheratos[2,5], Panagiotis Nastos[2,5], Thomais Papazoi[1], Konstantinos Fragkos[3], Andreas Kazantzidis[4], Vassilis Amiridis[6], and Christos Zerefos[1,5,7,8] — [1]Academy of Athens, Greece — [2]University of Athens, Greece — [3]The Cyprus Institute, CARE-C, Nicosia, Cyprus — [4]University of Patras, Greece — [5]Biomedical Research Foundation of the Academy of Athens, Greece — [6]National Observatory of Athens, Greece — [7]Navarino Environmental Observatory, Messenia, Greece — [8]Mariolopoulos-Kanaginis Foundation, Athens, Greece

The purpose of this study is to evaluate satellite- and reanalysis-based retrievals of the UV effective dose for cutaneous vitamin D production using ground-based measurements over Athens, Greece. We evaluate data from (1) the climatology by Fragkos et al., (2024) based on CAMS information combined with OMI and MSG satellite data, and (2) the UV climatology of TEMIS also based on data from various sensors analyzing air quality. Ground-based spectral solar UV irradiance measurements performed with a Brewer MKIV spectrophotometer operating at the Academy of Athens have been used for the evaluation, as well as AOD measurements from a co-located CIMEL sun-photometer, part of the AERONET network. The analysis covers 2008 - 2021 when both the CIMEL and the Brewer were operating side-by-side.

UP 3.4 Tue 12:15 MER/0002

Observations of double aerosol layers below an altitude of 30 km with different causes of formation — •Christian Löns[1], Ronald Eixmann[2], and Christian von Savigny[1] — [1]University of Greifswald, Germany — [2]Leibniz-Institute of Atmospheric Physics at the University of Rostock, Germany

In December 2011, it was possible to observe a second layer with an increased Mie signal above the stratospheric aerosol layer in measurements taken with a Doppler lidar in the southern high latitudes during the collapse of the polar vortex. The signature descends from an altitude of 28 km within a few days and can be observed as a broad aerosol layer after about a week. The signature is also observable in satellite measurements of the aerosol extinction coefficient by

OSIRIS and SCIAMACHY. In December 2018, the Kamchatka asteroid, approximately 10 m in diameter, exploded over the Bering Sea. It was the third largest recorded impact on Earth after the Tunguska event and the Chelyabinsk meteor. The expected transport path can be modelled using trajectory analyses. Using measurements of the aerosol extinction coefficient from OMPS-LP, signatures of the Kamchatka asteroid can be observed at an altitude of 26 km one week after its explosion. The signature can be observed on several consecutive days as an increase in the extinction coefficient at an altitude of ~26-28 km during its transport over the North Atlantic from America towards Europe.

UP 3.5 Tue 12:30 MER/0002

Validation of Airborne HALO Wind and Aerosol Measurements Using Ground-Based Lidar and Radar Observations in Kühlungsborn — •Ronald Eixmann[1], Gerd Baumgarten[1], Frederik Ernst[1], Jan Froh[1], Josef Höffner[1], Philipp Joppe[2], Christian Löns[3], Thorben Lüke-Mense[1], Alsu Mauer[1], Mira Pöhlker[4], Pablo Saavedra Garfias[1], Marina Schimpf[5], and Marius Zecha[1] — [1]Leibniz-Institute of Atmospheric Physics, Kühlungsborn, Germany — [2]Max Planck Institute for Chemistry, Mainz, Germany — [3]University of Greifswald, Greifswald, Germany — [4]Leibniz Institute for Tropospheric Research, Leipzig, Germany — [5]German Aerospace Center, Germany

On 20 August 2025, a scientific research flight was conducted over northern Germany with destination Kühlungsborn as part of the HALO-South mission and its preparatory activities. Flight operations were led by the Leibniz Institute for Tropospheric Research (TROPOS), Leipzig, with coordination by the Max Planck Institute for Chemistry, Mainz, in collaboration with the German Aerospace Center (DLR), Oberpfaffenhofen. Ground-based measurements were carried out by the Leibniz Institute of Atmospheric Physics (IAP), Kühlungsborn.

This contribution presents the first validation results combining ground-based lidar and radar observations with airborne HALO measurements at the tropopause level to assess wind fields and aerosol distributions. The campaign demonstrates the potential of coordinated airborne and ground-based observations to provide a comprehensive, multi-dimensional characterization of atmospheric dynamics and aerosol variability at a single site.

UP 4: Members' Assembly

Agenda:

- Annual Report of PA Environmental Physics
- Upcoming Conferences
- Awards and Appointments
- Miscellaneous

Time: Tuesday 13:00–13:45 Location: MER/0002

30 min break

UP 5: Modelling and Prediction Across Scales

Seamless prediction and boundary-layer physics; the session then broadens to cross-cutting modelling, multiscale methods, data assimilation, computational techniques, and optimization of fuel combustion.

Time: Tuesday 14:00–15:30 Location: MER/0002

Invited Talk UP 5.1 Tue 14:00 MER/0002

A path to seamless modelling of the convective atmospheric boundary layer — •Mirjana Sakradzija — Ludwig Maximilian University of Munich, Germany

Numerical weather prediction (NWP) has reached operational grid spacings of less than 1 km at several leading weather centres. The possibility of using the same model configuration across various applications and spatial scales, ranging from local large-eddy-resolving cases to global NWP and climate simulations, is now a reality. I will explore one such possibility by using an operational NWP model at sub-km resolutions and examining its ability to represent relevant processes in the atmospheric boundary layer (ABL) compared with standard large-eddy simulations, and micro- and sub-mesoscale meteorological observations. Next, I will discuss the current state of development of a unified parameterization of ABL turbulence, convection, and clouds, and the prospects for a smooth transition from parameterized to resolved scales. The importance of land-atmosphere coupling emerges at all spatio-temporal scales as the key forcing factor for the ABL and one of the largest sources of uncertainty in both modelling and observations.

UP 5.2 Tue 14:30 MER/0002

Projected variability of solar resources in the Eastern Mediterranean and Middle East — •Nikolaos Papadimitriou[1,2], Kostas Douvis[2], Stergios Misios[2], Antonis Gkikas[2], Andreas Kazantzidis[1], Christos Zerefos[3,4,5], and Ilias Fountoulakis[2] — [1]Department of Physics, University of Patras, Patras, Greece — [2]Research Centre for Atmospheric Physics and Climatology, Academy of Athens, Athens, Greece — [3]Biomedical Research Foundation, Academy of Athens, Athens, Greece — [4]Navarino Environmental Observatory (N.E.O.), Messinia, Greece — [5]Mariolopoulos-Kanaginis Foundation for the Environmental Sciences, Athens, Greece

Climate change is expected to alter key atmospheric parameters influencing downwelling solar irradiance, including cloudiness and aerosol concentration. The Eastern Mediterranean and Middle East region, identified as a climate hotspot and known for its high levels of solar exposure, constitutes a particularly relevant case study for assessing future variability of solar energy potential. We use data from three global climate models that participated in the 6th phase of the Climate Model Intercomparison Project (CMIP-6): CNRM-CM6-1-HR, INM-CM5-0, and MPI-ESM1-2-HR. Projections were evaluated under three different Shared Socioeconomic Pathways (SSPs 245, 370, 585). In this study, we analyzed trends in surface downwelling solar irradiance and associated climatic drivers and estimate the photovoltaic (PV) power potential by performing simulations with the climate data interface of the GSEE model.

UP 5.3 Tue 14:45 MER/0002

An optimization-based approach to track the Asian summer monsoon anticyclone across daily and interannual variability — •Oleh Kachula, Bärbel Vogel, Gebhard Günther, and Rolf Müller — Forschungszentrum Jülich, 52428 Jülich, Germany

The Asian summer monsoon anticyclone (ASMA) is an upper troposphere-lower stratosphere (UTLS) meteorological circulation system that develops over Asia during summer months in the Northern Hemisphere. It strongly influences regional weather, particularly monsoon rainfall, and shapes the climate of densely populated regions such as India and Southeast Asia. The ASMA also plays a major role in transporting near-surface anthropogenic pollutants to the UTLS, with important implications for air quality and stratospheric chemistry. Improving our understanding of this complex system is essential for enhancing weather prediction capabilities and for better assessing climate and environmental impacts.

We present a novel method based on the absolute vortex moments that defines the ASMA boundary by solving an optimization problem. Here, we address the ASMA's climatology (1980-2023), interannual variability, the variability of the start and end dates and the duration of the anticyclone peak phase calculated with help of the defined novel method by using the ERA5 reanalysis provided by ECMWF. Our findings show that the ASMA area decreases at 370, 390 and 410 K over the period 1980-2023 in contrast to previous studies. Further, we provide evidence of possible bimodality of the ASMA.

UP 5.4 Tue 15:00 MER/0002

Differentiable Operators for Ocean Simulation and Inverse Problems — •Pauleo R. Nimtz[1,2], Vadim Zinchenko[1], Kubilay T. Demir[1], Anthony Frion[1], and David S. Greenberg[1] — [1]Helmholtz-Zentrum Hereon, Geesthacht, Germany — [2]Universität Potsdam, Potsdam, Germany

Gradient-based optimization is a powerful tool for fitting mechanistic simulations to observation data and is crucial for modern machine learning frameworks. However, in established numerical models of ocean hydrodynamics (e.g. NEMO, ICON-O, SCHISM) and biogeochemistry (e.g. ECOSMO, HAMMOC),

the required gradients with respect to model input are typically not available. To address this, we implemented a family of differentiable operators in PyTorch, focusing on the transport and interaction of tracers in fluid dynamical simulations. We provide key operations such as advection, turbulent mixing and biogeochemical processes, with native GPU support and efficient vectorized code. Gradients are computed automatically with memory-efficient custom backpropagation routines for implicit time integration. These operators enable auto-differentiable simulations, with applications including model tuning, data assimilation, physics-informed neural networks, and hybrid physical and data-driven models. We demonstrate their utility by performing data assimilation to identify initial conditions in simulations of inert tracer transport and spatially extended models of light- and nutrient-dependent aquatic ecosystems. These tools provide an essential step towards building and tuning differentiable ocean models, and fitting them to observation data.

UP 5.5 Tue 15:15 MER/0002

Approximating the universal thermal climate index using sparse regression with orthogonal polynomials — •Sabin Roman[1], Gregor Skok[2], Ljupco Todorovski[2,1], and Saso Dzeroski[1] — [1]Department of Knowledge Technologies, Jozef Stefan Institute — [2]Faculty of Mathematics and Physics, University of Ljubljana

The Universal Thermal Climate Index (UTCI) is widely used to quantify outdoor thermal comfort, but its standard sixth-degree polynomial approximation can yield substantial numerical errors, especially under extreme conditions. We present a new approximation method that preserves computational efficiency while offering markedly improved accuracy and stability. The method employs sparse regression with Legendre polynomial bases, whose orthogonality ensures well-conditioned models and a hierarchical coefficient structure. Adjusting sparsity constraints yields families of models that span a clear Pareto front between accuracy and complexity. Compared with the standard UTCI approximation, the proposed models substantially reduce mean, absolute, and root-mean-square errors and significantly limit large deviations. Training on only 20% of the data while testing on the remaining 80% demonstrates strong generalization, further supported by bootstrap analysis. The resulting representation acts as a Fourier-like expansion in an orthogonal basis, providing an efficient and highly accurate approximation of the UTCI.

UP 6: Upper Atmosphere, Polar Chemistry and Volcanic Aerosols

Upper-atmosphere, polar processes, volcanic aerosols, remote sensing, and dynamics.

Time: Wednesday 9:30–11:00 Location: MER/0002

UP 6.1 Wed 9:30 MER/0002

Twofold Chemical Properties of Premelting at Ice Surfaces — •Thorsten Bartels-Rausch[1], Jérôme Gabathuler[1], Yanisha Manoharan[1], Luca Artiglia[1], Markus Ammann[1], Rawan Abouhaidar[2], Céline Toubin[2], and Ivan Gladich[3] — [1]Paul Scherrer Institute, Villigen, Switzerland — [2]Universite de Lille, Lille, France — [3]University of Urbino, Urbino, Italy

The physical properties of ice surfaces are a longstanding subject of intense research motivated by their relevance in glacial flow, thunder, (anti-)freezing, and on-water catalysis. How water molecules re-arrange at the surface to minimize energy, going as far as evolving liquid-like features in premelting, is under ongoing investigation. Less elusive remains the impact of this disorder on chemistry. This is problematic considering the role of ice and snow interfaces in chemical processes, such as global geochemical cycles. This work presents hexylamine adsorption as a means to investigate the chemical characteristics of the ice- and water-air interface. By analyzing the X-ray photoemission spectra of the adsorbate at the air-ice interface against those at the air-water interface, we discovered experimental evidence indicating differing chemical interactions at these two interfaces. Molecular dynamics and core binding calculations linked these spectroscopic differences to an active interfacial proton transfer.

UP 6.2 Wed 9:45 MER/0002

Bromine Explosion signals in Arctic snow — •Stefanie Falk[1], Hogo El-Mansi[2], Ariane Le Cardinal[1], Luca Reissig[1,4], Bianca Zilker[3], Andreas Richter[3], Hans-Werner Jacobi[2], and Björn-Martin Sinnhuber[1] — [1]Karlsruhe Institute of Technology, Institute of Meteorology and Climate Reseach, Atmospheric Trace Gases and Remote Sensing, Karlsruhe, Germany — [2]nstitute of Environmental Geosciences (IGE), Université Grenoble Alpes / CNRS / Grenoble INP / INRAE / IRD, Grenoble, France — [3]University of Bremen, Institute of Environmental Physics, Bremen — [4]German Weather Service, Offenbach, Germany

Ozone (O_3) volume mixing ratios (VMR) below 5 ppb are frequently observed during springtime in the polar boundary layer. The destruction of O_3 is caused by reactive halogen compounds, likely dominated by bromine (Br_2) released from salty ice and snow. The driving mechanism leads to exponential growth in Br_2 VMR during so-called Bromine Explosions (BEs). Increased vertical column densities (VCD) of bromine monoxide (BrO) are regularly observed by remote sensing. Long-term observations of O_3 at Arctic coastal sites and BrO indicate emerging signals of a changing climate. We also compare modeled bromine deposition on snow to bromide concentrations determined in snow samples taken at Spitsbergen in 2024. To this end, we use the ECHAM/MESSy Atmospheric Chemistry (EMAC) model, including a treatment of bromine release, recycling on ice and snow-covered surfaces, and parameterized emissions from sea salt aerosols. We discuss implications for the assumed sources of Br_2 in the Arctic.

UP 6.3 Wed 10:00 MER/0002

Polar 6 airborne in situ aerosol and turbulence measurements in the Arctic and Antarctica — •Laura Köhler[1], Stephan Borrmann[2], Jörg Hartmann[1], Zsofia Juranyi[1], Christof Lübkes[1], Jonas Schäfer[3], David Simon[3], Frank Stratmann[3], and Andreas Herber[1] — [1]Alfred-Wegener-Institut, Bremerhaven, Germany — [2]Max Planck Institute for Chemistry, Mainz, Germany — [3]Leibniz Institute for Tropospheric Research, Leipzig, Germany

We present three aircraft campaigns conducted with the research aircraft Polar 6, all using similar configurations for in situ aerosol and turbulence measurements. Two campaigns, BACSAM I (autumn 2022) and BACSAM II (spring 2024), were carried out in the Arctic from Longyearbyen. The third campaign, SANAT, will take place in early 2026 from Neumayer III Station in Antarctica. These measurements provide one of the first aerosol profile datasets collected in the vicinity of Neumayer III.

A comprehensive suite of aerosol instruments enables measurements of aerosol parameters such as number concentrations and size distributions, while the aircraft*s nose boom provides high-frequency (100 Hz) meteorological and turbulence data. During all three campaigns, the Turbulence-Bird (T-Bird) was also deployed up to 80 m below the aircraft, carrying additional aerosol and turbulence sensors allowing for simultaneous observations at two altitudes.

This unique setup enables investigations such as airborne particle fluxes. We present the three campaigns, outline the measurement setup, and show examples of the atmospheric conditions encountered.

UP 6.4 Wed 10:15 MER/0002

Stratospheric aerosol size evolution after the Ruang volcanic eruptions in 2024 — •Felix Wrana, Christian von Savigny, and Sandra Wallis — Institute of Physics, University of Greifswald, Greifswald, Germany

The size of stratospheric aerosols is an important factor in their effect on Earth's radiative balance and on atmospheric chemistry. On April 17th and 30th 2024, the Ruang volcano (2.3 °N, 125.37 °E) had two eruptions with a volcanic explosivity index (VEI) of 4, both reaching the stratosphere. Although each eruption injected only around 0.26 Tg of SO_2, they had a considerable effect on the stratospheric aerosol size in the Junge layer, that was at that point in time still affected by the exceptional Hunga eruption of 2022. The evolution of the stratospheric aerosol size from before to after the Ruang eruptions is shown, based on a multi-wavelength retrieval from the satellite solar occultation measurements of the Stratospheric Aerosol and Gas Experiment III on the ISS (SAGE III/ISS). Similarities and differences with other volcanic eruptions that reached the stratosphere in the previous years are shown and discussed, adding to our current understanding of the main driving factors behind observed aerosol size increases vs decreases after volcanic eruptions. Also, the satellite retrieval is validated with balloon-borne in situ measurements.

UP 6.5 Wed 10:30 MER/0002

How long does H2O from a strong tropical volcanic eruption need to reach the polar summer mesopause? — •Sandra Wallis[1], Hauke Schmidt[2], and Christian von Savigny[1] — [1]University of Greifswald, Greifswald, Germany — [2]Max Planck Institute for Meteorology, Hamburg, Germany

It is assumed that the historic 1883 Krakatoa volcanic eruption emitted a large amount of water vapour into the tropical middle atmosphere (20 - 100 km). According to a prominent hypothesis, this volcanic water vapour might have been transported to the polar summer mesopause resulting in the first ever sighting of noctilucent clouds (NLC) two years later. This discussion was recently revived after the 2022 Hunga eruption. We used simulations from the Hamburg Model of the Neutral and Ionized Atmosphere (HAMMONIA) to determine the transport time of water vapour from the tropics to the summer polar mesopause for different volcanic injection seasons and heights. The results suggest that a 1.5 to 2 year transport time period is plausible, strengthening the Krakatoa-NLC hypothesis.

UP 6.6 Wed 10:45 MER/0002

Is there a stratospheric airglow layer caused by the chemiluminescent reaction of NO and O_3? — •Christian von Savigny[1], Christoph G. Hoffmann[1], Wuhu Feng[2,3], and John Plane[2] — [1]Institute of Physics, University of Greifswald, Greifswald, Germany — [2]School of Chemistry, University of Leeds, Leeds, UK — [3]National Centre for Atmospheric Science, Leeds, UK

Airglow, i.e. non-thermal emissions caused directly or indirectly by solar radiation, is a ubiquitous phenomenon in the Earth's atmosphere and also other planetary atmospheres. Most airglow emissions in the terrestrial atmosphere occur in the mesosphere and thermosphere, but some emissions can also extend down to below the stratopause. The most prominent example is the $O_2(^1\Delta)$ dayglow emission at a wavelength of about 1270 nm. Another potential stratospheric emission is a nightglow emission by excited NO_2 that was reported three decades ago by Evans and Shepherd (1996) based on nightglow measurements with the Wind Imaging Interferometer (WINDII) on UARS and model simulations. This emission has not yet been confirmed in other studies. In this contribution we use nightglow simulations based on input from the Whole Atmosphere Community Climate Mode (WACCM) to investigate, (a) how intense the NO + O_3 chemiluminescence is at stratospheric altitudes, and (b) whether it can likely be identified with a satellite limb viewing spectrometer. Our results indicate that the NO + O_3 volume emission rates are orders of magnitude weaker than suggested earlier.

UP 7: Aquatic Systems: Limnology, Natural Waters, Wetlands and Soilmoisture

Cohesive freshwater and wetland focus, combining circulation, properties, biogeochemistry, and innovative sensing/quantification.

Time: Wednesday 11:15–12:30 Location: MER/0002

UP 7.1 Wed 11:15 MER/0002

One Dimensional Thermobaric Mixing in a Deep Lake — •Joshua Marks[1,2], Kazuhisa A. Chikita[3], and Bertram Boehrer[1,2] — [1]Department of Lake Research, Helmholtz Centre for Environmental Research - UFZ, Magdeburg, Germany — [2]Department of Physics and Astronomy, Heidelberg University, Heidelberg, Germany — [3]Arctic Research Center, Hokkaido University, Sapporo, Japan

Thermobaricity is defined as the temperature dependence of the compressibility of water. It leads to a decrease of the temperature of maximum density T_{md} with increasing pressure. This effect has significant impacts in many deep lakes, like Lake Shikotsu, Hokkaido, Japan. Despite this, it is often not implemented in lake models, except in combination with external forcing. We created a simplified 1D model with the surface temperature input as only external forcing, excluding salinity and any other competing influences. For stability considerations, we used the in-situ density. The model recreated the one dimensional deep water renewal with the following key features: (1) at the intersection of the temperature profile with the T_{md} line diffusion induces cabbeling which leads to thermobaricity driven deep water circulation, (2) this deep water circulation cell is detached from the surface, (3) the deep water stays isothermal, (4) and after the winter stratification the temperature profile aligns with the T_{md} line. The results emphasize the necessity and the feasibility of the implementation of thermobaricity in lake models to ensure correct behaviour of the deep water renewal.

UP 7.2 Wed 11:30 MER/0002

Sound Speed Contributions of Solutes in Water — •Ivan Selyakov, Lutz Hrdlicka, and Bertram Boehrer — Helmholtz Centre for Environmental Research, Magdeburg, Germany

This study provides a structured investigation of the fundamental property of sound speed in limnic waters, presenting systematic experimental data on the contributions of various electrolytes over a temperature range from 1 °C to 30 °C and concentrations up to 0.05 mol L-1. While established approaches such as the UNESCO formula and the TEOS-10 package describe sound speed in oceanic waters, information on the contributions of specific solutes in freshwater environments remains limited. We observed no evidence of nonlinearities in either temperature or concentration dependences within the studied range and accuracy. Coefficients for calculating sound-speed excess are provided for a range of salts containing all major ions commonly found in natural waters. Contributions in mixtures of salts can be directly added, and a numerical approach is introduced for predicting sound speed in arbitrary mixtures of the investigated ions, including unusual combinations found in volcanic or meromictic conditions. Using our data, isothermal and adiabatic compressibility as well as in-situ density can be calculated with enhanced accuracy. These findings are valuable for applied fields such as acoustic sensing and environmental monitoring, and for advancing theoretical understanding in physical limnology and aquatic thermodynamics. The numerical tool implementing this approach has been validated against the UNESCO formula.

UP 7.3 Wed 11:45 MER/0002

First Observations of Extreme Gas Accumulation in Meromictic Lake Kilevann — •Bertram Reventlow[1,2], Bertram Boehrer[2], Florian Meienburg[1], Joshua Marks[2], Marius Feuerle[1], Martina Schmidt[1], and Werner Aeschbach[1] — [1]Institute of Environmental Physics, Heidelberg, Germany — [2]Helmholtz Centre for Environmental Research - UFZ, Magdeburg, Germany

Lake Kilevann in southern Norway is a former fjord that became isolated from the sea about 8000 years ago due to isostatic rebound. In its deepest basin, a strongly stratified layer of ancient seawater remains trapped between 60 and 100 m depth. Such isolated layers in meromictic lakes tend to accumulate gases, which can lead to limnic eruptions. In Lake Kilevann, we measured methane concentrations among the highest ever recorded in lakes. Isotopic analyses of CO_2 and CH_4 indicate long carbon residence times, a biogenic origin, and active methanogenesis in the water column. Preliminary noble gas measurements suggest strong depletion, supporting the hypothesis of bubble-mediated gas transfer, which could potentially trigger an eruption. On the other hand, the water column is strongly stratified, except for a single double-diffusive convection cell near the lake bottom. Major ions exhibit fractionated depletion relative to oceanic values, indicating that molecular diffusion over the lake's lifetime is a key mechanism driving the dilution of the seawater.

UP 7.4 Wed 12:00 MER/0002

Airborne Lidar Measurements of Methane over Canada — •Arunima Das[1,2,3], Christoph Kiemle[2,3], Sabrina Zechlau[1,2], Martin Wirth[2], and Andreas Fix[2] — [1]Ludwig Maximilian University of Munich — [2]Deutsches Zentrum für Luft- und Raumfahrt — [3]Technical University of Munich

Methane(CH4) is a key greenhouse gas with an atmospheric lifetime of about 10 years and high mitigation potential. Wetlands, coastal zones and offshore oil and gas facilities are major CH4 sources yet quantifying emissions over these remains challenging. Passive sensors struggle over low-albedo water surfaces and in-situ data are sparse. The French-German MERLIN mission aims to address this gap. Its Integrated Path Differential Absorption(IPDA) lidar will retrieve global column-averaged CH4 independent of sunlight. IPDA maintains high precision over dark water, flooded wetlands, and high-latitude regions with low sun angles. A robust retrieval algorithm performing accurately across diverse surfaces is crucial for detecting small CH4 gradients. CHARM-F, MERLIN's airborne demonstrator provides essential testing. During the CoMet 2.0 campaign, it measured XCH4 across Arctic wetlands and lake systems in the Hudson Bay Lowlands with agreement to in-situ vertical profiles within 1%. Further analysis shows negligible bias over land and higher biases over water, majorly driven by varying signal-to-noise ratio. The upcoming campaign CoMet 3.0 will broaden environmental coverage over tropical wetlands in Brazil, further testing CH4 retrieval performance over extensive water-dominated regions. These observations significantly reduce gaps in global CH4 monitoring.

UP 7.5 Wed 12:15 MER/0002

Environmental monitoring with cosmic-ray neutrons: new experiments on ships, blimps, and trains — •Martin Schrön[1], Lasse Hertle[1], Daniel Altdorff[1,2], Solveig Landmark[1], Bernd Heber[3], Sascha Oswald[2], Peter Dietrich[1], and Steffen Zacharias[1] — [1]UFZ - Helmholtz Centre for Environmental Research, Leipzig — [2]Institute of Environmental Science and Geography, University of Potsdam — [3]Institute of Experimental and Applied Physics, University of Kiel

Cosmic-ray neutron sensing (CRNS) technology has emerged as a robust technique for measuring root-zone soil moisture and snow water equivalent at the hectare scale, addressing many limitations of traditional electromagnetic and remote-sensing methods. Here we will present three new applications that utilize mobile cosmic-ray neutron detectors to explore (i) Earth's geomagnetic field with the "Polarstern" research vessel from Bremerhaven to Antarctica, (ii) the soil moisture distribution of inaccessible regions in Germany using hot-air blimps, and (iii) country-scale soil moisture patterns using CRNS on trains along German railway networks. The three experiments showcase recent advancement in CRNS research which may contribute to new applications in hydrology, environmental physics, and even space wheather.

UP 8: Poster

Time: Wednesday 15:00–17:00 Location: P1

UP 8.1 Wed 15:00 P1

Defect-Driven Photoluminescence Quenching in WO3 Micro-Flakes: A simple approach for Bisphenol A Detection — •Hamood Al Shidhani[1], Sumesh Pillai[1], Basim Al Farsi[1], Zainab Al Ruqaishi[2], and Abey Issac[1] — [1]Department of Physics, College of Science, Sultan Qaboos University, P.O Box 36, Al Khoud, Muscat, PC 123, Oman. — [2]Department of Chemistry, College of Science, Sultan Qaboos University, P.O Box 36, Al Khoud, Muscat, PC 123, Oman.

This study presents a novel approach utilizing photoluminescence (PL) spectroscopy of tungsten trioxide (WO*) micro-flakes to detect Bisphenol A(BPA). The WO* was synthesized via a solution phase route, with enhanced sensitivity achieved through controlled annealing. The annealing process increases oxygen vacancy concentrations, which are directional-dependent within the crystal lattice. These vacancies act as emission centers, whose PL response is modulated by BPA concentrations, resulting in measurable quenching effects. The method achieves a detection limit of 0.025 μmol/L, demonstrating sensitivity comparable to other complex analytical techniques, while offering advantages in simplicity and real-time monitoring. The underlying quenching mechanism involves electron transfer from oxygen vacancies to BPA*s H* ions, confirming a static quenching pathway. This work provides an efficient and practical platform for environmental and health monitoring of biohazardous molecules.

UP 8.2 Wed 15:00 P1

Solar and Geomagnetic Forcing Effects on Middle Atmospheric Dynamics Simulated with ICON-ART*LINOZ — •Amrutha Vasudevan — karlsruhe Institute of Technology — Geomar Helmholtz Centre for Ocean Research Kiel

The paper discusses the effect of solar forcing and geomagnetic forcing on middle atmospheric dynamics, using the ICON general circulation model with ART simulations and LINOZ simulations. Simulations are carried out under solar forcing conditions at solar maximum and minimum, and with and without the upper boundary condition NOy, focusing on the role of energetics forced odd nitrogen. Solar forcing is imposed through irradiance spectra, and geomagnetic forcing through particle precipitation and ionization. In the chemistry-dynamics model, the interaction between ozone and NOy and wind and wave forcing has been considered. The paper finds important middle atmospheric responses in the mesosphere and lower thermosphere regarding zonal wind, wave mean flow, and the distribution of ozone, and there are large differences in the UBC(NOy) simulations compared with the non-UBC simulations. The paper emphasizes the crucial role played by the influx of NOy in simulating the solar and geomagnetically forced middle atmospheric variability.

UP 8.3 Wed 15:00 P1

Laboratory studies of the charging state of giant mineral dust — •Lea Sophie Ebel[1,2], Alexei Kiselev[1], Thomas Leisner[1], and Martina Klose-Albinger[2] — [1]IMKAAF, Karlsruhe Institute of Technology, Germany — [2]IMKTRO, Karlsruhe Institute of Technology, Germany

Giant mineral dust particles, characterized by a diameter ≥ 63 μm, are observed to travel thousands of kilometers in the atmosphere from the Sahara across the Atlantic ocean to America. Mechanisms counteracting the expected fast gravitational settling of giant aerosols and, therefore, enabling their long-range transport are not yet sufficiently understood. The charging state of mineral dust and its interaction with the atmospheric electric potential gradient are proposed as a force potentially large enough to counteract gravity.

To assess the role of charge in long-range dust transport, single mineral dust particles collected from various desert dust sources are charged and inserted into acoustic and electrodynamic traps to measure charge decay and their aerodynamic properties. Additionally, the morphology and mineralogical composition of the particles are characterized via Scanning Electron Microscopy and Energy-dispersive X-ray spectroscopy to link the charge decay to these properties.

Understanding the exact mechanisms behind the long-range transport of giant mineral dust is crucial to improving the dust representation in weather and climate models and to better quantifying dust climate impacts.

UP 8.4 Wed 15:00 P1

The role of sea salt aerosols in Arctic bromine explosion events — •Ariane Le Cardinal[1], Stefanie Falk[1], Hugo El-Mansi[2], Hans-Werner Jacobi[2], and Björn-Martin Sinnhuber[1] — [1]Karlsruhe Institute of Technology, Institute of Meteorology and Climate Research, Atmospheric Trace Gases and Remote Sensing, Karlsruhe, Germany — [2]Institute of Environmental Geosciences (IGE), Université Grenoble Alpes / CNRS / Grenoble INP / INRAE / IRD, Grenoble, France

Ozone depletion events (ODEs) during Arctic springs are caused by halogen compounds, dominated by bromine (Br). Sea salt aerosols provide an important reservoir of bromide (Br^-). During bromine explosion events, the reaction of atmospheric HOBr with Br^- in the snow or sea ice surface releases molecular bromine Br_2 in the gas phase. Photolysis of Br_2 then rapidly amplifies the amount of reactive Br, causing ozone loss. As polar tropospheric bromine chemistry is currently not included by default in most chemistry climate models, a better understanding of the sea salt distribution in the Arctic snow is needed to better predict ODEs. We compare modelled sea salt emission, transport, and deposition, using ICON-ART at a 13 km resolution (R03B07) with Br_2 released from salty snow. Model results are evaluated using snow samples taken at Spitzbergen (Ny-Ålesund) in 2024, together with satellite observations.

UP 8.5 Wed 15:00 P1

The Impact of Ionic Conductivity on Device Performance in Perovskite Solar Cells — •Immo Petersen[1,2], Aaron Schüller-Ruhl[1,2], Tim Timewell[1,2], Ali Reza Nazari Pour[1,2], Lukas Wagner[1,2], and Jan Christoph Goldschmidt[1,2] — [1]Physics of Solar Energy Conversion Group, Department of Physics, Marburg University, Germany. — [2]mar.quest Marburg Center for Quantum Materials and Sustainable Technology, Marburg University, Germany.

Perovskite solar cells (PSCs) are a promising candidate for cost-effective climate change mitigation; however, their relatively low operational stability remains a major challenge. Recent studies identified mobile ions to be one of the main causes for operational efficiency losses. This work investigates how the density of migrating ions affects the electrical device performance.

For determining the density and mobility of migrating ions, Fast Hysteresis, Mott-Schottky analysis and dark-CELIV measurements are performed. In these methods, a defined voltage protocol is applied to the PSC and the resulting current response is recorded. The measurements are carried out on PSCs with varying electrode materials and different hole transport layers. These layers influence the properties of migrating ions and the surface-recombination rate. In a second step, drift-diffusion simulations are used to model ion dynamics and their influence on the electrical behavior of PSCs.

We found that the magnitude of surface recombination strongly modifies the impact of accumulating ions. Untangling the underlying mechanisms is a central objective of this work.

UP 8.6 Wed 15:00 P1

Evaluation of UA-ICON simulations of Gravity Waves in the Middle Atmosphere for Northern Hemispheric Winter 2016 — •Arwin Marbini, Hella Garny, and Natalie Kaifler — German Aerospace Center (DLR) Oberpfaffenhofen

Gravity waves in middle atmospheric regions are poorly understood, making them a significant scientific object in atmospheric physics. Using numerical simulations, with high horizontal resolution, an understanding of their sources in stratospheric and mesospheric regions becomes a possibility. Here, we evaluate high resolution UA-ICON simulations (20 km horizontal grid size), with JAWARA reanalysis data and lidar observations.

We study the temperature and wind profiles of zonal means for a characterization of the background structure of ICON data. This reveals a warmer stratopause in the ICON simulations, compared to JAWARA.

Furthermore, we analyze temperature perturbations in comparison to the lidar observations in Sodankylä, Finland, to characterize gravity wave activity. With this we test the ability of ICON to simulate realistically gravity wave activity, a prerequisite to study their processes.

This approach aims at closing the gap in our understanding of gravity wave sources, and their influence in our atmosphere.

Working Group on Accelerator Physics
Arbeitskreis Beschleunigerphysik (AKBP)

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Overview of Invited Talks and Sessions

(Lecture hall SCH/A117; Poster P4)

Topical Talks

AKBP 1.1	Mon	9:30–10:00	SCH/A117	**Recent Developments at S-DALINAC** — •D. Schneider, M. Arnold, J. Birkhan, U. Bonnes, A. Brauch, L. B. Dingeldein, J. Enders, R. Grewe, K. Ide, L. Jürgensen, M. Meier, C. M. Nickel, N. Pietralla, V. Pruy, F. Schliessmann, T. Zimmermann
AKBP 1.2	Mon	10:00–10:30	SCH/A117	**Status of Source and Delivery of Spin-Polarized Electron Beams at ELSA** — •Michael Switka, Klaus Desch, Dennis Proft, Axel Spreitzer
AKBP 2.1	Mon	11:00–11:30	SCH/A117	**From ELBE to DALI - Superconducting Electron Accelerators in Dresden** — •Andreas Wagner, Ulf Lehnert, Andre Arnold, Manfred Helm, Sebastian Mährlein, Raffael Niemczyk, Rong Xiang
AKBP 5.1	Tue	9:30–10:00	SCH/A117	**Generation and Acceleration of In-Target Gold Fission Fragments using the ATLAS-3000 Laser System** — •Laura D. Geulig, Veronika Kratzer, Erin Grace Fitzpatrick, Maximilian J. Weiser, Jörg Schreiber, Peter G. Thirolf
AKBP 6.1	Tue	11:00–11:30	SCH/A117	**Efficient high energy and high-repetition-rate proton acceleration from cryogenic hydrogen foil targets** — •Stefan Assenbaum, Martin Rehwald, Paweł Ordyna, Joshua Schilz, Maximilian Müller, Thomas Streil, Julian Garreis, Thomas Kluge, Sebastian Göde, Maxence Gauthier, Christopher Schönwälder, Ulrich Schramm, Karl Zeil
AKBP 10.1	Wed	15:00–15:30	SCH/A117	**Multiscale longitudinal electron bunch characteristics of LWFA bunches determined by single-shot CTR spectroscopy** — •Alexander Debus, Maxwell LaBerge, Omid Zarini, Susanne Schöbel, Jessica Tiebel, Finn-Ole Carstens, Nico Wrobel, Richard Pausch, Klaus Steiniger, Yen-Yu Chang, Jurjen Couperus Cabadağ, Alexander Köhler, Thomas Kurz, Rafal Zgadzaj, Michael Downer, Michael Bussmann, Ulrich Schramm, Arie Irman
AKBP 12.1	Thu	9:30–10:00	SCH/A117	**Cutting-edge research and technology at KIT's advanced accelerator facilities** — •Erik Bründermann

Sessions

AKBP 1.1–1.3	Mon	9:30–10:45	SCH/A117	**Electron Accelerators and Sources I**
AKBP 2.1–2.5	Mon	11:00–12:30	SCH/A117	**Electron Accelerators and Sources II**
AKBP 3.1–3.6	Mon	15:00–16:30	SCH/A117	**Diagnostics**
AKBP 4.1–4.5	Mon	16:45–18:00	SCH/A117	**Beam Dynamics**
AKBP 5.1–5.4	Tue	9:30–10:45	SCH/A117	**Plasma Accelerators, Ions I**
AKBP 6.1–6.5	Tue	11:00–12:30	SCH/A117	**Plasma Accelerators, Ions II**
AKBP 7.1–7.6	Tue	14:00–15:30	SCH/A117	**Ion and Medical Accelerators**
AKBP 8.1–8.10	Wed	9:30–11:00	P4	**Poster AKBP**
AKBP 9.1–9.6	Wed	11:00–12:30	SCH/A117	**RF Cavities I**
AKBP 10.1–10.4	Wed	15:00–16:15	SCH/A117	**Plasma Accelerators, Diagnostics I**
AKBP 11.1–11.4	Wed	16:30–17:30	SCH/A117	**Plasma Accelerators, Diagnostics II**
AKBP 12.1–12.5	Thu	9:30–11:00	SCH/A117	**Novel Accelerators I**

AKBP 13.1–13.4	Thu	11:30–12:30	SCH/A117	**Novel Accelerators II**
AKBP 14.1–14.3	Thu	15:00–15:45	SCH/A117	**RF Cavities II**
AKBP 15.1–15.3	Thu	16:00–17:30	SCH/A117	**AKBP Prize Talks**
AKBP 16	Thu	18:00–19:00	SCH/A117	**Members' Assembly**

Members' Assembly of the Working Group on Accelerator Physics

Thursday 18:00–19:00 SCH/A117

Sessions

– Topical Talks, Contributed Talks, and Posters –

AKBP 1: Electron Accelerators and Sources I

Time: Monday 9:30–10:45 Location: SCH/A117

Topical Talk AKBP 1.1 Mon 9:30 SCH/A117

Recent Developments at S-DALINAC — •D. Schneider, M. Arnold, J. Birkhan, U. Bonnes, A. Brauch, L. B. Dingeldein, J. Enders, R. Grewe, K. Ide, L. Jürgensen, M. Meier, C. M. Nickel, N. Pietralla, V. Pruy, F. Schliessmann, and T. Zimmermann — Institut für Kernphysik, TU Darmstadt

The superconducting Darmstadt electron linear accelerator S-DALINAC is a thrice-recirculating accelerator [1] which can be operated as an energy recovery linac [2].

Two novel experimental set-ups are being implemented at the S-DALINAC: The study of electron-induced fission reactions of actinides and a demonstrator for Compton backscattering in ERL operation. We have further improved the overall beam quality and the diagnostic capabilities of the accelerator: A streak camera has been implemented for bunch length measurements. Monitoring the beam position with a system of high-speed cameras and a novel feedback-driven beam stabilization, the beam stability was increased significantly. A cavity for a double-chopper setup for the injector has been implemented. This contribution gives an overview on the activities at the S-DALINAC.

[1] N. Pietralla, Nucl. Phys. News, Vol. 28, No. 2, 4 (2018).
[2] F. Schliessmann et al., Nat. Phys. 19, 597-602 (2023).
[3] A. Brauch et al., Rev. Sci. Instrum. 96(11), 113303 (2025).
[4] D. Schneider et al., Nucl. Inst. Phys. A. 1077, 170540 (2025).

*Work supported by State of Hesse within GRK 2891 'Nuclear Photonics' (Project-ID 499256822).

Topical Talk AKBP 1.2 Mon 10:00 SCH/A117

Status of Source and Delivery of Spin-Polarized Electron Beams at ELSA — •Michael Switka, Klaus Desch, Dennis Proft, and Axel Spreitzer — University of Bonn, Physics Institute, Bonn, Germany

Operation of the 50 kV GaAs-based photoinjector source for spin-polarized electrons at the electron stretcher accelerator (ELSA) has been re-established and its usage for regular machine operation is being prepared. This includes the recommissioning of a Compton backscattering polarimeter located in the 3.2 GeV fast ramping storage ring to monitor the effects depolarizing resonances and their countermeasures during the energy increase. An overview of the latest achievements and upcoming improvements is presented.

AKBP 1.3 Mon 10:30 SCH/A117

Simultaneous Beam Extraction at ELSA — •Max Ammann, Klaus Desch, Dennis Proft, Michael Switka, and Leonardo Thome — Physikalisches Institut der Universität Bonn

At the electron accelerator facility ELSA, electrons with energies up to 3.2 GeV are extracted to multiple experimental stations at two distinct beamlines via slow resonant extraction, serving hadron-physics experiments, detector tests, and medical research. In the past, only one beamline could be served at a time. A new machine-operation mode has been developed that enables extraction to one of the hadron-physics experiments and, simultaneously, to the detector test beamline, where typically lower electron rates are required. This allows more efficient use of the available beam time. The properties and underlying beam dynamics of this machine mode are presented, along with sophisticated methods for rate control at the second beamline.

AKBP 2: Electron Accelerators and Sources II

Time: Monday 11:00–12:30 Location: SCH/A117

Topical Talk AKBP 2.1 Mon 11:00 SCH/A117

From ELBE to DALI - Superconducting Electron Accelerators in Dresden — •Andreas Wagner[1,2], Ulf Lehnert[1], Andre Arnold[1], Manfred Helm[3,4], Sebastian Mährlein[1,4], Raffael Niemczyk[1], and Rong Xiang[1] — [1]Institute of Radiation Physics, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Institute of Radiation Physics — [3]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum D — [4]Dresden University of Technology, Dresden, Germany

The Helmholtz-Zentrum Dresden-Rossendorf successfully operates the superconducting ELBE (Electron LINAC with High Brilliance and Low Emittance) accelerator to produce a variety of secondary photon and particle beams. ELBE serves an international user community involved in fundamental studies in nuclear physics, radiation biology, solid-state physics, chemistry, materials science, detector characterisation, positron interactions with matter, and materials control using high-field THz radiation. Based on the experience of the existing user facility and after more than 20 years of operations, the DALI (Dresden Advanced Light Infrastructure) concept for a successor facility with an enhanced frequency range for high-field THz radiation ranging from 0.1 to 30 THz, a high intensity positron source, and ultra-fast electron diffraction has been developed. In 2025, DALI was promoted to the national shortlist of research infrastructures. This contribution will cover the scientific motivations, the implementation of the machine, and the proposed auxiliary instruments and end stations.

AKBP 2.2 Mon 11:30 SCH/A117

CW e- beam from SRF gun for multifunctional accelerator facility ELBE — •Rong Xiang, André Arnold, Andreas wagner, Stefan Gatzmaga, Petr Murcek, Raffael Niemczyk, Anton Ryzhov, Jochen Teichert, and Gowrishankar Hallilingaiah — Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany

The ELBE center for high-power radiation sources is a compact, accelerator-based facility that provides a wide range of radiation types to its users, including gamma rays, IR- Free-Electron Lasers (FELs), THz radiation, positrons and electron beams, for various applications in materials science, medicine, and nuclear physics.

The development of new continuous-wave (CW) electron source with high bunch charges represents a significant advancement in enhancing the overall performance of ELBE. By combining the well-established radio-frequency (RF) with superconducting (SC) technology, it is able to realize CW operation at high gradient. The robust semiconductor photocathode Cs2Te shows a stably high quantum efficiency (QE) during the gun operation.

SRF Gun II has been routinely operated since 2018 for THz user experiments, delivering high bunch charges (200 pC at 100 kHz) with excellent stability and reliablity. In 2024, SRF Gun II achieved a record current of 0.6 mA in CW mode and drove the IR-FEL for a highly sensitive s-SNOM experiment. Recently the first ultrafast electron diffraction (UED) patterns of MoO3 sampple were obtained, demonstrating its outstanding stability and high beam quality.

AKBP 2.3 Mon 11:45 SCH/A117

Status and Perspectives of the Photo-CATCH Photocathode Test Stand* — •Maximilian Herbert, Joachim Enders, Markus Engart, Robin Petry, and Vincent Wende — Institut für Kernphysik, Technische Universität Darmstadt, Darmstadt, Germany

TU Darmstadt's test stand for Photo-Cathode Activation, Testing and Cleaning using atomic-Hydrogen Photo-CATCH faciliates dedicated research on GaAs photocathodes for electron-beam production at accelerators. Recent results include successful tests of automatized activation [1] and improved photocathode lifetime using an enhanced Cs-O-Li surface layer [2,3]. This contribution will present the current status of Photo-CATCH and work planned in the near future.

[1] M. Herbert et al., PoS(PSTP2022), Vol. 433, p. 003 (2023).
[2] N. Kurichiyanil et al., J. Instrum. 14 (8), P08025 (2019).
[3] M. Herbert et al., Phys. Rev. Accel. Beams 28, 013401 (2025).

*Work supported by DFG (Project-ID 264883531 - GRK 2128 "AccelencE", and Project-ID 499256822 - GRK 2891 "Nuclear Photonics")

AKBP 2.4 Mon 12:00 SCH/A117

Status of the Hybrid Electron Gun Development at ELSA — •Samuel Kronenberg, Klaus Desch, Ben Simon Gatzsche, Philipp Hänisch, Dennis Proft, Yannick Schober, and Michael Switka — Physikalisches Institut, Universität Bonn

A redesign of the injector beamline for the S-band linac at ELSA is underway, including the replacement of the existing electron gun by a hybrid gun that

combines thermionic emission and thermally assisted photoemission in a single setup. The goal is to offer a new single-bunch injection mode alongside the long pulse mode already provided by the current gun. Measurements have been conducted to verify this emission technique using caesium dispenser cathodes. The development of a dedicated test stand is currently being carried out to facilitate more detailed studies and serve as a prototype for the future injector section. Recent research has concentrated on the lattice and magnet design, as well as on evaluating suitable beam-diagnostic instrumentation.

AKBP 2.5 Mon 12:15 SCH/A117

First demonstration of MeV electron diffraction with the ELBE SRF Gun: towards an MeV-UED instrument — •Louis Stein[1,2], André Arnold[1], Michael Klopf[1], Raffael Niemczyk[1], Anton Ryzhov[1], Jochen Teichert[1], Ece Uykur[1], Andreas Wagner[1], Stephan Winnerl[1], Rong Xiang[1], and Sebastian Maehrlein[1,2] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden — [2]TU Dresden

Ultrafast electron diffraction (UED) is a unique technique for measuring structural and electronic dynamics with sub-picosecond time resolution in a pump-probe arrangement. In most state-of-the-art UED setups, beams with keV electron energy are utilized. The project presented here aims to step up to MeV electron beams with the help of a superconducting radio frequency photo electron injector (SRF gun). The most promising argument for MeV-UED is its ability to access higher-order diffraction, which provides high sensitivity to small atomic displacements. Using the current HZDR ELBE SRF electron gun in continuous wave (CW) operation with megahertz repetition rates, a first demonstration of an MeV electron diffraction is presented. This presentation will summarize the SRF gun parameters and shows the current status of the electron diffraction setup at the ELBE SRF Gun. In future, the combination of MeV-UED with high-intensity tunable THz pump beams will open up exciting new possibilities for time-resolved studies of types of light-driven ultrafast structural dynamics in quantum matter, correlated systems, and other types of complex matter.

AKBP 3: Diagnostics

Time: Monday 15:00–16:30 Location: SCH/A117

AKBP 3.1 Mon 15:00 SCH/A117

Broadband Cavity BPM Design for MESA — •Robin Wolf — Institut für Kernphysik, Mainz, Germany

The MESA accelerator's Energy Recovery Linac (ERL) mode requires a fast and sensitive beam position monitor (BPM) capable of distinguishing between accelerated and decelerated electron bunches in diagnostic pulse mode. This talk will present the design of the proposed cavity BPM for the MESA requirements.

The proposed design is an adaptation of the SACLA BPM, optimised for operation at 2.6GHz (the 2nd harmonic of MESA's 1.3GHz RF frequency) for increased sensitivity and smaller physical size. The tailored cavity design integrates a monopole-mode cavity (for phase and intensity measurements) with an dipole-mode cavity (for position measurements). Key enhancements include the splitting of the X and Y planes with implementation of mode separators, which maximises orthogonal plane decoupling. Furthermore, integrated waveguides are employed in the dipole-part to suppress the monopole-mode, while offering increased freedom in antenna coupling to the dipole field.

AKBP 3.2 Mon 15:15 SCH/A117

Compact Beam Position Monitor using a Segmented Toroidal Coil — •Lars Festring — RWTH Aachen University, Germany

A compact beam position monitor based on a segmented toroidal coil surrounding a charged particle beam has been investigated (F. Abusaif et al., Rev. Sci. Instrum. 1 March 2025; 96 (3): 033302, https://doi.org/10.1063/5.0240076).

It uses the induced voltages in the windings. We theoretically investigate the response of the coils to a bunched particle beam based on a lumped-element model and a Gaussian beam model. Then, we compare the model to measurements taken in the laboratory and the storage ring COSY. In addition, we devise a way to measure the covariance of the transversal beam profile and test it via a simulation. The resonant behavior in the coils' frequency response may be exploited to further increase the sensitivity of the device.

The resolution of the position measurement presently achieved is about 5 μm in a 1 s time interval for a beam current of 0.5 mA.

AKBP 3.3 Mon 15:30 SCH/A117

Design, installation and commissioning of an optical real-time diagnostic system for the BESSY II Injection LINAC — •Pauline Ahmels — Helmholtz-Zentrum Berlin, Hahn-Meitner-Platz 1, 14109 Berlin — Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin

In order to improve the present LINAC injection line diagnostic system at BESSY II, a non-destructive source point imaging system is being developed.

Until now, these source point imaging have primarily relied on retractable fluorescence screens (FOMs),which are inherently destructive due to the direct imaging of the electron beam. This talk presents the conceptual design, including technical requirements, simulation results, mechanical integration and commissioning of an optical diagnostic instrument for real-time monitoring at the injection line.

The design aims to ensure beam quality during operation using synchrotron radiation emitted from the dipole magnet. The primary components of this beamline are a CCD camera and a lens system designed to operate under high vacuum conditions. To enable precise positioning, the optical system is equipped with a motorized linear feed through. A basic, fixed focal length setup is initially employed to experimentally validate the simulation results, using the same CCD camera as in the final beamline setup. This new setup must be adapted to the spatial constraints, make use of existing materials as much as possible, and be simple to construct and install.

AKBP 3.4 Mon 15:45 SCH/A117

Error investigations of longitudinal phase space measurements using tomography — •Marc P. Kerstan, Christopher J. Richard, and Namra Aftab — Deutsches Elektronen-Synchrotron DESY, Zeuthen, Germany

The Longitudinal Phase Space (LPS) characterization is important in beam dynamics, especially in Free-Electron Lasers (FELs), where the slice energy spread is a key parameter to evaluate lasing performance and brightness.

The Photo Injector Test facility at DESY in Zeuthen (PITZ) is a test stand to condition and characterize electron sources for EuXFEL and FLASH. Measurement of the LPS directly after the electron source at PITZ is not possible due to unavailability of a dedicated diagnostics setup. Alternatively, the LPS can be measured 2.33 m from the cathode using tomography with the booster cavity as a rotating element. The aim of this project is to better understand the measured reconstructed LPS by refining the simulation model to better represent the measurement process. The current model is simplified. It only consists of a drift space with the correct length and does not include a dispersive element or many of the systematic error sources, that contribute to the real measurement.

Presented here are the results of an updated beamline model including a dipole and transverse focusing elements. This improved model allows for studies of the systematic errors on the reconstructed LPS including noise cuts and measurement camera resolution.

AKBP 3.5 Mon 16:00 SCH/A117

Compton Polarimetry with a Timepix3 ASIC at ELSA — •Tobias Schiffer, Michael Switka, Dennis Proft, and Klaus Desch — Physikalisches Institut der Universität Bonn, Bonn, Germany

The Electron Stretcher Facility (ELSA) in Bonn can provide spin polarized electrons to its users. During acceleration depolarising resonances have to be crossed reducing the achievable degree of polarization.

For a non-destructive in situ measurement of the beam polarization in the storage ring a Compton polarimeter is available. It utilizes a high intensity cw-laser beam scattering off the electron beam. The back scattered photon profile is measured with a detector. Depending on the polarization of the laser and the electron beam a vertical shift of the intensity profile can be observed. This is currently measured with a in-house custom-built silicon strip sensor.

However, to improve the detector setup and to obtain 2D information, a detector using a pixelized readout chip (Timepix3) with a 500 μm thick silicon sensor is in development.

The current status of the detector and first results of the performance are presented.

AKBP 3.6 Mon 16:15 SCH/A117

Automated In-Situ Ion Beam Characterization During Ion Implantation — •Ali Kosari Mehr, René Heller, Oliver Steuer, and Slawomir Prucnal — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstr 400, 01328 Dresden, Germany

Ion implantation is a key technique for materials modification, especially in semiconductor processing. However, high-current industrial implanters often struggle to distinguish ion species and energies when projectiles have similar mass-to-charge ratios, such as Al and N*. Because industrial implantation relies on fast throughput and simple mass-analysis stages, ambiguous beam composition can compromise process reliability. This motivates the development of an automated in-situ diagnostic tool. A compact apparatus combining Rutherford backscattering spectrometry and ionoluminescence was therefore developed. It is inserted into the beam path for only a few seconds before implantation and comprises a beam-entry aperture, a dummy target of known composition, an RBS detector, and an ionoluminescence module with mirrors, optical fibres, and

a miniature spectrometer. The dual-modality concept enables cross-checked identification of ion species, energies, and molecular fractions. For automated beam-quality decisions, a machine-learning evaluation scheme based on an artificial neural network was implemented and trained on simulated RBS spectra. The optimised model reliably distinguishes target ions under realistic noise and intensity fluctuations, enabling real-time ion beam characterisation.

AKBP 4: Beam Dynamics

Time: Monday 16:45–18:00 Location: SCH/A117

AKBP 4.1 Mon 16:45 SCH/A117

Improving Energy spread of MESA beam in ERL operation — Esraa Khidr and •Florian Hug — Johannes Gutenberg university Mainz

Precise control of longitudinal beam dynamics is crucial at the Mainz Energy-Recovering Superconducting Accelerator (MESA), particularly in support of the MAGIX experiment, which operates in ERL mode. Comprehensive simulations were conducted using the elegant tracking code; starting with 4 ps bunch length, the full acceleration and deceleration process in ERL was modeled by optimizing the RF phase and the accelerating gradient field in off-crest operation, resulting in the desired energy gain in each linac section. At low energies, improved energy spread is required with a short bunch length; therefore, the injection arc was optimized for a 2 ps bunch by adjusting the arc momentum compaction R56 and introducing an energy*position correlation (chirp) downstream of MAMBO. The resulting optimization provides enhanced bunch compression and reduces the longitudinal phase-space width, while preserving longitudinal emittance and thereby enhancing overall beam quality not only at the lowest but also at all energies.

AKBP 4.2 Mon 17:00 SCH/A117

Determining the influence of transversal beam excitation on beam size and dynamics at KARA — •Simon Braner[1], Marvin-Dennis Noll[1], Johannes Steinmann[1], Erhard Huttel[1], Anke-Susanne Müller[1], Erik Bründermann[1], and Michele Caselle[2] — [1]IBPT, KIT, Karlsruhe — [2]IPE, KIT, Karlsruhe

Significant beam dynamics parameters, such as energy spread or transversal beam size, can be calculated from the transversal bunch profile. At the Karlsruhe Research Accelerator (KARA), located at the Karlsruhe Institute of Technology (KIT), the beam size in the storage ring is being investigated using the KArlsruhe Linear arraY detector for MHz rePetition rate SpectrOscopy (KALYPSO), a line array that examines the synchrotron radiation emitted at a five-degree port of a dipole magnet. Trench-Isolated Low-Gain Avalanche Diode (TI-LGAD) technology provides superior sensitivity compared to conventional silicon detectors, thereby facilitating the study of low-charge bunches. As the KALYPSO system can be triggered at several megahertz, turn-by-turn analysis can be performed at KARA, which has a revolution frequency of 2.7 MHz. In addition to the study of the energy spread, the analysis of beam size and position modulations can be performed. These can either occur naturally or be induced by a white noise signal on a strip line. In this contribution, the influence of transversal beam excitation on beam size and time-resolved dynamics at KARA is investigated.

AKBP 4.3 Mon 17:15 SCH/A117

Coulomb Crystallization in Free Electron Beams — •Valerio Di Giulio[1,2], Rudolf Haindl[1,2], and Claus Ropers[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]University of Göttingen, Göttingen, Germany

In the context of electron beams, the Coulomb repulsion experienced by the constituents of high-current probes is usually regarded as a detrimental effect, leading to emittance growth. However, under suitable conditions, electron-electron interactions can be exploited to produce phase space distributions with well-defined energy-time correlations, as recently observed in few-electron pulses photoemitted from a metallic nanotip and imaged in a transmission electron microscope (R. Haindl et al., 2023). Such correlations can be leveraged to harness specific beam properties by selecting a portion of the probe. Extending this concept to higher currents and larger particle numbers, the beam can enter a crystalline state, forming an electron lattice defined by Coulomb repulsion, a Wigner crystal. In this work, we employ Monte Carlo simulations to examine the conditions under which Coulomb crystallization can emerge in both few-particle and continuous electron beams, exploring the interplay between beam temperature, current, and electromagnetic confinement. We compute properties associated with different structural phases, revealing a strong enhancement of beam brightness in the crystalline regime. We also present new measurements of electron-electron energy correlations in pulses containing from 4 to 8 particles, demonstrating the transient formation of an ordered electron chain during propagation in the microscope.

AKBP 4.4 Mon 17:30 SCH/A117

Status of the Compton Backscattering Source COBRA at the S-DALINAC* — •Lisa B. Dingeldein, Michaela Arnold, Ruben Grewe, Julian Hauf, Maximilian Herbert, Katharina E. Ide, Lars Jürgensen, Maximilian Meier, Clemens M. Nickel, Norbert Pietralla, and Dominic Schneider — Institut für Kernpysik, Technische Universität Darmstadt, Darmstadt, Germany

The COBRA source (Compton Backscattering at a Recirculating Accelerator) utilizes a 100 W Yb:YAG laser, which is synchronized with the electron beam of the superconducting Darmstadt linear accelerator S-DALINAC [1] for head-on collisions. The backscattered photons can be collimated into a quasi-monochromatic beam for electron beam diagnostics and as a technology demonstrator. This contribution highlights recent upgrades and developments of the detector setup, the laser beamline and the beam-stabilization systems of COBRA. The first collision of the electron and laser beam is planned in an upcoming beamtime with multi-turn recirculation. Later, COBRA is foreseen to be operated during energy-recovery mode [2] serving as a demonstrator for future Compton scattering light sources.

[1] N. Pietralla, Nucl. Phys. News **28**(2), 4 (2018)
[2] F. Schliessmann *et al.*, Nat. Phys. **19**, 597-602 (2023)

*This work is supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) - Project-ID 499256822 - GRK 2891 'Nuclear Photonics'.

AKBP 4.5 Mon 17:45 SCH/A117

Towards plasma-wakefield photon acceleration and its potential applications — •Michael Quin[1], Tom Blackburn[1], and Mattias Marklund[2,1] — [1]Department of Physics, University of Gothenburg, SE-41296 Gothenburg, Sweden — [2]Department of Physics, Chalmers University of Technology, SE-41296 Gothenburg, Sweden

A laser pulse copropagating with a relativistic plasma wave (wakefield) can experience a continuous upshift in frequency known as "photon acceleration". Recent particle-in-cell (PIC) simulations have demonstrated how an optical laser pulse can be accelerated to extreme ultraviolet (XUV) frequencies in an electron-beam-driven plasma-wakefield using a tailored plasma density profile. Intense ($I_0 > 10^{17}$ W/cm^2) XUV laser light is highly sought after for collision experiments with multi-GeV electrons; the high photon and electron energy indicates the onset of effects in strong-field quantum electrodynamics, such as non-linear Compton scattering and Breit-Wheeler pair production. By combining PIC simulations of photon acceleration with Monte-Carlo simulations of the electron-photon collision, we show how the brilliance, yield, and polarization of the emitted γ-rays can be optimized for applications in nuclear and particle physics.

AKBP 5: Plasma Accelerators, Ions I

Time: Tuesday 9:30–10:45 Location: SCH/A117

Topical Talk AKBP 5.1 Tue 9:30 SCH/A117

Generation and Acceleration of In-Target Gold Fission Fragments using the ATLAS-3000 Laser System — •Laura D. Geulig, Veronika Kratzer, Erin Grace Fitzpatrick, Maximilian J. Weiser, Jörg Schreiber, and Peter G. Thirolf — Ludwig-Maximilians University Munich

In our experiment, the ATLAS-3000 laser system was used to accelerate ions from heated micrometer thing gold foils. A Thomson parabola spectrometer, optimized for high-resolution detection of heavy ions, was used to deflect ions with the same charge-to-mass (m/q) ratio on parabolic traces, which then can be matched to the ions with respective charge states. CR-39 track detectors were used to identify and characterize the accelerated ion species via their energy and charge states. In addition to remaining light contaminant species and highly-charged gold ions, an unexpected component of heavy (A 98) ions was observed in the m/q range below 2.5. We attributed those distinct pits to Au fission products. A similar in-target fission fragment component was observed in our previous experiment at the PHELIX laser. Details on our interpretation of the origin of these fragments will be presented.

AKBP 5.2 Tue 10:00 SCH/A117

Proton induced fission studies at CALA — •Maximilian J. Weiser, Erin G. Fitzpatrick, Laura D. Geulig, Runjia Guo, Jinbao Hong, and Syed A. Raza — Ludwig-Maximilians-Universität München

At the Centre for Advanced Laser Applications (CALA) we are investigating a novel fission-fusion reaction scheme [1] by employing the ATLAS-3000 laser with a central wavelength of 800 nm, energy per pulse < 60 J and a pulse duration of about 25 fs. This reaction scheme is in particularly interesting, as it could enable us to study extremely neutron-rich isotopes crucial for a quantitative understanding of the rapid neutron-capture, responsible for cosmic nucleosynthesis of heavy elements.

A necessary preparatory step for realizing this scheme is to gain a better understanding of the fission induced by laser accelerated protons in heavy elements. Therefore, we are improving a gas-flow transport system [2] and completed by aerosol-based transportation to transfer the fission products generated in laser-driven proton-induced fission of 238U to a shielded HPGe detector far from the EMP-contaminated experimental chamber. The status of fragment identification depending on laser and transport conditions will be presented.

Funded by the BMFTR under Grant No. 05P24WM2. We acknowledge the GSI target lab (Dr. Bettina Lommel) for providing the Uranium targets.

[1] D. Habs et al., Appl. Phys. B 103, 471-484 (2011)

[2] P. Boller et al., Sci. Rep. 10, 17183 (2020)

AKBP 5.3 Tue 10:15 SCH/A117

Pre-Expansion of Nano Rods in 2D PIC Simulations — •Franziska-Luise Paschke-Bruehl[1,2] and Thomas Kluge[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf — [2]Technische Universität Dresden

We present a computational study investigating the pre expansion of 10 um long, 100 nm thick nano rods under ultra-high intensity laser contrasts in 2D particle-in-cell simulations. We find that realistic contrasts, modelled by laser systems such as DRACO and ReLaX, lead to significant expansion, hindering the maximum intensities of the laser from seeing an intact rod structure. Based on that, we explore shorter pulse lengths and higher intensities of the laser pulse to ensure an intact rod structure at t_max.This shows that shorter pulse lenghts seem to be a promising alternatvie while higher intensities lead to more pre expansion, despite considering the relativistic critical density.

AKBP 5.4 Tue 10:30 SCH/A117

Characterization of Reflected Light Properties in PIC Simulations — •Vidisha Rana[1,2], Milenko Vescovi[1,2], Richard Pausch[1], Marvin E.P. Umlandt[1,2], Franziska Paschke-Brühl[1,2], Pengjie Wang[1], Tim Ziegler[1], Karl Zeil[1], Ulrich Schramm[1,2], and Thomas Kluge[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf — [2]Technische Universität Dresden

Laser-driven ion accelerators offer several advantages over the conventional ones due to their potential of achieving high accelerating gradients over small distances. Recent experiments have demonstrated that one can achieve significantly high proton energies by modifying the temporal profile and controlling the spectral phase of laser pulses, specifically using Group Delay Dispersion (GDD) and Third Order Dispersion (TOD).

Reflected light properties provide a powerful diagnostic tool for understanding these interactions and optimizing proton energies. Experiments involving ultrashort laser pulses interacting with glass targets reveal prominent spectral shifts across changing dispersion values. These shifts can offer valuable insights into plasma dynamics, relativistic surface motion, and laser contrast effects, which have a direct impact on proton energies but remain difficult to interpret solely through experiments. This challenge can be addressed by employing Particle-in-Cell codes to simulate these interactions to analyze the underlying mechanisms. By bridging the gap between experimental observations and theoretical predictions, this work aims to advance our understanding of laser-plasma interactions and optimize laser-driven ion acceleration.

AKBP 6: Plasma Accelerators, Ions II

Time: Tuesday 11:00–12:30 Location: SCH/A117

Topical Talk AKBP 6.1 Tue 11:00 SCH/A117

Efficient high energy and high-repetition-rate proton acceleration from cryogenic hydrogen foil targets — •Stefan Assenbaum[1,2], Martin Rehwald[1], Paweł Ordyna[1,2], Joshua Schilz[1,2], Maximilian Müller[1,2], Thomas Streil[1,2], Julian Garreis[1,2], Thomas Kluge[1], Sebastian Göde[3], Maxence Gauthier[4], Christopher Schönwälder[4], Ulrich Schramm[1,2], and Karl Zeil[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]TU Dresden, Dresden, Germany — [3]European XFEL, Schenefeld, Germany — [4]Stanford Linear Accelerator Center, Menlo Park, CA, USA

Laser plasma-based ion accelerators have not yet reached their full potential in producing high radiation doses at high particle energies, mainly due to the lack of a suitable high-repetition-rate targets that also provide adequate control of the plasma conditions. Cryogenic, solid hydrogen jet targets are being developed to fill this gap, as they combine many favourable properties for studying advanced laser ion acceleration regimes, such as low solid density, single ion species composition and ease of probing in experiments, with repetition-rated operation capability by being self-replenishing and debris-free. In a recent experiment, a new foil-like geometry of this cryogenic hydrogen target is used to accelerate proton bunches at 1 Hz repetition rate. Using the Draco PW laser at reduced laser energy, we report stable, continuous acceleration of ion beams over thousands of consecutive shots. Despite the low laser energy of only 1.6 J, we observe maximum proton energies of up to 50 MeV, indicating outstanding acceleration efficiency.

AKBP 6.2 Tue 11:30 SCH/A117

Hybrid study of the prepulse impact on cryogenic hydrogen target — •Arthur Hirsch Passicos[1], Stefan Assenbaum[1,2], Pawel Ordyna[1,2], Constantin Bernert[1], Thomas Kluge[1], and Martin Rehwald[1] — [1]Helmholtz-Zentrum Dresden - Rossendorf, 01328 Dresden, Germany — [2]Technical University Dresden, Dresden, Germany

Laser-driven ion accelerators have become more prominent in many fields of applications but are very sensititive to the target density profile in order to to determine the acceleration scheme of the main interaction. At HZDR, we demonstrated the use of cryogenic hydrogen jet targets shaped with controlled prepulse in order to optimise the proton acceleration.

Based on these results, we will present an hydrid study of the target shaping combining hydrodynamic and Particle-in-Cell simulations. By combining the two types of codes, we can correctly simulate and analyse the laser absorption processes, the target expansion as well as the acceleration schemes at play over a large range of pre-pulse intensities and delays.

AKBP 6.3 Tue 11:45 SCH/A117

PIC simulation study of highly efficient, high proton energy laser ion acceleration from cryogenic hydrogen jet targets — •Paweł Ordyna[1,2], Stefan Assenbaum[1,2], Thomas Kluge[1], Karl Zeil[1], and Ulrich Schramm[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Deutschland — [2]Technische Universität Dresden, Dresden, Deutschland

Recent experiments on laser ion acceleration using planar cryogenic hydrogen jet targets have demonstrated high laser to proton coupling efficiency and maximum proton energies that far exceed expected scaling (over 50 MeV at 1.6 J laser energy on target).

We present an accompanying particle-in-cell simulation study that incorporates an approximately 30 ps long laser pedestal and the resulting plasma pre-expansion. Our results reproduce both a highly directional fast proton-beam as well as a return current driven, low-energy, high-charge, nearly isotropic proton emission; both features are observed experimentally. Additionally, we discuss a surprisingly strong influence of small variations in jet orientation on the emission angle of the fast protons.

AKBP 6.4 Tue 12:00 SCH/A117

Investigation of the temporal laser contrast by optical probing of cryogenic hydrogen jet targets — •Thomas Streil — Helmholtz Zentrum Dresden Rossendorf — Technische Universität Dresden

Precise control of experimental parameters in laser-plasma-based ion accelerators is essential for improving acceleration performance. Temporal laser contrast is particularly critical, as it determines pre-plasma formation on the target before the main pulse. Understanding the onset of plasma pre-expansion is therefore vital for realistic simulations and insight into acceleration mechanisms. We investigated this onset by observing laser-induced breakdown, seen as a transition of the target to an opaque state once the electron density exceeds the critical density for the probe wavelength.

Using the DRACO petawatt laser, we scanned intrinsic contrast on a cryogenic hydrogen jet. The method provides a useful correction factor for autocorrelator-based contrast measurements, and additional target characterization and development are presented.

AKBP 6.5 Tue 12:15 SCH/A117

Human-Explainable, Compact, Clustering-based Latents for Fast Proton Energy Spectra Estimation — •Vedhas Pandit[1], Jeyhun Rustamov[1], Martin Rehwald[1], Stefan Assenbaum[1], Vidisha Rana[1], Hans-Peter Schlenvoigt[1], Michael Bussmann[1,2], Ulrich Schramm[1,3], Thomas Kluge[1], and Jeffrey Kelling[1,4] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Center for Advance Systems Understanding (CASUS),

Görlitz, Saxony, Germany — [3]Technische Universität Dresden, Faculty of Physics, Dresden, Saxony, Germany — [4]Technische Universität Chemnitz, Institute of Physics, Chemnitz, Saxony, Germany

A bottleneck in gaining a deeper understanding of the complex laser-plasma interaction that generates laser-accelerated protons is the lack of robust and near real-time information extraction from high frequency shot-data, due to human intervention required in the process. Here, we present an approach to employ deep learning methods to reduce the need for human input into the analysis of Thomson Parabola Spectrometer (TPS) measurements of proton energy spectra given relatively limited labelled data. Our approach builds on deep feature extraction using general pre-trained autoencoders, self organizing map-based clustering of global image features and the spectra that are available as labels, to effectively reduce the dimension of input and output modalities. Lower dimensional representations then enable a small model to be trained on limited data to estimate proton spectra and to help with spectrometer re-calibrations.

AKBP 7: Ion and Medical Accelerators

Time: Tuesday 14:00–15:30 Location: SCH/A117

AKBP 7.1 Tue 14:00 SCH/A117

Theoretical and Numerical Studies of the Effects of Ultra-High Dose Rate Pulses — •Athanasios Koutsostathis, Miriam Brosi, and Anke-Susanne Müller — Karlsruhe Institute of Technology, Karlsruhe, Germany

The understanding of the interaction of high-intensity particle beams with matter is an important aspect for the development of novel accelerator instrumentation. Recently, methods for delivery of ultra-high dose rate radiation have become an increasingly important area of accelerator technology, for example, in the context of FLASH radiotherapy, dosimetry, and particle detector development. In this paper, theoretical models and numerical simulations have been implemented to determine the thermal and subsequent mechanical response of materials subjected to sub-millisecond irradiation with high-intensity particle beams. Emphasis is placed on the identification of phenomena with the potential to drive the development of next-generation accelerator technologies.

AKBP 7.2 Tue 14:15 SCH/A117

Dosimetry for FLASH Radiotherapy with High-Energy Electrons at ELSA — •Anne Stähler, Klaus Desch, Dennis Proft, Michael Switka, and Leonardo Thome — Physikalisches Institut der Universität Bonn

At the electron accelerator facility ELSA, FLASH radiotherapy is being studied. This treatment concept utilises high dose rates in nanosecond to microsecond pulses, which may reduce damage to healthy tissue and improve treatment for deep-seated tumours. Experiments are performed with high-energy electrons between 1.2 GeV and 3.2 GeV, to investigate the underlying beam properties. By applying a newly implemented extraction mode, spill durations of around 330 ns can be achieved. The electromagnetic shower and beam profile throughout water are characterised with Gafchromic films and Cherenkov-light measurements. These results provide, for the first time at energies up to 3.2 GeV, an understanding of the beam properties under FLASH conditions for future radiation studies.

AKBP 7.3 Tue 14:30 SCH/A117

Laser cooling of bunched relativistic ion beams at the FAIR SIS100 — •Danyal Winters[1], Michael Bussmann[2,3], Tamina Grunwitz[4], Jens Gumm[4], Volker Hannen[5], Thomas Kühl[1,6], Sebastian Klammes[1], Benedikt Langfeld[4], Ulrich Schramm[2,7], Denise Schwarz[4], Mathias Siebold[2], Peter Spiller[1], Thomas Stöhlker[1,6,8], Ken Ueberholz[5], and Thomas Walther[4,9] — [1]GSI Darmstadt — [2]HZDR Dresden — [3]CASUS Görlitz — [4]TU-Darmstadt — [5]Uni Münster — [6]HI-Jena — [7]TU-Dresden — [8]Uni-Jena — [9]HFHF Campus Darmstadt

The heavy-ion synchrotron SIS100 is (at) the heart of the Facility for Antiproton and Ion Research (FAIR) in Darmstadt, Germany. It is designed to accelerate intense beams of heavy highly charged ions up to relativistic velocities and to deliver them to unique physics experiments, such as those planned by the APPA/SPARC collaboration. In order to cool these extreme ion beams, bunched beam laser cooling will be applied using a dedicated facility at the SIS100. We will use a novel 3-beam concept, where laser beams from three complementary laser systems (cw and pulsed) will be overlapped in space, time and energy to interact simultaneously with a very broad ion velocity range in order to maximize the cooling efficiency. We will present this project and give an update of its current status. We will also give an overview of the laser and detector systems that will be used.

AKBP 7.4 Tue 14:45 SCH/A117

Acceletor Physics at ESR — •Areso Sherjan[1], Aaron Heinz[2], Giuliano Franchetti[1,2,3], Bernd Lorentz[1], Sergey Litvinov[1], Regina Hess[1], Claude Krantz[1], Jon Rossbach[1], Claudius Peschke[1], Ronald Joseph[1], and Ulrich Popp[1] — [1]GSI Darmstadt — [2]Goethe Universität Frankfurt — [3]HFHF

The ESR (experimental storage ring) at GSI can store and decelerate heavy ion beams with different charge states covering a wide range of energy. Hence, the ESR facility provides suitable conditions for various atomic physics experiments, which requires a very precise control on the machine optics during operation. It is therefore of paramount importance the excellent optics control on the machine and the assessment of all the parameters to prevent beam degradation during the deceleration ramp. This talk reviews the accelerator physics activity of the ESR group for delivering high brightness beam to the low energy experiments.

AKBP 7.5 Tue 15:00 SCH/A117

Dosimetry and beam monitoring for laser-accelerated protons — •Joshua Schilz, Florian Kroll, Karl Zeil, Ulrich Schramm, and Josefine Metzkes-Ng — Helmholtz-Zentrum Dresden-Rossendorf, Germany

Laser-driven plasma accelerators (LPAs) provide multi-10 MeV proton bunches at extremely high instantaneous dose rates, offering unique opportunities for application-oriented studies such as radiobiology. To use these beams effectively, a dedicated experimental environment is required. The ALBUS-2S beamline at the Helmholtz-Zentrum Dresden–Rossendorf delivers such proton beams and is already qualified for irradiating millimeter-scale *in vivo* samples. Building on initial pilot work, we investigate improved methods for beam monitoring and dosimetry of single, ultra-short proton bunches delivering multi-Gy doses.

Two detector concepts were tested at ALBUS-2S. The miniSCIDOM scintillator tomograph enables online 3D dose reconstruction in volumes of about 1 cm^3 with sub-500 μm resolution and 100 mGy sensitivity, including characterization of scintillator quenching at LPA dose rates. A complementary time-of-flight detector records transmitted proton spectra, allowing Monte Carlo-based depth–dose predictions; recent studies have established an optimized detector configuration for routine use.

Together, these diagnostics enable precise characterization of laser-accelerated proton beams, supporting reliable radiobiological experiments under the extreme conditions produced by LPAs.

AKBP 7.6 Tue 15:15 SCH/A117

Advancements in Fast Extraction Methods of Short High Ity Pulses at ELSA for FLASH-RT Researchntensi — •Leonardo Thome, Klaus Desch, Dennis Proft, and Michael Switka — Physikalisches Institut der Universität Bonn

Studies investigating the FLASH effect for radiotherapy (FLASH-RT) are currently being carried out at the electron accelerator facility ELSA. In an initial operation mode, the booster synchrotron provides 1.2 GeV electron pulses of 250 ns duration for the irradiation of cell samples. To access higher beam energies up to 3.2 GeV and pulse lengths spanning from the nanosecond to the millisecond regime, this is complemented with a new developed fast extraction scheme from the stretcher ring. Current work focuses on repurposing the existing injection kickers to achieve single-turn or few-turn extraction. The extracted beam is characterized with charge and profile monitors. In parallel, the feasibility of faster resonant extraction techniques to provide spill durations up to several milliseconds is being investigated.

AKBP 8: Poster AKBP

Time: Wednesday 9:30–11:00 Location: P4

AKBP 8.1 Wed 9:30 P4

Status of the Automated Activation of GaAs Photocathodes at Photo-CATCH* — •Markus Engart, Joachim Enders, Maximilian Herbert, Robin Petry, Julian Schulze, and Vincent Wende — Institut für Kernphysik, TU Darmstadt, Germany

Photocathodes based on the III-V seminconductor GaAs are used as photoelectron sources to supply spin-polarized electron beams for accelerator applications. In order to achieve a sufficient electron yield, a thin surface layer of cesium combined with an oxidant is applied onto the cathode surface in a process called the cathode activation. It is typically done manually by an experienced operator.

This contribution presents the current status in the development and testing of an adaptive algorithm for automated activation at the Photo-CATCH test stand.

*Work supported by DFG (GRK 2128 *AccelencE *, project number 264883531 and Project-ID 499256822 * GRK 2891 'Nuclear Photonics')

AKBP 8.2 Wed 9:30 P4

Status of the beam dynamics design of the bunch compressor for DALI — •Arthur Delan[1], Ulf Lehnert[1], Atoosa Meseck[2], Najmeh Mirian[1], Raffael Niemczyk[1], and Andreas Wagner[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Helmholtz-Zentrum Berlin, Berlin, Germany

Dresden Advanced Light Infrastructure (DALI), a new 50 MeV superconducting linear accelerator at the Helmholtz-Zentrum Dresden-Rossendorf on the national shortlist of research infrastructures, is envisaged as the successor to ELBE, which has served users for over 20 years. Improving on the capabilities of ELBE, DALI contains a superradiant THz source designed to operate between 0.1 and 3 THz, driven by bunch charge increased up to 1 nC. Achieving the required form factor for superradiant emission demands sub-wavelength bunch lengths. The combination of high bunch charge and medium energy causes collective effects such as space charge forces and coherent synchrotron radiation emission to be significant contributions to the beam dynamics. Simulations of the compression and the status of the design for this bunch compressor are presented.

AKBP 8.3 Wed 9:30 P4

Gaussian Process Regression and Bayesian Optimization for a 90 MeV Laser-Plasma Injector for the cSTART Storage Ring — •David Squires, Elias Sailer, Joseph Natal, Alexander Saw, Nathan Ray, and Matthias Fuchs — Karlsruhe Institute of Technology, Kaiserstraße 12 76131 Karlsruhe

Laser-plasma accelerators (LPAs) generate ultrashort high intensity electron bunches from a compact source size. At the Karlsruhe Institute of Technology (KIT), we will use an LPA as one of the injectors for the compact, high-acceptance, non-equilibrium storage ring cSTART.

The LPA injector will be based on an ionization trapping scheme in combination with a tailored plasma density profile to produce an electron beam with small energy spread that maximizes the charge at our target energy, which is at (for LPAs) comparably low energies of 50-90 MeV. Moreover, the LPA injector must produce controlled electron beams with a high shot-to-shot stability and avoid high-energy runaway electrons. These goals can be achieved largely by the detailed design of the plasma density profile and the laser pulse parameters.

In an LPA, small changes across the high-dimensional parameter space can have an outsized influence on overall performance. To handle this challenge, we perform particle-in cell (PIC) simulations and use machine-learning driven approach using Gaussian Process Regression (GPR) and Bayesian Optimization (BO). This procedure allows us to both optimize our gas target design and characterize the effects of the interaction parameters, giving us a functional LPA with a simple tuning mechanism.

AKBP 8.4 Wed 9:30 P4

Programmable Focal Elongation and Shaping of High-Intensity Laser Pulses using Adaptive Optics — •Peter Blum[1], Anna Puchert[1], Emily Archer[1], Sören Jalas[1], Spencer W. Jolly[2], Jens Osterhoff[1,3], Wim P. Leemans[1], Manuel Kirchen[1], Andreas R. Maier[1], and Rob J. Shalloo[1] — [1]Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany — [2]Service OPERA-Photonique, Université libre de Bruxelles (ULB), Brussels, Belgium — [3]now at Lawrence Berkeley National Laboratory

Controlling the intensity distribution of laser pulses in the focal region is becoming increasingly important across many areas of high-intensity laser-matter interactions. Rather than focusing light to a single longitudinal point, like a parabolic mirror, it is often desirable to focus light to a line segment along the optical axis, allowing for the generation of extended regions of high laser intensity. Optics for generating such intensity structures, sometimes referred to as *axioptics*, include the axicon, the axilens, and the more recently proposed axi-parabola.

In laser-plasma accelerators, *axioptics* are essential for forming optically-generated plasma waveguides and for enabling advanced plasma acceleration techniques, including dephasingless wakefield acceleration. Current solutions of tailoring the focal region rely on custom off-axis solutions or diffractive/refractive optics which can be expensive and senstive misalignment and/or aberrations. Here, we present an alternative approach for programmatically generating and shaping extended regions of high intensity, utilising common optical components; an adaptive optic and an off-axis parabolic mirror.

AKBP 8.5 Wed 9:30 P4

Towards spectroscopic characterization of in-target gold fission fragments — •Syed A. Raza[1,2], Maximilian J. Weiser[1], Erin G. Fitzpatrick[1], Laura D. Geulig[1], and Peter G. Thirolf[1] — [1]Ludwig-Maximilians-Universität München, Garching, Germany — [2]University of Bologna, Bologna, Italy

The fission fusion reaction mechanism aims to produce neutron-rich nuclei near the magic neutron number N = 126, which are important for understanding the r-process. A key prerequisite for enabling this mechanism is achieving high bunch densities of accelerated heavy ions, which is why laser-based acceleration is used [1].

In recent experiments at CALA on the acceleration of gold from 300-600 nm foils, using a Thomson parabola spectrometer and CR39 track detectors as diagnostics, we unexpectedly observed a heavy-ion component in the region of $m/q = 2 - 2.5$, where only light ions were expected. This component could be determined to be $A \approx 98$ and attributed to in-target fission fragments [2].

In our experiment in order to unambiguously identify these heavy ions as Au fission fragments, we will use gold target foils ($\approx 300nm - 2\,\mu$m) at CALA and implement a down-stream Mylar catcher foil in front of TPS with a central hole on the target-normal axis to allow accelerated ions to reach the TPS, while the rest will be implanted in the catcher foil and transported out of the vacuum to a well-shielded HPGe detector for characterization of (long-lived) species.

[1] D.Habs et al., Appl. Phys. B 103, 471–484 (2011).

[2] L. D. Geulig, Dissertation LMU, Munich 2025

AKBP 8.6 Wed 9:30 P4

MeV-UED: An instrument for experiments on the atomic scale in space and time — Jakob Krämer[1], Verena Kümper[1], Moritz Pfeiffer[1,2], •Christoph Quitmann[1], and Ariane Ufer[1,2] — [1]RI Research Instruments GmbH Friedrich-Ebert-Str. 75 51429 Bergisch Gladbach — [2]III. Physikalisches Institut B, RWTH Aachen, 52056 Aachen

Current research focuses on investigating promising materials that are potential candidates for applications as nano, quantum and energy technologies. For these kind of materials information about static atomic structures and how they change in time is of crucial importance. Such changes happen upon absorption of energy, during chemical reactions, or in phase transitions. In order to observe these changes, it is necessary to measure atomic positions with sub-Å spatial and sub-ps temporal resolution. RF-Photocathodes excited with ultra-short laser pulses allow generation of electron pulses with MeV energies. Such pulses can be used for diffraction experiments where they create Bragg peaks with ca. mrad angles.

We introduce a commercial robust MeV-UED instrument aimed at ultra-fast electron diffraction with 100fs temporal and sub Å spatial resolution based on a 2.5-cell warm RF-gun and a commercial Ti:Sa laser. This instrument is compatible with solid , liquid or gaseous samples (incl. cryogenic option). We present the main design considerations, electron beam dynamics simulations, and the engineering design of the RI-Bornite MeV-UED instrument.

AKBP 8.7 Wed 9:30 P4

Advancing Resolution in LWFA-Driven X-ray Probing of Laser-Nanostructure Interactions — •Maurice Zeuner[1], Moritz Foerster[1], Florian Haberstroh[1], Johannes Zirkelbach[1], Felipe Peña[1,3], Sonja Gerlach[1], Enes Travac[1], Sanchita Sharan[1], Mohamed Ayache[1], Marius S. Schollmeier[2], Gregor Schilling[1], Andreas Döpp[1], Daniel E. Rivas[2], and Stefan Karsch[1] — [1]Ludwig-Maximilians-Universität München, Fakultät für Physik, Am Coulombwall 1, Garching 85748, Germany. — [2]Marvel Fusion, Theresienhöhe 12, 80339 Munich, Germany — [3]Department of Physics, University of Oslo, Olso, Norway

A novel inertial fusion concept (by Marvel Fusion) proposes the use of nanostructured targets in the form of arrays of thin rods that are irradiated by high-intensity laser pulses. The resulting interaction potentially enables heating and compression of mixed solid fusion fuels. Experimental validation of this approach is crucial, but the underlying dynamics unfold on femtosecond time scales and nanometer length scales, posing significant diagnostic challenges. In the framework of the VANLIFE collaboration, this work investigates the feasibility of probing nanostructured targets during the laser-target interaction using laser-driven plasma-wakefield accelerators for X-ray generation, delivering ultrashort and high-brightness pulses via Betatron radiation. We want to explore possibilities to use these radiation sources to probe the interaction at such nano targets and gain a better understanding of diagnostic challenges in probing rapidly expanding, high-density laser-plasma interactions.

AKBP 8.8 Wed 9:30 P4

A Roadmap towards Direct Imaging of Plasma Targets during Laser Acceleration using Computation X-Ray Holography — •Ritz Ann Aguilar[1], Long Yang[1], Yangzhe Cui[1], Lingen Huang[1], Martin Rehwald[1], Toma Toncian[1], Karl Zeil[1], Michael Bussmann[1,2], Ulrich Schramm[1,3], Thomas Cowan[1,3], and Jeffrey Kelling[1,4] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]CASUS, Görlitz, Germany — [3]TU Dresden, Germany — [4]TU Chemnitz, Germany

Accurate density diagnostics of laser-driven targets are essential for optimizing high-intensity experiments in laser-plasma acceleration (LPA) and inertial-confinement fusion (ICF). We apply a computational X-ray imaging workflow based on single-shot, in-line coherent holography that records diffraction patterns with strong phase contrast and reconstructs spatial phase, and thus density, from intensity-only data. We use differentiable optical propagators and physics-informed machine-learning-assisted phase retrieval to recover fine-scale struc-

tures. As a proof of concept, we present reconstructions of laser-irradiated hydrogen gas jets, resolving features relevant to plasma tailoring and injection control. This is compatible with external light sources and compact plasma-based X-ray sources, supporting feedback-oriented operation on LPA platforms. We also outline an application to ICF: XFEL-based coherent diffraction imaging of shock-compressed solid hydrogen. At the European XFEL's HED-HIBEF instrument, the approach targets resolving fuel-compression dynamics down to sub-micron scales, addressing a central diagnostic need for high-gain implosion studies.

AKBP 8.9 Wed 9:30 P4

Preliminary Studies for a Colliding Beam Møller Polarimeter — •Philipp J. Kompa — JGU Mainz

The Colliding Beam Møller Polarimeter is a proposed setup for measuring the spin polarisation of electron beams with high precision. The proposed setup promises improved systematic uncertainties compared to existing polarimeters which have uncertainties around 0.5%. There are some experimental challenges, one of them being the low cross section of Møller scattering and the therefore low scattering rate even with the high average currents needed for experiments at MESA.

This work discusses the experimental challenges, focusing on background measurements and estimations of how far the background may be suppressed by using coincident measurement of the scattered electrons.

AKBP 8.10 Wed 9:30 P4

Development of a precision timing system for beam background characterization using plastic scintillators — •Florian Eisele[1], Fabian Hummer[1], and Luca Scomparin[2] — [1]Institute for Data Processing and Electronics, KIT — [2]SLAC National Accelerator Laboratory

Many facilities employ beam loss monitors that report time-averaged loss rates and do not support precise time-of-arrival measurements. We developed an FPGA-based read-out system that, in combination with plastic scintillator detectors, enables beam loss measurements with sub-nanosecond time resolution over multi-second acquisitions. After calibrating the system with cosmic particles, we commissioned this system at the (50 - 500 MeV) booster synchrotron of the Karlsruhe Research Accelerator (KARA). This measurement campaign demonstrated the potential of this new technique. First, we characterized the beam background with nanosecond-level timing precision. Second, we acquired the accelerator clock and injection triggers, in order to correlate the beam background with beam injection, storage and extraction. We prove that the revolution timing structure of the beam current is present in the beam loss. In addition, we showed versatility of the readout system to sample the signals of a stripline sensor at the KARA main ring. In this contibution, we present the FPGA based data acquisition system, first commissioning results and discuss future applications of this technique.

AKBP 9: RF Cavities I

Time: Wednesday 11:00–12:30 Location: SCH/A117

AKBP 9.1 Wed 11:00 SCH/A117

RF characterization of superconducting samples with the UHH QPR at DESY — •Carl Weiss[1], Ricardo Monroy-Villa[2], Manuela Schmökel[3], Marc Wenskat[1,3], and Wolfgang Hillert[1] — [1]Institut für Experimentalphysik, Universität Hamburg — [2]Institut für Kernphysik, Johannes Gutenberg-Universität Mainz — [3]Deutsches Elektronen-Synchrotron DESY

Superconducting materials are indispensable for modern accelerators, for example highest acceleration fields are achieved with superconducting radio-frequency cavities made out of niobium. To further advance the development of superconducting materials for accelerators, an RF testing of samples is essential. The quadrupole resonator (QPR) is such a testing system, which allows the RF characterization of samples in the range of typical operational parameters of accelerators, such as a temperature range of 2-20 K, magnetic fields up to 120mT and for three different frequencies: 425 MHz, 860 MHz and 1300 MHz. In this report, the very first measurement of a sample in two different QPRs will be reported, which will proof the reliability and accuracy of such a system. Furthermore, fully exploiting the fact that the very same surface is tested at three different frequencies, the slow vs. fast superconductor model and non-equilibrium superconductivity will be investigated. This is of significant importance to study the so-called mid-T recipe developed for 1.3 GHz and test its transferability to other frequencies.

AKBP 9.2 Wed 11:15 SCH/A117

Atomic layer deposition of silicon nitride as an insulator layer for use in multilayer coating of cavities — •Ana Katharina Steffens[1], Isabel Díaz-Palacio[1], Robert Zierold[1], Marc Wenskat[2], and Wolfgang Hillert[1] — [1]Universität Hamburg, Hamburg, Deutschland — [2]Deutsches Elektronen Synchrotron (DESY), Hamburg, Deutschland

Multilayer coatings of superconducting cavities provide a strategic route to superconducting radio frequency surfaces engineered to surpass the performance limits of conventional bulk Nb. Particular attention is paid to SIS structures consisting of thin superconducting (S) and insulating layers (I), as these can prevent global vortex penetration and allowing for higher surface magnetic fields before the loss of the Meissner state. However, previous SIS structures consisting of Nb bulk, AlN, and NbTiN show diffusion of aluminum into the NbTiN layer upon annealing at high temperatures, compromising the SIS-performance. Herein, SiN is investigated as an alternative due to its greater thermal stability. Plasma-enhanced atomic layer deposition (PEALD) is used to deposit thin SiN and NbTiN layers, enabling controlled growth of homogeneous, conformal layers at low process temperatures. This study focuses on the development of a PEALD process for SiN and the characterization of various layer configurations, with initial results being presented.

AKBP 9.3 Wed 11:30 SCH/A117

Comparison of co-sputtered Nb_3Sn thin films grown on copper, sapphire and fused silica — •Amir Farhood[1], Alexey Arzumanov[1], Márton Major[1], Mohammad Khodakarami[1], Amin Matin Javid[1], Michaela Arnold[2], Norbert Pietralla[2], and Lambert Alff[1] — [1]Institute of Materials Science, Technical University of Darmstadt, — [2]Institute of Nuclear Physics, Technical University of Darmstadt, Darmstadt, Germany

Pure Niobium is still the main choice for superconducting RF cavities; however, it must be operated at around 2 K, which significantly increases cooling requirements. Nb_3Sn with a much higher T_c of approximately 18.2 K enables operation at 4.2 K. Applying Nb_3Sn coatings onto copper cavities through co-sputtering is expected to enhance the quality factor and to suppress quenching at elevated accelerating fields. In this work, Nb_3Sn layers were co-sputtered onto different substrates to examine their critical temperature and lower critical field (H_{c1}). Film growth was carried out under controlled conditions, followed by characterization through X-ray diffraction, resistivity measurements, and SQUID magnetometer. On all substrates, Nb_3Sn exhibits a clear superconducting transition. For films deposited on *r*-cut sapphire, a T_c of 17.8 K was achieved, which is close to the value for bulk Nb_3Sn. On copper, the films showed a T_c of about 15 K. Importantly, H_{c1} exceeded not only that of bulk Nb_3Sn but also that of pure niobium.

AKBP 9.4 Wed 11:45 SCH/A117

Texture investigations of Nb_3Sn thin films grown for SRF cavity application — •Márton Major[1], Alexey Arzumanov[1], Amir Farhood[1], Michaela Arnold[2], Norbert Pietralla[2], and Lambert Alff[1] — [1]Institute of Materials Science, Technical University of Darmstadt, Darmstadt, Germany — [2]Institute of Nuclear Physics, Technical University of Darmstadt, Darmstadt, Germany

Superconducting (SC) RF cavity technology is dominated by bulk Nb due to its proven physical performance and mature production technology. Needs for reducing the energy consumption of particle accelerators, however, call for alternative SC materials, such as Nb_3Sn, to allow their operation at higher temperatures at lower cryogenic costs. The Nb_3Sn coating of carrier structures has the potential to reach high acceleration gradients even at 4.2 K. Utilising thin film technology enables to use copper, an excellent heat conductor, for the bulk of the cavity to which Nb_3Sn can be sputtered for high-quality SC coatings. At our group, based on a low-temperature magnetron co-sputtering process, the direct deposition of SC Nb_3Sn on Cu became possible. The grown films had high critical fields and critical temperatures. Films co-sputtered on different substrates (single crystalline sapphire, polycrystalline copper, amorphous glass) show different superconducting properties. In this contribution we present a detailed analysis of the texture and local order of the grown Nb_3Sn thin films based mainly on x-ray diffraction measurements and discuss possible causes of observed differences.

AKBP 9.5 Wed 12:00 SCH/A117

Successfull Refurbishment of TESLA Cavities for MESA — •Paul Plattner — JGU Mainz - Institut für Kernphysik, Mainz, Germany

Two TESLA cavities that were previously operated in the decommissioned ALICE project have been successfully refurbished in the clean room and tested at the AMTF. They now meet the requirements for the Mainz Energy-recovering Siperconducting Accelerator (MESA) and will be used to test Higher Order Mode (HOM) antenna upgrades for the MESA Energy Recovering (ER) mode.

AKBP 9.6 Wed 12:15 SCH/A117

V-Band Microwave Cavities for Pulse Compression in an Ultrafast Transmission Electron Microscope — •Johann Toyfl[1,2], Dennis Naraschkewitz-Epp[1,2], Armin Feist[1,2], and Claus Ropers[1,2] — [1]Department of Ultrafast Dynamics, Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]4th Physical Institute, University of Göttingen, Göttingen, Germany

Ultrashort electron bunches are a unique source of coherent radiation, but utilizing their short matter wavelength for nanoscale probing was only recently achieved in ultrafast electron microscopes (UEM). However, their temporal resolution is typically limited by electron pulse dispersion to a few hundred femtoseconds [1].

In this contribution, we explore high-frequency V-band microwave cavities to compress the longitudinal phase space of electron pulses generated by femtosecond photoemission, either in the temporal or energy domain [1, 2, 3]. We characterize the microwave reflection coefficient and use our ultrafast transmission electron microscope (UTEM) [1] to obtain electric-field maps by spectroscopic imaging.

The integration of cavity-based phase-space control will enhance the temporal and spectral resolution of UEM, enabling the study of ultrafast dynamics that are currently accessible only in large-scale free-electron laser facilities.

[1] A. Feist *et al.*, Ultramicroscopy **176**, 63 (2017) [2] T. van Oudheusden *et al.*, Phys. Rev. Lett. **105**, 264801 (2010) [3] R. P. Chatelain *et al.*, Appl. Phys. Lett. **101**, 081901 (2012) [4] J. Kuttruff *et al.*, Sci. Adv. **10**, eadl6543 (2024)

AKBP 10: Plasma Accelerators, Diagnostics I

Time: Wednesday 15:00–16:15 Location: SCH/A117

Topical Talk AKBP 10.1 Wed 15:00 SCH/A117

Multiscale longitudinal electron bunch characteristics of LWFA bunches determined by single-shot CTR spectroscopy — •Alexander Debus[1], Maxwell LaBerge[1], Omid Zarini[1,2], Susanne Schöbel[1], Jessica Tiebel[1,2], Finn-Ole Carstens[1,2], Nico Wrobel[1,2], Richard Pausch[1], Klaus Steiniger[1], Yen-Yu Chang[1], Jurjen Couperus Cabadağ[1], Alexander Köhler[1,2], Thomas Kurz[1,2], Rafal Zgadzaj[3], Michael Downer[3], Michael Bussmann[1], Ulrich Schramm[1], and Arie Irman[1] — [1]HZDR, Dresden, Germany — [2]TU Dresden, Germany — [3]UT Austin, USA

The longitudinal structure of ultra-short electron bunches produced in laser-wakefield accelerators (LWFAs) is strongly influenced by the rapid injection dynamics as well as by ongoing interactions between the driving laser and the accelerated beam. Gaining a detailed picture of these bunch structures is key for progressing toward compact FELs and other advanced secondary light sources.

We report experimental findings derived from single-shot broadband coherent transition radiation (CTR) spectroscopy (spanning UV to mid-IR, 250 nm - 11.35 μm) generated as LWFA electron bunches traverse a metal foil. Through analysis of the CTR spectra, we reconstruct the corresponding electron bunch profiles. Our results reveal that electron bunches originating from different injection processes exhibit intricate longitudinal structures spanning multiple temporal scales, from the overall envelope down to sub-micrometer features. These patterns vary systematically with the injection regime and align with signatures observed in the electron spectrometer.

AKBP 10.2 Wed 15:30 SCH/A117

Novel approaches of using transition radiation to diagnose driver dynamics in plasma wakefield accelerators — •Nico Wrobel[1,3], Finn-Ole Carstens[1,3], Alexander Debus[1], Arie Irman[1], Maxwell La Berge[1], Susanne Schöbel[1], Ulrich Schramm[1,3], Klaus Steiniger[1,2], Jessica Tiebel[1,3], Patrick Ufer[1], and Richard Pausch[1] — [1]Helmholtz-Zentrum Dresden - Rossendorf e.V., DE — [2]Center for Advanced Systems Understanding, Görlitz, DE — [3]TU Dresden, DE

LPWFA is a new hybrid accelerator concept which combines laser wakefield accelerators (LWFA) and plasma wakefield accelerators (PWFA), resulting in an ultra-compact form factor while promising improved beam quality, compared to LWFA. The dynamics of the PWFA driver are investigated due to their impact on the capabilities to accelerate particles in the plasma wake. Since the driver beam dynamics cannot be directly observed in experiment, new diagnostic methods had to be explored, which we will present here.

Coherent transition radiation (CTR) was investigated to diagnose longitudinal and transversal driver dynamics with the help of the open-source particle-in-cell code PIConGPU. We were able to detect the breakup of the driving bunch through the emitted CTR spectrum and developed a novel diagnostic approach, which may be able to reconstruct time-dependent driver dynamics, like driver oscillation, from CTR measurements.

AKBP 10.3 Wed 15:45 SCH/A117

From studying to controlling injection dynamics in laser wakefield accelerators — •Jessica Tiebel[1,2], Richard Pausch[1], Michael Bussmann[1], Finn-Ole Carstens[1,2], Alexander Debus[1], Klaus Steiniger[1], René Widera[1], and Ulrich Schramm[1,2] — [1]Helmholtz-Zentrum Dresden - Rossendorf — [2]Technische Universität Dresden

Laser Wakefield Accelerators (LWFAs) enable the generation of highly relativistic, high charge, low emittance electron beams within only a few millimeters of acceleration. Their compactness and favorable electron beam properties make them attractive for many applications, like compact plasma wakefield drivers, synchrotron sources or free electron lasers. Enabling application-ready operation requires precise control over the sensitive and non-linear acceleration process, and therefore a deep understanding of the injection process and bunch evolution.

We used the open-source, multi-GPU particle-in-cell code PIConGPU to perform a comprehensive investigation of the acceleration and injection process. This enabled us to explain discontinuities in the injection process of self-truncated ionization injection (STII) and their consequent impact of the spatial and spectral charge distribution of the electron bunch. Based on these findings, we provide a practical guide for controlling STII to achieve the targeted electron beam parameters.

AKBP 10.4 Wed 16:00 SCH/A117

Time-Resolved Interferometry Measurement of Ultrasound Pulses generated by Laser-Accelerated Ions in Water — •Hannah Forsthuber, Julia Liese, Florian Schweiger, Alexander Prasselsperger, Sonja Gerlach, Xiang Chen, Kumudini Pagare, and Jörg Schreiber — LMU München, Fakultät für Physik - Medizinische Physik, Am Coulombwall 1, 85748 Garching

Recent progress in laser-driven ion acceleration and its applications in radiation-therapy research demands sensitive techniques to probe processes like ionoacoustic pressure waves. Building on earlier work using optical detection of refractive-index changes caused by ion beams in water, this project investigates a Mach-Zehnder interferometric approach operated near destructive interference. By combining high optical intensities with a balanced-detection scheme, the setup aims to enhance sensitivity to the weak acoustic signatures generated by laser-accelerated ion bunches at LMU's Center for Advanced Laser Applications. The method targets temporally and spatially resolved measurements of the pressure-wave evolution within the interaction volume, providing complementary information to transducer-based diagnostics [1]. The performance of the interferometric system will be evaluated in forthcoming experiments, with initial results expected by the time of the conference. Ultimately, this optical technique aims to deepen the understanding of ion-induced acoustic phenomena and to advance diagnostic capabilities for laser-accelerated ion sources in radiation-research environments.[1] S. Gerlach et al., High Power Laser Science and Engineering 11, 38 (2023)

AKBP 11: Plasma Accelerators, Diagnostics II

Time: Wednesday 16:30–17:30 Location: SCH/A117

AKBP 11.1 Wed 16:30 SCH/A117

Time-Resolved Optical Probing of Water Vapor Effects in Laser-Driven Ion Acceleration — •Kumudini Devendra Pagare, Florian Schweiger, Julia Liese, Alexander Prasselsperger, Sonja Gerlach, Hannah Forsthuber, and Jörg Schreiber — LMU München, Fakultät für Physik-Medizinische Physik, Am Coulombwall 1, 85748 Garching

Applications in laser-driven ion acceleration demand stable and reproducible ion beams with well-controlled properties. The quality of these ion beams depends critically on the dynamics of laser-target interactions, which are determined by both laser and target parameters. Time-resolved optical probing provides insight into these rapid interaction dynamics, revealing the processes responsible for ion acceleration and the mechanisms involved. Here, we examine how water vapor emitted from a recently implemented liquid-leaf target at the Centre for Advanced Laser Applications (CALA) influences the acceleration process. We employ interferometric diagnostics to quantify spatiotemporal vapor density profiles in front of the target surface. This allows us to assess how the expand-

ing vapor interacts with the main laser pulse and affects ion acceleration. These findings elucidate the complex dynamics of laser-target interactions and help optimize the resulting ion beam properties. This work was supported by the DFG under Grant Number 558546291 and CALA.

AKBP 11.2 Wed 16:45 SCH/A117

Active mirror cooling concept for high average power, high peak power Ti:Sapphire laser amplifiers — •Anneli Dick[1,2], Juan B. Gonzalez-Diaz[1], Thomas Hülsenbusch[1], Leonie Jaworski[1], Lutz Winkelmann[1], Andreas R. Maier[1], and Guido Palmer[1] — [1]Deutsches Elektronen Synchrotron DESY, Hamburg, Germany — [2]University of Hamburg, Hamburg, Germany

Advancing laser plasma accelerators from a few-hertz repetition rate to the kHz-regime is essential for unlocking next-generation applications, including free-electron lasers and direct synchrotron injection. Moreover, a high-repetition rate enables direct active stabilization of crucial laser parameters which will support sub-percent energy spread from the plasma accelerator. For efficient electron acceleration, 100 TW-level laser pulses are required, which are commonly generated by chirped pulse Ti:Sapphire amplifier systems. The Kaldera laser system at DESY is being developed to drive such a high-repetition-rate plasma accelerator. It is currently providing J-level energies at 100 Hz repetition rate. However, one major challenge of power scaling this material is the thermal load generated at high repetition rates and pump energies due to its high quantum defect. To control the resulting thermal effects more efficiently, new cooling concepts are required. Theoretical investigations on cryogenically cooled active mirror amplifiers have shown they can be a promising method to achieve this. The presented work evaluates this approach experimentally with respect to further power scaling of the Kaldera laser towards the multi-100 W range.

AKBP 11.3 Wed 17:00 SCH/A117

Patch-MLP-Based Predictive Control: Simulation with an Upstream Pointing Stabilization for PHELIX Laser System — •Jiaying Wang[1], Jonas Benjamin Ohland[3], Yen-Yu Chang[4], Vedhas Pandit[1], Stefan Bock[1], Andrew-Hiroaki Okukura[6], Udo Eisenbarth[3], Arie Irman[1], Michael Bussmann[1], Ulrich Schramm[1,2], and Jeffrey Kelling[1,5] — [1]HZDR, Dresden,Germany — [2]Technische Universität Dresden, Dresden, Germany — [3]GSI Helmholtzzentrum für Schwerionenforschung, Germany — [4]Amplitude laser group - Dresden operations, Germany — [5]Chemnitz University of Technology, Chemnitz, Germany — [6]Extreme Light Infrastructure - Nuclear Physics, National Institute for Physics and Nuclear Engineering, Ilfov, Romania

High-energy laser facilities such as PHELIX at GSI require excellent beam-pointing stability to ensure reproducibility and reliable operation. Conventional PID control mitigates slow drift but is fundamentally limited by diagnostic latency and mirror inertia. We introduce a predictive control scheme in which beam-pointing errors are forecast using a patch-based multilayer perceptron, and the predicted errors are converted into correction signals via a PID controller. This feed-forward strategy compensates for system delay and is trained directly on diagnostic time-series data. Simulations with an upstream correction mirror at the PHELIX pre-amplifier bridge show reduced residual jitter compared with conventional PID control. Across a 10-hour dataset, the predictive controller remained drift-free and improved pointing metrics by approximately 10%-20%.

AKBP 11.4 Wed 17:15 SCH/A117

2D Measurements of Laser Angular Chirps for the DRACO CPA Laser system — •Mohamed Samir[1,2], Maxwell Laberge[1], Susanne Schöbel[1], Yen-Yu Chang[1], Patrick Ufer[1,2], Franziska Marie Herrmann[1,2], Stefan Bock[1], Ulrich Schramm[1,2], and Arie Irman[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf (HZDR) — [2]Technische Universität Dresden

Controlling spatio-temporal properties of ultrashort, high-power laser pulses is essential for laser-matter interactions, particularly Laser Wakefield Acceleration (LWFA). For such broadband pulses, angular dispersion (AD) becomes detrimental due to unavoidable transmissive optics or misalignment in the chirped-pulse amplification (CPA) chain. This dispersion induces wave-front tilt (WFT), degrading the focal spot, lowering the peak intensity on target, and introducing wakefield asymmetries that deflect the accelerated electron beam, thereby reducing the efficiency and stability of the acceleration process.

To quantify this for efficient LWFA and to support next-generation, dephasingless LWFA (DLWFA) concepts, we implemented a compact optical setup and conducted measurements at various positions along the 100-TW DRACO laser chain and inside the target chamber. The laser's AD and WFT were fully characterized in 2D and subsequently corrected at the target-chamber focal plane using the main TW compressor. The setup also enables precise spectral measurements, highly compact (~20 cm), lens configurable, and easily integrated.

These characterizations will support more stable, efficient laser wakefields, while serving as key diagnostics for DLWFA schemes.

AKBP 12: Novel Accelerators I

Time: Thursday 9:30–11:00 Location: SCH/A117

Topical Talk AKBP 12.1 Thu 9:30 SCH/A117

Cutting-edge research and technology at KIT's advanced accelerator facilities — •Erik Bründermann — IBPT Accelerator Team, KIT, Karlsruhe, Deutschland

The Institut für Beschleunigerphysik und Technologie (IBPT) at the Karlsruhe Institute of Technology (KIT) operates a unique suite of accelerator facilities. These include the Karlsruhe Research Accelerator (KARA) with its electron storage ring (0.5-2.5 GeV) and booster synchrotron (50-500 MeV), the short-pulse linear accelerator FLUTE (40-90 MeV), and the KITTEN test center for energy-efficient research infrastructures. In addition, IBPT is developing compact laser-plasma accelerators (LPAs). Together with its Magnet and Cryogenics Facilities of the Accelerator Technology Platform (ATP), KIT offers an outstanding environment for accelerator research and technology transfer. Looking ahead, the compact storage ring cSTART will be established to explore non-linear and non-equilibrium physics, with FLUTE and LPAs serving as injectors.

In this group report, we present the current and upcoming accelerator test facilities at KIT and highlight key results in accelerator physics and technology, including the first superconducting THz undulator, ultra-high-dose operation modes of FLUTE, and innovative diagnostic techniques.

AKBP 12.2 Thu 10:00 SCH/A117

Simulations of a Plasma Booster for the European XFEL — •Anna Krivkova[1], Tianyun Long[1], Alexander Sinn[1], Maxence Thevenet[1], Stephan Wesch[1], Matthew Wing[1,2], and Jonathan Wood[1] — [1]Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany — [2]University College London, London WC1E 6BT, United Kingdom

Proposed upgrades of the European XFEL include continuous-wave operation, which requires lowering maximum beam energy from 17.5 GeV to about 8 GeV to facilitate a large increase in repetition rate. A beam-driven plasma accelerator offers a compact and efficient solution to compensate for this energy loss. By integrating a plasma booster into an existing beamline, the European XFEL could restore its nominal beam energy and potentially exceed the current 17.5 GeV limit. To evaluate the feasibility and performance of such a booster, we perform particle-in-cell simulations in HiPACE++ using several gas species over a range of plasma densities. The accelerating gradients consistently reach the multi-GV/m regime, with realistic peak values of about 8 GV/m. The simulations further show that the 5 kA, high-brightness XFEL bunches present challenges for plasma wakefield acceleration due to strong ion motion and beam-induced ionization, increasing the emittance and energy spread of the accelerated witness bunch. Mitigation strategies, including optimization of the initial driver and witness emittance, will be presented.

AKBP 12.3 Thu 10:15 SCH/A117

all-optical In-plasma multi-staging of Laser-Wakefield Accelerators using density tailoring — •Xingjian Hui, Alberto Martinez de la ossa, Alexander Sinn, Ángel Ferran pousa, Rob Shalloo, and Maxence Thévenet — DESY, Hamburg, Germany

The staging of laser-driven plasma accelerators (LPAs) could open up energy frontiers, but achieving in- and out-coupling of laser pulses while preserving beam quality remains a challenge. In this work, we present an all-optical, in-plasma staging scheme that uses refraction in a transverse plasma density gradient to couple the incoming laser into the next LPA stage, eliminating the need for mirrors and magnets. This design can in principle support significant ion motion without substantial emittance degradation, making it well-suited for a broad energy range. With realistic 3D simulations using the quasistatic particle-in-cell code HiPACE++ on GPU, we observe 98% capture efficiency and 15+3+3 GeV energy gain per within 3 stages with emittance preserved and proper bean loading, driven by a ~20J for first stage and ~10 J laser pulse for followings guided by a hydrodynamic optical-field-ionized (HOFI) channel of matched spot size 30 microns. These results represent a significant step toward practical multistage plasma acceleration, paving the way for the generation of ultra-high-energy electron beams for a wide range of scientific and technological applications.

AKBP 12.4 Thu 10:30 SCH/A117

Microsecond-timescale plasma density growth by electron beam energy deposition in plasma-wakefield accelerators — •Judita Beinortaite[1], Jonas Björklund Svensson[1], Lewis Boulton[1], Greg Boyle[2], Brian Foster[1,3], Pau González Caminal[1], Harry Jones[1], Advait Kanekar[1,4], Anna Křivková[1], Gregor Loisch[1], Jens Osterhoff[1], Felipe Peña[1,4], Sarah Schröder[1], Stephan Wesch[1], Matthew Wing[1,5], Jonathan Wood[1], and Richard D'Arcy[1,3] — [1]DESY, Germany — [2]James Cook University, Australia — [3]J.A.I, UK — [4]University of Hamburg, Germany — [5]University College London, UK

High-repetition-rate operation of plasma-wakefield accelerators is essential for their suitability in the design of particle colliders and Free-Electron Lasers (FELs). Energy remaining in the plasma after the wakefield acceleration event can limit the repetition rate of the plasma accelerator as the plasma takes time to relax to its initial state. This relaxation is dominated by two ion-driven effects: their redistribution after the wakefield event and potential further collisional ionisation caused by this motion. In this work, we investigated argon plasma at a variety of working points with two different diagnostics: the pump-probe electron-beam-based technique and optical-emission spectrometry. In some regimes, both diagnostics indicated additional ionisation occurring on the nanoseconds-to-microsecond timescale for specific initial plasma conditions, which increased the recovery time. This can inform the design of the highest-repetition-rate plasma sources for future colliders and FELs.

AKBP 12.5 Thu 10:45 SCH/A117

Radiation Signatures from Injection Lasers in Plasma Wakefield Accelerators — •Finn-Ole Carstens[1,2], Alexander Debus[1], Klaus Steiniger[1], Michael Bussmann[1], Fabia Dietrich[1,2], Maxwell LaBerge[1], Susanne Schoebel[1], Jessica Tiebel[1,2], Patrick Ufer[1,2], Nico Wrobel[1,2], Arie Irman[1], Ulrich Schramm[1,2], and Richard Pausch[1] — [1]Helmholtz-Zentrum Dresden - Rossendorf, Dresden, Germany — [2]Dresden University of Technology, Dresden, Rossendorf

Plasma-wakefield acceleration driven by electron beams from laser-wakefield accelerators enables compact, two-stage schemes of electron accelerators. The trojan horse injection method uses a transverse, femtosecond laser pulse to ionize electrons inside the first plasma cavity and promises high-brightness electron bunches. Unexpectedly, experiments showed a distinct radiation feature in shadowgraphy images whenever this injection laser interacted with the plasma wake. This effect that turned out to be crucial for timing calibration but was not understood.

We investigate this signal using particle-in-cell simulations equipped with an in-situ imaging plugin based on Fourier propagation, which models the shadowgraphy diagnostic directly during runtime. This approach allows tracing the formation of the observed feature and reveals that it originates from Thomson scattering of the injection laser of the sheath electrons of the PWFA cavity. In this contribution, we present the mechanism behind the signal and show how it can be used to infer structural properties of the plasma cavity.

AKBP 13: Novel Accelerators II

Time: Thursday 11:30–12:30 Location: SCH/A117

AKBP 13.1 Thu 11:30 SCH/A117

High-Repetition-Rate Electron Beams from a Multi-kHz LPA Driven by an Industrial Laser System — Bonaventura Farace[1], Kristijan Poder[1], •Taegyu Pak[1], Esmerando Escoto[1], Nikita Khodakovskiy[1], Christoph Heyl[1], and Wim Leemans[1,2] — [1]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany — [2]University of Hamburg, Department of Physics, Jungiusstr. 9, 20355 Hamburg, Germany

Laser-plasma accelerators (LPAs) provide a compact platform for generating ultrashort, high-brightness electron beams and are gaining attention as next-generation electron sources. For practical use, the driving laser must operate stably at high repetition rates with high average power and scalability. Here, we report the first demonstration of electron acceleration using an industrial Yb-based laser compressed via a multi-pass cell (MPC) post-compression stage. The Yb:YAG laser was spectrally broadened in a 2-m long MPC and compressed from 1.3 ps to 49 fs, delivering 9 mJ on target at repetition rates up to 12.5 kHz. With these post-compressed pulses, we generated high-repetition-rate electron beams and characterised their charge, energy spectrum and transverse beam profile. The source produced 10 pC per shot with a thermal-like spectrum extending up to 5 MeV and operated robustly in the multi-kHz regime. These results demonstrate a new technological route for generating high-repetition-rate electron beams with industrial Yb lasers. They also open pathways toward applications that require high repetition rates and ultrashort pulses, including ultrafast electron diffraction and FLASH-type irradiation schemes.

AKBP 13.2 Thu 11:45 SCH/A117

Temperature diagnostics for MHz-repetition-rate plasma accelerator sources — •Juan Pablo Díaz[1,2], Judita Beinortaite[1], Maryam Huck[1], Harry Jones[1], Anna Křivková[1], Gregor Loisch[1], Gudrid Moortgat-Pick[1,2], Lukas Müller[1], Trupen Parikh[1], Stephan Wesch[1], Matthew Wing[3,1], and Jonathan Wood[1] — [1]DESY, Hamburg, Germany — [2]Universität Hamburg, Germany — [3]University College London, UK

Electron-bunch-driven plasma-wakefield accelerators promise to revolutionize particle acceleration by providing compact and cost-effective energy boosters for electron linacs which could, for example, significantly enhance the photon energies produced by free-electron lasers. The FLASHForward facility at DESY has made substantial progress, demonstrating that accelerated electron bunches can maintain their charge, energy spread, and emittance during plasma acceleration. A major challenge remains in achieving high-repetition-rate operation. Reaching MHz-level repetition rates, necessary to match superconducting RF linac bunch patterns, means generating reproducible plasma acceleration events at MHz frequencies. Doing so poses significant challenges: keeping the plasma density uniform over these rapid cycles and dealing with the high heat load placed on the plasma cell by the plasma formation process and the drive beam. In this contribution, we report on recent efforts to characterize the long-term heating effects arising in a discharge plasma source at repetition rates up to 1 kHz. We will present measurements of the time evolution of the discharge plasma source and discuss the implications of these results.

AKBP 13.3 Thu 12:00 SCH/A117

Statistical analysis of sources of instability in electron beam quality in laser plasma accelerators preparing for Bayesian optimization — •Franziska Marie Herrmann[1,2], Maxwell Laberge[1], Yen-Yu Chang[1], Amin Ghaith[1], Jeffrey Kelling[1], Susanne Schöbel[1], Patrick Ufer[1,2], Ulrich Schramm[1,2], and Arie Irman[1] — [1]HZDR, Dresden, Germany — [2]Technische Universität Dresden, Dresden, Germany

Laser-electron accelerators are emerging as novel, compact sources of high-quality relativistic electron beams for a wide range of applications. Each experimental application requires unique electron parameters. Additionally, all the input parameters are interconnected, resulting in a highly complex parameter space. To address this issue, we have developed a semi-automated Bayesian optimization loop that adjusts six input parameters simultaneously to achieve optimal electron beam parameters. However, the high nonlinearity of laser wakefield acceleration poses a challenge for automated optimization, as even minor fluctuations in input parameters can lead to significant changes in electron beam properties. To quantify and mitigate the effects of these statistical fluctuations, we have compiled an extensive dataset through systematic studies of their characteristics and influence on the electron beam quality. Alongside demonstrating an initial prototype for semi-automated Bayesian optimization, this work will enhance the understanding of the underlying sources of instability in laser-plasma acceleration experiments, which are essential for more complex machine learning experiments.

AKBP 13.4 Thu 12:15 SCH/A117

Characterization of kinetic instabilities in high-intensity, short-pulse, laser-driven solid-density plasmas — •Jannis Schulz — TU Dresden — HZDR

We present a study of instabilities in plasmas generated by the interaction of electron beams accelerated by intense femtosecond laser pulses with dense solid targets. At intensities exceeding 10^{18} W/cm^2, the beam-plasma system develops collective processes that strongly influence energy and particle transport. As an overarching framework, the analysis of linear stability properties is used to systematically describe the emergence and evolution of characteristic structures. The main emphasis lies on transverse filamentation instabilities, in particular the collisional-resistive regime, whose growth is strongly affected by electrical conductivity and current distribution. In addition, longitudinal processes such as the two-stream instability are examined, arising from counter-propagating electron populations. The classification relies on analytically derived dispersion relations, which allow the comparison of growth rates and wavelengths with numerical simulations and latest experiments performed at LCLS and EuropeanXFEL. The objective is to clarify the mechanisms that drive the development of these instabilities, connect them to the structures observed in the simulations, and ultimately connect them to the underlying plasma conditions (e.g. beam and background densities and effective temperatures).

AKBP 14: RF Cavities II

Time: Thursday 15:00–15:45 Location: SCH/A117

AKBP 14.1 Thu 15:00 SCH/A117

Development and Realization of a new Chopper Cavity for the S-DALINAC* — •Vincent Pruy, Arnold Michaela, Ruben Grewe, Katharina E. Ide, Lars Jürgensen, Lisa Dingeldein, Clemens M. Nickel, Norbert Pietralla, and Dominic Schneider — Institut für Kernphysik, Technische Universität Darmstadt, Darmstadt, Germany

The operation of the superconducting radio-frequency cavities of the S-DALINAC [1] relies on a bunched electron beam. Currently, the continuous beam generated by the thermionic gun is divided into bunches using a chopper system incorporating a single deflecting cavity. However, this system induces nonlinear curvatures in the beam trajectory. A second, identically constructed deflecting cavity can be employed to re-bend the beam thus counteracting the nonlinear distortions. Comprehensive electromagnetic and particle-tracking simulations aimed at optimizing the cavitiy's deflection behavior and quality factor have already been completed. This work further concluded the in-house fabrication of the cavity and its commissioning in the injector beamline of the S-DALINAC. In this contribution, we report on the manufacturing process and the measured properties of the cavity. In addition, we propose a viable concept realizing a double chopper system based on the existing components.

[1] N. Pietralla, Nucl. Phys. News, Vol. 28, No. 2, 4 (2018).

*This work is supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) * Project-ID 499256822 * GRK 2891 'Nuclear Photonics'.

AKBP 14.2 Thu 15:15 SCH/A117

Development of a New Prebuncher for the 26 MeV S-band Linac at ELSA — •Nicholas Treska, Klaus Desch, Jerome Orbons, Michael Switka, Dennis Proft, and Philipp Hänisch — Physikalisches Institut der Universität Bonn

A new prebuncher for the 26 MeV S-band linac at ELSA is being developed. A range of CST simulations and prototype measurements indicate the potential for improvements in transfer efficiency, vacuum performance, and electric field characteristics. A test stand for the characterization of prototypes is set up. The work focuses on assessing the feasibility and performance of the new design.

AKBP 14.3 Thu 15:30 SCH/A117

Design of a fast reactive tuner for 1.3 GHz TESLA cavities at MESA — •Ricardo Monroy-Villa[1], Ilan Ben-Zvi[2], Florian Hug[1], and Timo Stengler[1] — [1]Institute for Nuclear Physics, Johannes Gutenberg-Universität Mainz, Mainz, Germany — [2]Physics and Astronomy Department, Stony Brook University, New York, USA

We present a state-of-the-art design of a Ferroelectric Fast Reactive Tuner (FE-FRT), capable of modulating high reactive power in TESLA-type cavities on a microsecond time scale. The Mainz Energy-Recovering Superconducting Accelerator employs 1.3 GHz superconducting radio-frequency (SRF) cavities, achieving quality factors of the order of 10^10. However, detuning of 25 Hz induced by microphonics has led to the use of strong coupling for the fundamental power coupler, requiring high-power amplifiers, orders of magnitude above the intrinsic dissipation. Current solutions to mitigate microphonics rely on piezoelectric tuners, which are not fast enough for the spectral range of the microphonics. A novel alternative is the FE-FRT, a technology made possible by low-loss ferroelectric materials, which offer sub-microsecond response times. Analytical results are provided along with their validation through finite-element simulations. The FE-FRT can handle substantial reactive power while offering a tuning range of 50 Hz in SRF cavities, resulting in a reduction in peak forward RF power by about an order of magnitude.

AKBP 15: AKBP Prize Talks

Time: Thursday 16:00–17:30 Location: SCH/A117

AKBP 15.1 Thu 16:00 SCH/A117

Master course accelerator research - a joint effort of the Rhein Main Universities (RMU) — •Aulenbacher Kurt — Institut für Kernphysik Universität Mainz

Goethe-University Frankfurt, Johannes Gutenberg-University Mainz and TU-Darmstadt have developed a new educational concept in the field of accelerators. It is based on the unique situation in the Rhein-Main area where three universities are not only contributing to the GSI/FAIR project but also operate particle accelerators on their respective campus. This creates a unique opportunity to educate students coming from different areas, such as electric engineering or physics, towards a master degree in accelerator research. This qualification will address the needs for qualified accelerator personnel in industry and science. The talk will present the structure of the educational program and the specific possibilities of the contributing universities.

AKBP 15.2 Thu 16:30 SCH/A117

Young Investigator Prize AKBP — •N N — NN

Prize talk tbd

AKBP 15.3 Thu 17:00 SCH/A117

Horst Klein Prize Talk — •N N — NN

Prize Talk tbd

AKBP 16: Members' Assembly

Time: Thursday 18:00–19:00 Location: SCH/A117

All members of the Working Group on Accelerator Physics are invited to participate.

Working Group on Equal Opportunities
Arbeitskreis Chancengleichheit (AKC)

Agnes Sandner
Sprecherin des AKC
sandner@akc.dpg-physik.de

Overview of Invited Talks and Sessions

(Lecture hall MER/0002)

Invited Talks

AKC 1.1	Thu	11:15–11:45	MER/0002	**From Taboo to Transformation: Addressing Gender-Based Violence in Academia** — •Anja Wiede
AKC 1.2	Thu	11:45–12:15	MER/0002	**Leadership, Cooperation and Conflicts in Physics: Research Leaders' Perspectives** — •Maike Reimer
AKC 1.3	Thu	12:15–12:45	MER/0002	**Die Physikidentität von Schüler:innen stärken: Erkenntnisse zu Theorie und Praxis** — •Paula Becker, Peter Wulff

Sessions

AKC 1.1–1.3	Thu	11:00–12:45	MER/0002	**AKC**
AKC 2	Thu	13:00–13:45	MER/0002	**Women in Physics Lunch**

Sessions

– Invited Talks –

AKC 1: AKC

Time: Thursday 11:00–12:45 Location: MER/0002

Begrüßung durch Agnes Sandner, Sprecherin des AKC

Invited Talk AKC 1.1 Thu 11:15 MER/0002

From Taboo to Transformation: Addressing Gender-Based Violence in Academia — •Anja Wiede — TU Dresden, Dresden, Germany

Gender-based violence in academia is not a side issue but part of how power and inequality are reproduced within universities. According to recent UniSAFE findings, around 62% of respondents have encountered at least one form of such violence since joining their institution. Psychological violence and sexual harassment are particularly common, while reporting remains rare.

This lecture treats sexualised discrimination and violence not as individual misbehaviour or desire, but as a way power is exercised through everyday academic relations. It examines how universities with their status hierarchies, insecure employment paths, male-centred norms, and self-image as progressive spaces, create conditions in which these forms of harm are downplayed, rendered invisible, or dealt with inadequately. These structural features interact with individual tendencies of perpetrators, making violence both possible and easy to hide.

The lecture explores why such violence persists despite equality and diversity rhetoric and how gender-based violence operates as a form of power abuse in academic systems. Participants will gain concrete insights into the structural and cultural conditions that enable these dynamics, and they will be invited to reflect on their own institutional contexts. The session offers practical ideas for creating safer academic environments from strengthening accountability and reporting structures to developing everyday practices that confront power imbalances.

Invited Talk AKC 1.2 Thu 11:45 MER/0002

Leadership, Cooperation and Conflicts in Physics: Research Leaders' Perspectives — •Maike Reimer — Bayerisches Staatsinstitut für Hochschulforschung und Hochschulplanung (IHF), Arnulfstraße 56, 80335 München

"Can Germany rein in its academic bullying problem?" This question was recently raised prominently in a nature article. Anecdotal evidence as well as systematic surveys among researchers indeed paint a bleak picture of research leadership and institutional structures for conflict prevention and management in research settings in Germany and its German-speaking neighbouring states. However, the perspectives and voices of senior researchers are conspicuously absent from this discourse. Therefore, in collaboration with the DPG, we conducted 11 interviews and a survey among all members with leadership experience, about one crucial aspect and challenge of leadership: dealing with conflicts in their research teams. Here, we will present results from the full report on the frequency, kind, antecedents and consequences of conflicts and the ways they were resolved with or without institutional support. In addition, we investigate gender specific patterns in conflict experience. We hope to contribute to a more nuanced discussion and ultimately an improvement in research institutions conflict management structures.

Invited Talk AKC 1.3 Thu 12:15 MER/0002

Die Physikidentität von Schüler:innen stärken: Erkenntnisse zu Theorie und Praxis — •Paula Becker und Peter Wulff — Pädagogische Hochschule Ludwigsburg

Im Fach Physik zeigen sich weiterhin geschlechterspezifische Disparitäten entlang von Bildungswegentscheidungen. Die Frage, ob Physik als etwas erlebt wird, das zur eigenen Person passt, spielt dabei eine zentrale Rolle dafür, ob Schüler:innen sich ein langfristiges Engagement in Physik vorstellen können. In der Physikdidaktik wurde dies in der Physikidentitäts-Theorie konzeptionalisiert, die bedeutsame motivationstheoretische Forschungsstränge zusammenführt und die Bedeutung der sozialen Situiertheit von Lernen und Engagement explizit adressiert. Der Vortrag stellt diese Theorie vor und analysiert Fördermaßnahmen, die empirische Befunde zur Stärkung von Physikidentiät berücksichtigen. Wir berichten die Entwicklung und Evaluation von a) einem Programm zur Förderung von hochleistenden Schüler:innen und b) einer fünftägigen Projektwoche für Oberstufenschülerinnen. Unsere Ergebnisse zeigen, dass gezielte Maßnahmen positive Effekte auf Physikidentiät und Studienaspirationen haben können. Gleichzeitig wird deutlich, dass diese Potenziale begrenzt sind, wenn sie auf punktuelle Förderformate beschränkt bleiben. Um auszuschärfen, wie die Erkenntnisse in den schulischen Alltag integriert werden können, wird ein Ausblick auf ein Projekt gegeben, das untersucht, wie Lehrkräfte dabei unterstützt werden können, die Physikidentität ihrer Schüler:innen zu stärken.

AKC 2: Women in Physics Lunch

Time: Thursday 13:00–13:45 Location: MER/0002

Female physicists of all career stages are cordially invited to join our meet-and-greet networking lunch or snack. Diverse and all kinds of interested colleagues are also welcome!

Working Group on Industry and Business
Arbeitskreis Industrie und Wirtschaft (AIW)

Hans-Georg Grothues
Chairman of the AIW
hg.grothues@dlr.de

The Industry Day will be held as part of the DPG Spring Conference, which usually has over 6,000 participants. Around 250 people (mostly students and doctoral candidates) taking part in the Industry Day, which is organized and carried out by the Industry and Economy Working Group (AIW) of the DPG. The aim of the events is to inspire students and PhD candidates for careers in business and industry. Following the Industry Day the DPG Technology Transfer Award will be conferred.

Overview of Invited Talks and Sessions

(Lecture hall BAR/SCHÖ)

Invited Talks

AIW 1.2	Wed	14:10–14:30	BAR/SCHÖ	**From Particle Physics to Patient Care – The Evolution of Accelerator-Based Tumor Therapy in Germany** — •Andrea Denker
AIW 1.3	Wed	14:30–14:50	BAR/SCHÖ	**High Energy X-rays: Pioneering Hope and Success in Cancer Therapy** — •Stefan Scheib
AIW 1.4	Wed	14:50–15:10	BAR/SCHÖ	**A Compact Accelerator Driven Neutron Source for Industry and Medicine** — •Holger Höltermann
AIW 2.2	Wed	16:00–16:20	BAR/SCHÖ	**Accelerating Research with Particle Accelerators** — •Christoph Quitmann
AIW 2.3	Wed	16:20–16:40	BAR/SCHÖ	**Advancements in Superconductor Technology for High-Energy Accelerators and Fusion Applications** — •Klaus Schlenga
AIW 2.4	Wed	16:40–17:00	BAR/SCHÖ	**Application of Electron Accelerators for the Crosslinking of Polymers in Industry** — •Andreas Ostrowicki

Invited Talks of the joint Symposium The Sustainability Challenge: A Decade of Transformation (SYSC)

See SYSC for the full program of the symposium.

SYSC 1.1	Mon	15:00–15:30	HSZ/AUDI	**Open-Endedness and Community-Based Approaches to Sustainability Challenges** — •Hiroki Sayama
SYSC 1.2	Mon	15:30–16:00	HSZ/AUDI	**Education as a Social Tipping Element: Evidence from Climate and Physics Education Research** — •Thomas Schubatzky
SYSC 1.3	Mon	16:00–16:30	HSZ/AUDI	**Mechanistic and Material Perspectives on Enzymatic Hydrolysis of Semicrystalline Polyesters** — •Birte Höcker
SYSC 1.4	Mon	16:45–17:15	HSZ/AUDI	**Decarbonization Options for Industry** — •Uwe Riedel
SYSC 1.5	Mon	17:15–17:45	HSZ/AUDI	**Impacts of Cosmic Dust and Space Debris in the Terrestrial Atmosphere** — •John Plane

Sessions

AIW 1.1–1.5	Wed	14:00–15:30	BAR/SCHÖ	**Medical Applications – Accelerators in the Service of Health**
AIW 2.1–2.5	Wed	15:55–17:20	BAR/SCHÖ	**Medical Applications – Accelerators in the Service of Health**
AIW 3	Wed	17:20–18:00	BAR/SCHÖ	**Ceremony of the DPG Technology Transfer Award & Presentation**
AIW 4	Wed	18:00–19:30	BAR/SCHÖ	**Open Reception of the AIW for the winners**

Sessions

– Invited Talks, Discussions, and Contributed Talks –

AIW 1: Medical Applications – Accelerators in the Service of Health

Time: Wednesday 14:00–15:30 Location: BAR/SCHÖ

AIW 1.1 Wed 14:00 BAR/SCHÖ

Welcome and greeting — •Hans-Georg Grothues[1] and •John Kettler[2] — [1]Chairman of the AIW — [2]actimondo eG, Inden

Invited Talk AIW 1.2 Wed 14:10 BAR/SCHÖ

From Particle Physics to Patient Care – The Evolution of Accelerator-Based Tumor Therapy in Germany — •Andrea Denker — Helmholtz-Zentrum für Materialien und Energie, Berlin

The origins of particle therapy in Germany lay in 1998: In July, the treatment of ocular tumours with protons started in a collaboration of Helmholtz-Zentrum Berlin and Charité – Universitätsmedizin Berlin and in August clinical studies using carbon ions began at GSI Helmholtzzentrum für Schwerionenforschung. In both cases accelerators, originally built for particle physics, were used.

Now, more than 25 years later, five centres provide particle therapy for cancer treatment and more than 30000 patients have been treated in Germany. This is an excellent example of an extremely successful technology transfer from fundamental research to health care.

In parallel to routine treatment, accompanying research is on-going. This comprises, among others, new forms of beam delivery with the hope to reduce side effects while maintaining tumour control. Examples are FLASH-irradiations, where the dose is applied in a very short time, and the spatial fractionation of the irradiation, the so-called minibeam. This new irradiation forms create new challenges for the (existing and future) accelerators.

Invited Talk AIW 1.3 Wed 14:30 BAR/SCHÖ

High Energy X-rays: Pioneering Hope and Success in Cancer Therapy — •Stefan Scheib — Varian Medical Systems Imaging Lab GmbH, Zürich

Non-communicable diseases such as cancer represent one of the greatest challenges in global healthcare. Radiation therapy is a cornerstone of cancer treatment, applied in approximately 50% of all cases worldwide. This presentation will outline the fundamental principles of radiation therapy and explore the production and clinical application of high-energy X-rays within modern treatment workflows. Advances in high-energy X-ray technology have significantly contributed to improved outcomes, including enhanced tumor control and increased overall survival rates. Finally, emerging research directions in high-energy X-ray–based radiation therapy will be discussed, underscoring the promise of continued progress and success in cancer care.

Invited Talk AIW 1.4 Wed 14:50 BAR/SCHÖ

A Compact Accelerator Driven Neutron Source for Industry and Medicine — •Holger Höltermann — Bevatech GmbH, Mörfelden-Walldorf

The use of neutrons is established since decades and essential for industry, medicine, life sciences, and research. Classical neutron sources are mainly neutron generators, with low neutron flux, or research reactors and spallation sources, which are large and cost intensive installations. A cost efficient, effective, and compact neutron source with neutron yields up to 1e13 neutrons per second could bridge the gap existing. It will offer potential users either a dedicated standalone version for high demands of a single application such as BNCT or a full variable user facility.

Discussion AIW 1.5 Wed 15:10 BAR/SCHÖ

Panel discussion: Precision, Particles, Patients – The Future of Accelerator-Based Therapies — •Andrea Denker[1], •Stefan Scheib[2], •Holger Höltermann[3], and •John Kettler[4] — [1]Helmholtz-Zentrum für Materialien und Energie — [2]Varian Medical Systems Imaging Lab GmbH — [3]Bevatech GmbH — [4]actimondo eG, Inden

AIW 2: Medical Applications – Accelerators in the Service of Health

Time: Wednesday 15:55–17:20 Location: BAR/SCHÖ

AIW 2.1 Wed 15:55 BAR/SCHÖ

Find your way: Career orientation and support from the DPG — •Gabriele Becker — Advisor to the DPG Board, Bad Honnef

Invited Talk AIW 2.2 Wed 16:00 BAR/SCHÖ

Accelerating Research with Particle Accelerators — •Christoph Quitmann — RI Research Instruments, Bergisch Gladbach

Particle accelerators are fundamental for our understanding of the universe and for improving the human condition. Whether you want to understand the standard model of particle physics, sterilize surgical instruments, polymerize plastics or cure cancer, you need a particle accelerator.

Working in the design, fabrication and installation of such accelerators requires teams combining the knowledge of all fields in natural science, engineering and computer science. This team then interacts with customers from all areas of science, technology and society.

It is possibly the most fun and diverse job awaiting any curious and engaged physicist.

Invited Talk AIW 2.3 Wed 16:20 BAR/SCHÖ

Advancements in Superconductor Technology for High-Energy Accelerators and Fusion Applications — •Klaus Schlenga — Bruker Energy & Supercon Technologies, Hanau

Progress in Superconductor performance was significantly challenged and influenced by requirements for large scale physics projects. Experimental Fusion reactors and Accelerators up to LHC used superconducting magnets based on NbTi wires, while ITER Toroidal Field (TF) as well as Central Solenoid (CS) magnets use Nb3Sn wires with technologies from the 1990ies. Exploiting further progress in wire designs the LHC High Luminosity upgrade progressed to Nb_3Sn wires with 3x the performance of ITER Nb_3Sn.

Magnets for next generation Fusion reactors challenge again cost and performance of superconductors. The talk will give an overview of current status and future outlook of wire and magnet technology including High Temperature Superconductors (HTS).

Invited Talk AIW 2.4 Wed 16:40 BAR/SCHÖ

Application of Electron Accelerators for the Crosslinking of Polymers in Industry — •Andreas Ostrowicki — BGS Beta-Gamma-Service, Wiehl

The modification of polymers using electron accelerators has evolved from a specialized niche to a versatile industrial technology with applications in numerous areas. This presentation introduces the basic mechanisms and polymer classes that are best suited for radiation crosslinking. Using examples from industry, it provides an overview of established and new applications and the technical implementation of irradiation. Current research results, challenges, and technological trends are discussed.

Discussion AIW 2.5 Wed 17:00 BAR/SCHÖ

Panel discussion: Accelerating Innovation – Industrial Applications of High-Energy Physics — •Christoph Quitmann[1], •Klaus Schlenga[2], •Andreas Ostrowicki[3], and •John Kettler[4] — [1]RI Research Instruments — [2]Bruker Energy & Supercon Technologies — [3]BGS Beta-Gamma-Service — [4]actimondo eG, Inden

AIW 3: Ceremony of the DPG Technology Transfer Award & Presentation

Time: Wednesday 17:20–18:00 Location: BAR/SCHÖ

AIW 4: Open Reception of the AIW for the winners

Time: Wednesday 18:00–19:30 Location: BAR/SCHÖ

Working Group "Young DPG"
Arbeitskreis junge DPG (AKjDPG)

Pauleo Nimtz
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Overview of Invited Talks and Sessions

(Lecture hall SCH/A101)

Invited Talks of the joint Symposium The Sustainability Challenge: A Decade of Transformation (SYSC)

See SYSC for the full program of the symposium.

SYSC 1.1	Mon	15:00–15:30	HSZ/AUDI	**Open-Endedness and Community-Based Approaches to Sustainability Challenges** — •Hiroki Sayama
SYSC 1.2	Mon	15:30–16:00	HSZ/AUDI	**Education as a Social Tipping Element: Evidence from Climate and Physics Education Research** — •Thomas Schubatzky
SYSC 1.3	Mon	16:00–16:30	HSZ/AUDI	**Mechanistic and Material Perspectives on Enzymatic Hydrolysis of Semicrystalline Polyesters** — •Birte Höcker
SYSC 1.4	Mon	16:45–17:15	HSZ/AUDI	**Decarbonization Options for Industry** — •Uwe Riedel
SYSC 1.5	Mon	17:15–17:45	HSZ/AUDI	**Impacts of Cosmic Dust and Space Debris in the Terrestrial Atmosphere** — •John Plane

Invited Talks of the joint Symposium AI and Data Challenges behind Emerging Self-Driving Laboratories (SYAI)

See SYAI for the full program of the symposium.

SYAI 1.1	Thu	9:30–10:00	HSZ/AUDI	**Data and Experimental Foundations for Reliable Self-Driving Laboratories** — •Dr. Marcus Tze-Kiat Ng
SYAI 1.2	Thu	10:00–10:30	HSZ/AUDI	**Digital Catalysis - AI for Experiment Planning and Control** — •Christoph Scheurer
SYAI 1.3	Thu	10:30–11:00	HSZ/AUDI	**Autonomous, Data-Driven Workflows for Materials Acceleration Platforms with pyiron** — •Jan Janssen, Joerg Neugebauer
SYAI 1.4	Thu	11:15–11:45	HSZ/AUDI	**Machine Learning for Autonomous Optimization and Discovery of Materials** — •Pascal Friederich
SYAI 1.5	Thu	11:45–12:15	HSZ/AUDI	**Transforming Our View on Transformers in the Sciences** — •Kevin Maik Jablonka

Invited Talks of the joint Symposium Tipping Points in Social and Climate Systems (SYTP)

See SYTP for the full program of the symposium.

SYTP 1.1	Thu	15:00–15:30	HSZ/AUDI	**Social Tipping in Heterogeneous and Polarized Populations** — •Sara Constantino, Sonke Ehret, Elke Weber, Sonja Vogt, Charles Efferson
SYTP 1.2	Thu	15:30–16:00	HSZ/AUDI	**Tipping points and regime shifts in coupled social-climate systems** — •Chris Bauch
SYTP 1.3	Thu	16:00–16:30	HSZ/AUDI	**How to tune Earth system models toward tipping?** — •Sebastian Bathiany, Niklas Boers
SYTP 1.4	Thu	16:45–17:15	HSZ/AUDI	**Algorithmic amplification and contextual sensitivity in political information exposure** — Iris Damião, Ana Vranic, Paulo Almeida, Lília Perfeito, •Joana Gonçalves de Sá
SYTP 1.5	Thu	17:15–17:45	HSZ/AUDI	**The complex interplay between democracy and platform power** — •Philipp Lorenz-Spreen

Sessions

AKjDPG 1.1–1.4	Thu	9:30–11:30	SCH/A101	**Hacky Hour**

Sessions

– Talks –

AKjDPG 1: Hacky Hour

Time: Thursday 9:30–11:30 Location: SCH/A101

AKjDPG 1.1 Thu 9:30 SCH/A101

Using NOMAD as an Electronic Laboratory Notebook — •Ahmed E. Mansour[1], Siamak Nakhaie[1], Claudia Draxl[1], Martin Aeschlimann[2], and The FAIRmat team[1] — [1]Physics Department and CSMB, Humboldt-Universität zu Berlin, Germany — [2]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, Kaiserslautern, Germany

NOMAD (nomad-lab.eu) [1, 2] is an open-source, web-based research data management (RDM) platform that allows researchers in condensed-matter physics and materials science to organize, analyze, share, and publish their data. It also enables them to explore and reuse data provided by others.

The electronic laboratory notebook (ELN) functionality in NOMAD supports the documentation of research workflows and the management of experiments by creating structured records of samples, processing steps, measurements, results, and analyses. These searchable records can be accessed from any device, and enhance data integration, collaboration, and long-term recordkeeping.

In this talk, I will demonstrate how to use NOMAD as an ELN through its built-in templates for different record types, which can be accessed directly via the graphical user interface (GUI). I will also demonstrate how users can create custom templates using YAML-based schema definitions or Python-based plugins.

[1] Scheidgen, M. et al., JOSS 8, 5388 (2023).
[2] Scheffler, M. et al., Nature 604, 635-642 (2022).

AKjDPG 1.2 Thu 10:00 SCH/A101

Exploring and Publishing FAIR Research Data in NOMAD — •Siamak Nakhaie[1], Ahmed E. Mansour[1], Claudia Draxl[1], Martin Aeschlimann[2], and FAIRmat Team[1] — [1]Physics Department and CSMB, Humboldt-Universität zu Berlin, Germany — [2]Department of Physics and Research Center OPTIMAS, RPTU University Kaiserslautern-Landau, Kaiserslautern, Germany

Are you looking for a platform where you can explore physics and materials-science data with rich and well-structured metadata? Would you like to organize your own research data in an environment specifically tailored to the needs of physicists and materials scientists and aligned with the FAIR principles? Are you preparing a manuscript and need a simple way to share your data with reviewers via a single link, while keeping the underlying data modifiable so you can still update it based on their feedback, and later publish the final version with a DOI to cite in your paper? If so, this Hacky Hour is for you. We will introduce NOMAD as a practical platform for publishing and exploring FAIR research data. First, we will explore 19 million+ existing NOMAD entries and answer example scientific questions using the advanced yet user-friendly metadata filters provided by NOMAD. Next, we will upload example raw data files, manage access control, and inspect how NOMAD automatically extracts and structures useful information from these files. Finally, we will create a dataset and simulate the publication process, including DOI assignment.

Join us in this relaxed Hacky Hour to get introduced to NOMAD as a practical platform for managing FAIR research data.

AKjDPG 1.3 Thu 10:30 SCH/A101

Controlling experiments and recording FAIR data with NOMAD CAMELS - FAIR Data Workflow — •Alexander Fuchs[1,2], Michael Krieger[1], and Heiko Weber[1] — [1]Lehrstuhl für Angewandte Physik, Department Physik, Friedrich-Alexander Universität Erlangen-Nürnberg, Germany — [2]Physics Department and CSMB, Humboldt-Universität zu Berlin, Berlin, Germany

NOMAD CAMELS (Configurable Application for Measurements, Experiments and Laboratory Systems) [1, 2] is an open-source measurement orchestrator for easy control of lab instruments and recording of FAIR and fully self-describing measurement data directly from the experiment. CAMELS enables the definition of measurement protocols via a graphical user interface without requiring programming knowledge or deeper understanding of instrument communication. CAMELS provides the flexibility of controlling a large variety of measurement instruments in frequently changing experimental setups. Integrating the rich metadata of a measurement with a powerful ELN (e.g. NOMAD Oasis [3]) enables sophisticated research data management. This Hacky Hour contribution starts with a brief overview of CAMELS followed by a hands-on session on setting up CAMELS and performing measurements. To follow, bring your own laptop if possible. [1] A. Fuchs, J.A. F. Lehmeyer, H. Junkes, H.B. Weber, M. Krieger. NOMAD CAMELS: Configurable Application for Measurements, Experiments and Laboratory Systems. Journal of Open Source Software, 9(95), 6371 (2024), https://doi.org/10.21105/joss.06371 [2] NOMAD CAMELS documentation, https://fau-lap.github.io/NOMAD-CAMELS [3] Scheidgen et al., NOMAD: A distributed web-based platform for managing materials science research data. Journal of Open Source Software, 8(90), 5388 (2023), https://doi.org/10.21105/joss.05388

AKjDPG 1.4 Thu 11:00 SCH/A101

An exciting approach to electronic structure calculations — Hannah Kleine, •Kshitij Sinha, Martin Kuban, Marti Raya-Moreno, and Claudia Draxl — Humboldt-Universität zu Berlin, Berlin, Germany

With more than 30,000 scientific papers published annually on electronic-structure theory, navigating the landscape of theoretical approximations, ranging from ground-state density functional theory to advanced excited-state methods can be overwhelming, especially for early-career researchers [1]. This hacky hour aims to lower the barrier to advanced excited-state simulations and foster informed, critical use of modern electronic-structure tools on the example of the `exciting` code, an all-electron full-potential, open-source DFT package which is known to achieve μ-Ha precision [2,3]. Participants will be guided through practical workflows implemented in interactive notebooks that span multiple levels of theory, starting from ground- state calculations and extending to excited-state approaches such as time-dependent DFT and the Bethe-Salpeter equation. This session is designed as an interactive hacking workspace: with representative systems, direct comparison of methods within a unified code base and user-friendly workflows. Please, find more information about `exciting` and our session at https://exciting-code.org/dpg-hacky-hour-2026

[1] A. Pribram-Jones, D. A. Gross, and K. Burke, Annu. Rev. Phys. Chem. 66, 283 (2015).
[2] A. Gulans et al, J. Phys.: Condens. Matter 26, 363202 (2014).
[3] A. Gulans et al, Phys.: Rev. B, 97, 161105 (2018).

Working Group on Physics, Modern IT and Artificial Intelligence Arbeitskreis Physik, moderne Informationstechnologie und Künstliche Intelligenz (AKPIK)

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Overview of Invited Talks and Sessions

(Lecture hall BEY/0127; Poster P5)

Invited Talks

AKPIK 3.4	Tue	11:45–12:15	BEY/0127	**Model-free training of optical neural networks based on multimode semiconductor lasers** — •Anas Skalli, Satoshi Sunada, Mirko Goldmann, Marcin Gebski, Nasibeh Haghighi, Stephan Reitzenstein, James A. Lott, Tomasz Czyszanowski, Daniel Brunner
AKPIK 3.5	Tue	12:15–12:45	BEY/0127	**Virtual Reality Gamification for Photonics, AI and More** — •Arash Rahimi-Iman
AKPIK 4.1	Tue	14:00–14:30	BEY/0127	**Beyond the Hype: Can AI Truly Transform Photonics?** — •Mehdi K. Hedayati
AKPIK 4.2	Tue	14:30–15:00	BEY/0127	**Machine–learning assisted design of metasurfaces** — Lukas Mueller, Alexander Wolff, Janis Krieger, Steffen Klingel, Ralf Stemler, •Marco Rahm

Invited Talks of the joint Symposium The Sustainability Challenge: A Decade of Transformation (SYSC)

See SYSC for the full program of the symposium.

SYSC 1.1	Mon	15:00–15:30	HSZ/AUDI	**Open-Endedness and Community-Based Approaches to Sustainability Challenges** — •Hiroki Sayama
SYSC 1.2	Mon	15:30–16:00	HSZ/AUDI	**Education as a Social Tipping Element: Evidence from Climate and Physics Education Research** — •Thomas Schubatzky
SYSC 1.3	Mon	16:00–16:30	HSZ/AUDI	**Mechanistic and Material Perspectives on Enzymatic Hydrolysis of Semicrystalline Polyesters** — •Birte Höcker
SYSC 1.4	Mon	16:45–17:15	HSZ/AUDI	**Decarbonization Options for Industry** — •Uwe Riedel
SYSC 1.5	Mon	17:15–17:45	HSZ/AUDI	**Impacts of Cosmic Dust and Space Debris in the Terrestrial Atmosphere** — •John Plane

Invited Talks of the joint Symposium AI and Data Challenges behind Emerging Self-Driving Laboratories (SYAI)

See SYAI for the full program of the symposium.

SYAI 1.1	Thu	9:30–10:00	HSZ/AUDI	**Data and Experimental Foundations for Reliable Self-Driving Laboratories** — •Dr. Marcus Tze-Kiat Ng
SYAI 1.2	Thu	10:00–10:30	HSZ/AUDI	**Digital Catalysis - AI for Experiment Planning and Control** — •Christoph Scheurer
SYAI 1.3	Thu	10:30–11:00	HSZ/AUDI	**Autonomous, Data-Driven Workflows for Materials Acceleration Platforms with pyiron** — •Jan Janssen, Joerg Neugebauer
SYAI 1.4	Thu	11:15–11:45	HSZ/AUDI	**Machine Learning for Autonomous Optimization and Discovery of Materials** — •Pascal Friederich
SYAI 1.5	Thu	11:45–12:15	HSZ/AUDI	**Transforming Our View on Transformers in the Sciences** — •Kevin Maik Jablonka

Sessions

AKPIK 1.1–1.4	Sun	16:00–18:15	HSZ/0003	**Tutorial: Machine Learning Use Cases in Materials Science (joint session AKPIK/TUT)**
AKPIK 2.1–2.5	Tue	9:30–10:45	BEY/0127	**Machine Learning Prediction and Optimization Tasks**
AKPIK 3.1–3.5	Tue	11:00–12:45	BEY/0127	**Research with AI: Hardware, Software, Tools**
AKPIK 4.1–4.4	Tue	14:00–15:30	BEY/0127	**Focus: Deep Learning in Electromagnetics Research**
AKPIK 5.1–5.15	Thu	15:00–16:30	P5	**Poster**
AKPIK 6.1–6.7	Thu	16:45–18:30	BEY/0127	**AI Methods for Physics and Materials Science**

Sessions

– Invited Talks, Tutorials, Contributed Talks, and Posters –

AKPIK 1: Tutorial: Machine Learning Use Cases in Materials Science (joint session AKPIK/TUT)

Artificial intelligence (AI) tools are increasingly shaping research in materials science and physics by enabling advanced data analysis, modeling, and predictive capabilities.

This tutorial presents three practical use cases that demonstrate how machine learning methods can support materials science research.

Time: Sunday 16:00–18:15 Location: HSZ/0003

Tutorial AKPIK 1.1 Sun 16:00 HSZ/0003

Welcome Remarks Arbeitskreis Physik, moderne Informationstechnologie und Künstliche Intelligenz — DPG AKPIK and •Arash Rahimi-Iman — Deutsche Physikalische Gesellschaft e.V.

Inspired by last year's meeting program in Regensburg, March 2025, our interdisciplinary Working Group on Physics, Modern IT and Artificial Intelligence, the AKPIK, again offers a research-focused "AKPIK Day" on Tuesday during the upcoming conference. Together with the practical use cases of machine learning presented in this tutorial session, as well as the presentations and poster session planned for Thursday, we hope to encourage many conference attendees to engange scientifically in the areas of the AKPIK.

Tutorial AKPIK 1.2 Sun 16:05 HSZ/0003

A practical machine learning case study in materials science: Stumbling blocks, lucky breaks, and helpful colleagues — •Max Grossmann, •Malte Grunert, and Erich Runge — Institute of Physics and Institute of Micro- and Nanotechnologies, Technische Universität Ilmenau, 98693 Ilmenau, German

Machine learning projects in materials science are often exciting at first, but quickly encounter practical challenges. In this tutorial, we present a hands-on case study from our group and walk through the entire process, from the initial idea to building a dataset to training a working model. Rather than focusing solely on technical details, we highlight the stumbling blocks, unexpected insights, helpful colleagues, and lucky coincidences that shaped the project. We discuss the most important aspects of starting a machine learning project in physics or materials science, such as choosing a meaningful target property, designing a reliable dataset, avoiding common pitfalls, and identifying situations where simple approaches are as effective as advanced ones. Our goal is to provide an honest, accessible, and experience-driven introduction and guidance to researchers considering venturing into machine learning for the first time – the kind of guidance we wish we had when we started.

5 min. break

Tutorial AKPIK 1.3 Sun 16:50 HSZ/0003

Machine Learning-based Analysis of Electron Microscopy Images: Preprocessing and Synthetic Data Generation — •Amir Omidvarnia — Forschungszentrum Jülich, Jülich, Germany

In this tutorial session, participants will learn how to prepare electron microscopy (EM) images for machine learning (ML) analysis using a series of Jupyter Notebook demonstrations. The tutorial illustrates essential preprocessing steps such as denoising, normalization, and contrast enhancement using Python. The session then transitions to synthetic EM data generation, showing how classical augmentation and modern generative models can create controlled datasets that mimic real data. By observing these live examples, attendees will gain a conceptual understanding of how preprocessing pipelines and synthetic data strategies can be used for ML-based EM analysis.

5 min. break

Tutorial AKPIK 1.4 Sun 17:35 HSZ/0003

Machine Learning-based Analysis of Electron Microscopy Images: Segmentation — •Amir Omidvarnia — Forschungszentrum Jülich, Jülich, Germany

The second session focuses on segmentation of EM images using modern deep-learning architectures. Through a step-by-step Jupyter Notebook demonstration, the tutorial walks through the training and evaluation of a U-Net style segmentation model. Participants will see real examples of common challenges in EM segmentation, such as low contrast, overlapping nanoscale structures, and label ambiguity. By the end of the session, attendees will have an implementation-oriented understanding of how segmentation pipelines are built and validated in practice.

AKPIK 2: Machine Learning Prediction and Optimization Tasks

Time: Tuesday 9:30–10:45 Location: BEY/0127

AKPIK 2.1 Tue 9:30 BEY/0127

Bayesian Optimization for Mixed-Variable Problems in the Natural Sciences — •Yuhao Zhang[1], Ti John[2], Matthias Stosiek[1], and Patrick Rinke[1,3] — [1]School of Natural Sciences Physics Department, Technical University of Munich, Germany — [2]Department of Computer Science Aalto University, FInland — [3]Munich Center for Machine Learning, Germany

Optimizing expensive black-box objectives over mixed search spaces is a common challenge across the natural sciences. Bayesian optimization (BO) offers sample-efficient strategies through probabilistic surrogate models and acquisition functions. However, its effectiveness diminishes in mixed or high-cardinality discrete spaces, where gradients are unavailable and optimizing the acquisition function becomes computationally demanding. In this work, we generalize the probabilistic reparameterization (PR) approach of Daulton et al. to handle non-equidistant discrete variables, enabling gradient-based optimization in fully mixed-variable settings with Gaussian process surrogates. With real-world scientific optimization tasks in mind, we conduct systematic benchmarks on synthetic and experimental objectives to obtain an optimized kernel formulations and demonstrate the robustness of our generalized PR implementation. We additionally show that, when combined with a modified BO workflow, our approach can efficiently optimize highly discontinuous and discretized objective landscapes. This work establishes a practical BO framework for addressing fully mixed optimization problems encountered in the natural sciences.

AKPIK 2.2 Tue 9:45 BEY/0127

Overparametrization bends the landscape: BBP transitions at initialization in simple Neural Networks — •Brandon Livio Annesi, Chiara Cammarota, and Dario Bocchi — Sapienza Univeristy, Rome Italy

High-dimensional non-convex loss landscapes play a central role in the theory of Machine Learning. Gaining insight into how these landscapes interact with gradient-based optimization methods, even in relatively simple models, can shed light on this enigmatic feature of neural networks. In this talk, I will focus on a prototypical simple learning problem, which generalizes the Phase Retrieval inference problem by allowing the exploration of overparametrized settings. Using techniques from field theory, we analyze the spectrum of the Hessian at initialization and identify a Baik*Ben Arous*Péché (BBP) transition in the amount of data that separates regimes where the initialization is informative or uninformative about a planted signal. Crucially, we demonstrate how overparameterization can bend the loss landscape, shifting the transition point, even reaching the information-theoretic weak-recovery threshold in the large overparameterization limit, while also altering its qualitative nature. We distinguish between continuous and discontinuous BBP transitions and support our analytical predictions with simulations. In the case of discontinuous BBP transitions strong finite-N corrections allow the retrieval of information at a signal-to-noise ratio (SNR) smaller than the predicted BBP transition. In these cases we provide estimates for a new lower SNR threshold that marks the point at which initialization becomes entirely uninformative.

AKPIK 2.3 Tue 10:00 BEY/0127

Training convolutional neural networks with the forward - forward algorithm — •Matthias Schröter[1,2], Frauke Alves[3], and Riccardo Scodellaro[3] — [1]Institute for Diagnostic and Interventional Radiology, University Medical Center Göttingen, Robert Koch-Straße 40, 37075 Göttingen, Germany — [2]Max Planck Institute for Dynamics and Self-Organization, 37075 Göttingen, Germany — [3]Translational Molecular Imaging, Max Planck Institute for Multidisciplinary Sciences, 37075 Göttingen, Germany.

Recent successes in image analysis with deep neural networks are achieved almost exclusively with Convolutional Neural Networks (CNNs) trained using the backpropagation (BP) algorithm. In a 2022 preprint, Geoffrey Hinton proposed the Forward - Forward (FF) algorithm as a biologically inspired alternative, where positive and negative examples are jointly presented to the network and training is guided by a locally defined goodness function. Here, we extend the FF paradigm to CNNs. This talk compares FF and BP training across different datasets (MNIST, CIFAR 10, CIFAR 100) discusses different optimization strategies, and provides insights into the inner workings of FF trained networks using Class Activation Maps.

AKPIK 2.4 Tue 10:15 BEY/0127

Modeling resonant soliton interactions in the Kadomtsev-Petviashvili equation using PINNs — •Gerald Kämmerer — Universität Duisburg

Resonant two-soliton interactions in the Kadomtsev-Petviashvili (KP) equation are modeled using Physics-Informed Neural Networks (PINNs). This framework directly solves the KP equation by incorporating the governing partial differential equation residuals into the loss function, specifically focusing on Y-shaped resonances and web-like patterns that occur under specific resonance conditions. Comparisons with known algebraic solutions show a good agreement in capturing characteristic interaction patterns. To accelerate the learning of complex dynamics, progressive training strategies and symmetry-informed network architectures are implemented, embedding the equation's inherent coordinate symmetries. The results demonstrate that PINNs can capture the rich dynamics of resonant soliton interactions, offering a framework for exploring parameter regimes beyond traditional numerical methods.

AKPIK 2.5 Tue 10:30 BEY/0127

Phase Transitions reveal Accuracy Hierarchies in Deep Learning — •Ibrahim Talha Ersoy[1], Andrés Fernando Cardozo Licha[2], and Karoline Wiesner[1] — [1]Universität Potsdam, Institut für Astronomie und Physik, Potsdam, Deutschland — [2]Universidade Federal Fluminense, Instituto de Física, Niterói, Brazil

Training Deep Neural Networks relies on the model converging on a high-dimensional, non-convex loss landscape toward a good minimum. However, much of the phenomenology of training remains ill understood. We focus on three seemingly disparate phenomena: the observation of phase transitions akin to statistical physics, the ubiquity of saddle points, and mode connectivity which is key for the active research area of model merging. We bring these into a single explanatory framework, that of the geometry of the loss and error landscapes. We show analytically that phase transitions in DNN learning are governed by saddle points in the loss landscape. Furthermore, we present a simple, easy to implement and fast algorithm, using the L2 regularizer as a tool, to explore the geometry of error landscapes. We demonstrate its use for efficiently finding paths connecting global minima by confirming the mode connectivity for DNNs trained on the MNIST data set to then use it to show numerically that saddle points in DNN loss landscapes mark transitions between distinct models that encode distinct digits of the MNIST data. Our work establishes the geometric origin of key DNN training phenomena and reveals hierarchically ordered accuracy basins analogous to phases in statistical physics.

AKPIK 3: Research with AI: Hardware, Software, Tools

Time: Tuesday 11:00–12:45 Location: BEY/0127

AKPIK 3.1 Tue 11:00 BEY/0127

Agentic Exploration of Physics Models — •Maximilian Nägele[1,2] and Florian Marquardt[1,2] — [1]Max Planck Institute for the Science of Light — [2]FAU Erlangen

The process of scientific discovery relies on an interplay of observations, analysis, and hypothesis generation. Machine learning is increasingly being adopted to address individual aspects of this process. However, it remains an open challenge to fully automate the heuristic, iterative loop required to discover the laws of an unknown system by exploring it through experiments and analysis, without tailoring the approach to the specifics of a given task. Here, we introduce SciExplorer, an agent that leverages large language model tool-use capabilities to enable exploration of systems without any domain-specific blueprints, and apply it to physical systems that are initially unknown to the agent. We test SciExplorer on a broad set of models spanning mechanical dynamical systems, wave evolution, and quantum many-body physics. Despite using a minimal set of tools, primarily based on code execution, we observe impressive performance on tasks such as recovering equations of motion from observed dynamics and inferring Hamiltonians from expectation values. The demonstrated effectiveness of this setup opens the door towards similar scientific exploration in other domains, without the need for finetuning or task-specific instructions.

AKPIK 3.2 Tue 11:15 BEY/0127

Executable Manuscripts as Jupyter Notebooks: The Next Evolution in Scientific Publishing? — •Sebastian Rejman[1,2], Ina Vollmer[2], and Bert Marc Weckhuysen[2] — [1]Fritz-Haber-Institute of the Max-Planck-Society, Berlin, Germany — [2]Utrecht University, Utrecht, The Netherlands

The scientific paper as we know it today has remained largely unchanged for over a century. While color figures are now standard, and the supporting information contains more and more of the evidence, the manuscript itself remains a static pdf. The tools available to us, however, have drastically improved. Internet connections are faster, compute and storage are cheap, and high-level programming languages like Python make analysis automation accessible to the non-expert programmer.

Jupyter Notebooks, familiar to many students learning to program, allow to combine text with code and interactive figures. These notebooks, if used together with data repositories like OSF along with analysis code hosted on GitHub, allow for a transparent and reusable publication of research results. The reader can reproduce the analysis and figures at the push of the button, and easily re-purpose both analysis code and the underlying data - Paving the way for studies with large datasets in the field of chemistry and the natural sciences in general.

In this contribution, we demonstrate the executable version of our recent work on the role of external acidity in the cracking of plastics and provide practical guidance for implementation.

AKPIK 3.3 Tue 11:30 BEY/0127

PaperVerse: Disrupting the Peer-Review Process via AI-Driven Analysis and Reviewer Compensation — •Hendik Zobel, Oliver Mey, and René Stemmler — PaperVerse UG (haftungsbeschränkt), Dresden, Germany

The current scientific publishing model faces a systemic bottleneck: it relies on the uncompensated labor of volunteer researchers, resulting in significant delays and undervalued expertise. This talk introduces PaperVerse, a platform designed to disrupt this paradigm by treating peer review as valuable, billable work - supported by generative AI.

We propose a dual-layer architecture. First, our active AI Review Engine provides immediate, automated feedback on preprints (e.g., from arXiv) and private uploads, allowing authors to iteratively improve their manuscripts before submission. Second, and most critically, we outline our vision for a monetized marketplace that directly compensates human reviewers. By offloading structural and stylistic critique to AI, we free experts to focus on deep scientific validation, ensuring they are financially rewarded for their intellectual contribution.

We will discuss how AI-driven insights pave the way for this shift from volunteerism to a fair, incentivized economy. PaperVerse aims to establish a sustainable ecosystem where algorithmic efficiency meets human expertise, finally giving peer review the market value it deserves.

Invited Talk AKPIK 3.4 Tue 11:45 BEY/0127

Model-free training of optical neural networks based on multimode semiconductor lasers — •Anas Skalli[1], Satoshi Sunada[2], Mirko Goldmann[1], Marcin Gebski[3], Nasibeh Haghighi[4], Stephan Reitzenstein[4], James A. Lott[4], Tomasz Czyszanowski[3], and Daniel Brunner[1] — [1]FEMTO-ST Institute / Optics Department, CNRS & Université Marie et Louis Pasteur, 15B avenue des Montboucons, Besançon Cedex, France. — [2]Faculty of Mechanical Engineering, Institute of Science and Engineering, Kanazawa University, Kakuma-machi Kanazawa, Ishikawa, Japan. — [3]nstitute of Physics, Lodz University of technology, Wólczańska, Łódź, Poland — [4]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, Berlin, Germany

In this work, we demonstrate a fully autonomous and parallel optical neural network (ONN) based on a multimode VCSEL architecture using off-the-shelf components. The system is scalable in both network size and inference bandwidth, paving the way toward GHz-level computing. Our ONN supports in-situ learning, making it closer to true autonomous operation. To unlock the full potential of our hardware, we develop and benchmark several hardware-compatible optimization algorithms, including SPSA and PEPG, demonstrating their suitability for physical systems with limited computational resources, and showing how algorithmic choices impact convergence speed, scalability, and energy cost. Our ONN outperforms both a linear hardware baseline and a digital linear classifier on the MNIST task.

Invited Talk AKPIK 3.5 Tue 12:15 BEY/0127

Virtual Reality Gamification for Photonics, AI and More — •Arash Rahimi-Iman — I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

Amazing mixed or virtual reality (XR/VR) tools can boost excitement for various science topics across age groups. VR-enhanced lectures can visually address topics such as photonics or artificial intelligence, illustrate what space travel or a visit to periodic lattices of solids might be like, allow learners to play with beams and particles to solve quests, and do much more.

Game-like exploration environments can support self-paced learning and collaborative training, including multiplayer modes. This not only brings immersion, but also interaction and fun. Moreover, VR worlds can help circumvent typical limitations of traditional labs, such as access, safety, or resources. They promote an extraordinary variety of designs and implementations, such as toy experiments mimicking, for instance, laser optics, quantum and nanophysics, and more.

Here, I present in VR one example of a digital learning environment enabled by powerful computer game engines like UE5. Like a lab-on-a-chip combining several laboratory functions on a single integrated circuit, hence on a chip, my VR analog "lab-in-a-chip" (the virtual lab world) could bring together different virtual experiments and learning scenarios, with user-group–oriented gamification making them more tangible for learners and non-experts.

AKPIK 4: Focus: Deep Learning in Electromagnetics Research

Time: Tuesday 14:00–15:30 Location: BEY/0127

Invited Talk AKPIK 4.1 Tue 14:00 BEY/0127

Beyond the Hype: Can AI Truly Transform Photonics? — •Mehdi K. Hedayati — Durham University, Department of Engineering, Durham DH1 3LE, UK

AI has become a powerful enabler in photonics, offering new routes for accelerated design and materials discovery beyond conventional trial-and-error approaches. In our group, we have demonstrated several AI-driven photonic design frameworks, with selected results experimentally verified in the laboratory. These include AI-assisted metasurface design enabling direct mapping between geometry and structural colour*allowing multiple colours from a single geometry under strain*as well as machine-learning models that capture nonlinear relationships in amorphous metamaterials, leading to proof-of-concept devices such as metasurface perfect reflectors. Yet, alongside these successes, the field is increasingly shaped by exaggeration and misplaced expectations. In reality, AI rarely delivers deployable photonic technologies; instead, it proposes candidate materials, geometries, or structures that must still be fabricated and validated experimentally. Fabrication yield, scalability, and limited characterization throughput therefore remain the dominant bottlenecks, causing progress to saturate at the experimental stage. In this talk, we will review the current state of the art of AI in photonics, examine where the field is heading in the near future, identify the key limitations we are likely to face, and discuss realistic pathways forward to better align AI-driven design with experimental reality.

Invited Talk AKPIK 4.2 Tue 14:30 BEY/0127

Machine–learning assisted design of metasurfaces — Lukas Mueller, Alexander Wolff, Janis Krieger, Steffen Klingel, Ralf Stemler, and •Marco Rahm — RPTU Kaiserslautern-Landau, Erwin-Schroedinger-Strasse, 67663 Kaiserslautern, Germany

We present several applications of machine-learning-assisted metasurface design. The first study focuses on maximizing the received signal power for two users positioned at different angles relative to a reconfigurable intelligent surface (RIS) operating at 27 GHz and 31 GHz. The RIS must function as a frequency-selective yet independently tunable beam steerer, making the optimization of the varactor bias voltages a challenging task. The optimized voltage matrices successfully steered beams at both frequencies over angles from 10° to 45°. In parallel, the work explores metasurface designs with independent control of reflection amplitude and phase using physics-informed machine learning. To significantly reduce training data requirements, a Temporal Coupled Mode (TCM) model was introduced to capture the dynamic tuning behavior using only four simulations instead of hundreds. Machine-learning models predict TCM parameters directly from the metasurface geometry, enabling fast optimization. Furthermore, transfer learning was applied to composite unit-cell design, achieving comparable accuracy with far fewer simulations than direct training.

AKPIK 4.3 Tue 15:00 BEY/0127

Optical Human Action Recognition - Less can be more? — •Maximilian Zier, Stefan Sinzinger, Kathy Lüdge, and Lina Jaurigue — Technische Universität Ilmenau, Ilmenau, Germany

Automated recognition of human actions is becoming more relevant due to applications in areas such as surveillance and autonomous driving. Modern neural networks achieve nearly perfect classification accuracies across various action datasets. However, they rely on complex feature extraction methods that lead to long training times and significant computational demands. Focusing on sustainability and efficiency, Reservoir computing systems aim to deliver similar performance combined with reduced computational effort by only training the output layer. An optically implemented reservoir offers the prospect of processing at the speed of light and nearly unlimited scalability due to inherent parallelism. In this contribution, we present results of a human action recognition task using a hybrid opto-electronic set-up based on [1]. In contrast to previous works, we forgo common preprocessing and feature extraction methods and use raw video data as input to the reservoir. Our system lags behind large neural networks in terms of classification accuracy, but has very low hardware requirements. Additionally, we reduce the length of the video sequences to one second, thereby using less input data to perform classification than previous works.

[1] Antonik, P., Marsal, N., Brunner, D. et al., Nat Mach Intell 1, 530-537 (2019)

AKPIK 4.4 Tue 15:15 BEY/0127

Loss-Minimized Incoherent Photonic Computing with Interferometer Networks — •Mingwei Yang[1,2], Konrad Tschernig[1,2], Felix Kübler[1], Okan Akyüz[1], Lennart Mannteuffel[1], Enrico Stoll[1], and Janik Wolters[1,2] — [1]Technical University of Berlin, Berlin, Germany. — [2]German Aerospace Center (DLR), Berlin, Germany.

We present an algorithm for loss-minimized incoherent photonic multiplication of N-dimensional vectors with $N \times N$ matrices on standard Clements Mach-Zehnder interferometer (MZI) meshes [1]. By implementing arbitrary unitary transformations with incoherent light sources, the method avoids phase control and additional MZI blocks required by singular value decomposition in coherent schemes [2]. Optical energy per multiply and accumulate operation scales as $E = const$ in our approach, compared to $E \sim N$ in the crossbar architecture [3]. Experimentally, we implement a 4×4 photonic MVM and demonstrate an optical convolutional neural network for MNIST classification, achieving 28 correct predictions out of 31 images. Utilizing our loss-minimized architecture, we aim to reduce input intensity to the single photon regime to explore the limitations from shot noise.

[1] Clements, William R., et al. "Optimal design for universal multiport interferometers." Optica 3.12 (2016): 1460-1465.
[2] Shen, Yichen, et al. "Deep learning with coherent nanophotonic circuits." Nature photonics 11.7 (2017): 441-446.
[3] Feldmann, Johannes, et al. "Parallel convolutional processing using an integrated photonic tensor core." Nature 589.7840 (2021): 52-58.

AKPIK 5: Poster

Time: Thursday 15:00–16:30 Location: P5

AKPIK 5.1 Thu 15:00 P5

ARTIFICIAL INTELLIGENCE in the automotive industry — •Ilya Anufriev — Moscow, Russia

Modern automotive industry is a high-tech industry where production and management processes require constant improvement in efficiency and cost reduction. The use of robotic conveyors and artificial intelligence technologies allows for significant results in optimizing production processes, improving product quality, and reducing operational costs. The leading trends in the automotive industry include automation of production processes, data analysis and demand forecasting, product quality management, logistics and supply chain management, and decision support. I have developed a model for implementing artificial intelligence to optimize workflows within an automotive organization.

AKPIK 5.2 Thu 15:00 P5

Physics-based Reinforcement Learning for Balancing the Cart-Pole — •Igor Polonskiy, Atreya Majumdar, and Karin Everschor-Sitte — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany

Balancing a pole on a moving cart by applying lateral forces is a standard benchmark problem in reinforcement learning. Deep Q-Networks [1], which integrate reinforcement learning with neural networks, have been highly effective in solving this problem. Training the multiple hidden layers of Deep Q-Networks, however, is computationally expensive and thereby energy-demanding. Replacing these hidden layers with an Echo State Network reduces training costs while maintaining performance [2]. Echo State Networks have been shown to be re-

placeable by physical systems [3]. We explore the potential of solving the Cart-Pole problem with a physics-based Echo State Network.

[1] V. Mnih et al., Nature 518, 529 (2015)
[2] I. Polonskiy, Bachelor Thesis, University of Duisburg-Essen (11/2024)
[3] K. Everschor-Sitte et al., Nature Reviews Physics 6, 455 (2024)

AKPIK 5.3 Thu 15:00 P5

Stereovision-based angle and depth estimation for terahertz layer measurements — •Tim Arniko Meinhold[1,2], Dmytro Kharik[1], Joshua Hennig[1,2], Mirco Kutas[1,2], Jens Klier[1,2], Georg von Freymann[1,2], and Daniel Molter[1] — [1]Department for Materials Characterization and Testing, Fraunhofer Institute for Industrial Mathematics ITWM, 67663 Kaiserslautern, Germany — [2]Department of Physics and Research Center OPTIMAS, RPTU Kaiserslautern-Landau, 67663 Kaiserslautern, Germany

Terahertz systems can measure layer thicknesses with high precision in a fully contactless, non-destructive manner. However, reliable results require accurate alignment of the beam perpendicular to the surface, as even small angular deviations can affect the measurements. Many optical approaches still struggle to combine precision and real-time capability on demanding surfaces. Meanwhile, advances in stereo imaging and machine-learning methods provide a framework to support stable, interpretable measurement conditions.

Here, we report a compact stereovision-based setup within a framework that includes neural network-based approaches. Our goal is a practical and reliable method that delivers precise depth and angular information, which are expected to improve terahertz real-time thickness measurements.

AKPIK 5.4 Thu 15:00 P5

Exploring Reinforcement Learning for Particle Transport in the Presence of Inhomogeneities — •Finn Marten Boyer, Atreya Majumdar, and Karin Everschor-Sitte — University Duisburg-Essen, Duisburg, Germany

Classical transport theories typically assume homogeneous media, yet real materials often exhibit inhomogeneities that limit the applicability of such models. In particular, standard approaches like renormalization may fail when particles encounter defects whose characteristic energy scales are comparable to or larger than their kinetic energies. We investigate reinforcement learning as a data-driven framework for optimizing particle transport in strongly inhomogeneous environments. Our work indicates the potential of reinforcement-learning-based approaches for particle dynamics in more realistic and complex systems.

AKPIK 5.5 Thu 15:00 P5

Supporting Physical and Computational Biology with AI-Powered Multi-agent Model Generation — •Prerana Chandratre, Anjali Sharma, and Justin Bürger — TUD Dresden University of Technology, Dresden, Germany

Many open biological questions, from human embryogenesis to complex diseases like cancer, cannot be solved by experiments alone but require integration with biophysical and computational modeling. To address this, our group developed the software Morpheus (https://morpheus.gitlab.io/) which has become a widely used open-source platform (Starruß et al., 2014). Morpheus is based on a declarative modeling language, MorpheusML, and such models together with their biological context are collected in the MorpheusML model repository. Yet, creating MorpheusML models remains a barrier, especially for wet-lab researchers and students without programming expertise. To resolve this bottleneck, we are developing a model generation tool that uses a multi-agent workflow based on large-language models. Planned enhancements include a simulation-in-the-loop architecture enabling iterative, agent-driven model refinement and validation, expansion of the training dataset with model-text pairs from the MorpheusML model repository, and integration of automated validation and benchmarking metrics. The outcome will be the Morpheus.AI modeling assistant that enables robust generation of valid MorpheusML models from textual input sources, including PDF manuscripts. These AI-generated models will empower both research and education in physical and computational biology.

AKPIK 5.6 Thu 15:00 P5

Persistent Homology-Based Indicator of Orientational Ordering in Experimental Skyrmion Lattices — •Michiki Taniwaki[1,2], Thomas Winkler[1,3], Jan Rothörl[1], Raphael Gruber[1], Chiharu Mitsumata[4], Masato Kotsugi[2], and Mathias Kläui[1] — [1]Institute of Physics, Johannes Gutenberg University Mainz, 55099 Mainz, Germany — [2]Department of Materials Science and Technology, Tokyo University of Science, Niijuku 125-8585, Japan — [3]Institute of Molecules and Materials, Radboud University, Heyen- daalseweg 135, 6525AJ Nijmegen, The Netherlands — [4]Graduate School of Pure and Applied Sciences, University of Tsukuba, Tenodai 305-8571, Japan

Skyrmions are chiral spin textures whose topological protection makes them apt for low-power memory and logic devices. In two dimensions, skyrmion lattices can undergo topological phase transitions[1]. A central challenge is to quantify the configurational order of skyrmion lattices and to construct appropriate indicators that are sensitive to topological defects. Here we use persistent homology (PH), a method from topological data analysis, to characterize experimental two-dimensional skyrmion lattices. We define new scalar measures of translational and orientational order and compare them with the conventional measure of the ordering. Our approach captures the signatures of the softening of configurational order. These results demonstrate that PH provides a compact and robust indicator of the order and is well suited to the study of topological phase transitions. [1] R. Gruber et al., Nat. Nanotechnol. 20, 1405-1411 (2025).

AKPIK 5.7 Thu 15:00 P5

Hybrid Machine Learning Framework for Predicting Cycling-Induced Ageing in Lithium-Ion Batteries — •Sandhra Ganesh — University of Münster Institute of Physical Chemistry AK Heuer 48149 Münster, Germany

Predicting cyclical capacity fade is critical for assessing the long-term reliability and second-life potential of lithium-ion batteries. Traditional physics-based ageing models provide valuable interpretability but are often computationally expensive and depend on parameters that are difficult to obtain experimentally. Conversely, purely data-driven methods offer efficiency but typically struggle to generalise across operating conditions and lack physical grounding.This work proposes a hybrid modelling framework that integrates physics domain knowledge with deep learning to more accurately capture cycling-induced degradation. The framework incorporates physically meaningful feature extraction from voltage, capacity, and operational profiles, together with physics-guided constraints that ensure realistic degradation behaviour without requiring detailed mechanistic models. The approach aims to improve predictive accuracy, interpretability, and transferability across varying conditions and datasets. Its effectiveness will be evaluated through cross-condition generalisation studies and assessments of practical cycle-life prediction accuracy.

AKPIK 5.8 Thu 15:00 P5

Enabling high performance analog photonic computing using SFP transceivers — •Arvid Gansäuer[1], Mingwei Yang[1,2], Okan Akyüz[1,2], Lennart Mannteuffel[1], Felix Kübler[1], Konrad Tschernig[1], Enrico Stoll[1], and Janik Wolters[1,2] — [1]Technische Universität Berlin, Berlin, Germany — [2]Institute of Space Research, German Aerospace Center (DLR), Berlin, Germany

Photonic analog processors promise energy-efficient, parallel computing, specifically to tackle future machine learning and artificial intelligence (ML/AI) workloads. The fundamental mathematical operation of ML/AI computations, vector-matrix multiplication, is naturally suited to be performed in an optical setting [1]. However, many approaches utilize specialized, custom-made light sources and modulators to encode input vectors [1,2]. In this work we use commercial 1550 nm SFP transceivers to encode these vector inputs. We employ the incoherent excitation approach, which enables the use of light pulses generated by independent transceivers without any phase stabilization. To encode vector elements as incoherent light amplitudes, we generate sequences of 0- and 1-pulses within a time bin shorter than the integration time of the measuring photodiode. Using an FPGA, we achieve parallel transmission of photonic signals via 4 transceivers at 1.25 GHz/N, where N is the number of intensity levels to approximate the analog signal. Thus, our approach enables the use of robust, readily available SFP-transceiver modules for high-performance analog photonic computing. [1] Y. Shen et al. Nat. Photon. 11, no. 7, p. 441 (2017), [2] J. Feldmann et al., Nature 589, no. 7840, p. 52 (2021).

AKPIK 5.9 Thu 15:00 P5

Understanding phase transitions in information processing systems using Geometric Thermodynamics — •Jonas Maximilian Müller, Ibrahim Talha Ersoy, and Karoline Wiesner — University of Potsdam

Phase transitions are well understood phenomena which arise in many fields of physics. Near the transition point very different systems show identical behaviour in accordance to their universality class. The framework of Geometric Thermodynamics allows for a more abstract approach to the transitions. We have shown, that neural networks undergo phase transitions related to accuracy hierarchies. However, the full extent of the analogy is unclear and there is no direct mapping of the critical phenomena described for DNNs to a thermodynamical framework. Luckily, both systems can at least locally be described using information geometry. In this study we characterise the transition phenomenology of well known thermodynamical systems using Geometric Thermodynamics. Using the Fisher metric we then construct a precise mapping between information processing systems, specifically DNNs, and thermodynamic systems in the proximity of the transition point. This mapping will in turn help us explore the full extent of the phase transition analogy for DNNs and better understand how they process information by leveraging the knowledge and techniques of Thermodynamics and Statistical Physics.

AKPIK 5.10 Thu 15:00 P5

Advancing Machine Learning Optimization of Chiral Photonic Metasurface: Comparative Study of Neural Network and Genetic Algorithm Approaches — •Davide Filippozzi[1], Alexandre Mayer[2], Nicolas Roy[2], Wei Fang[3], and Arash Rahimi-Iman[1] — [1]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-University, Gießen, Germany — [2]Department of Physics,

Namur Institute for Complex Systems (naXys), University of Namur, Belgium — [3]College of Optical Science and Engineering, Zhejiang University, Hangzhou, China

We report on an advanced optimization framework for chiral photonic metasurfaces, comparing a refined Neural Network (NN) pipeline against a Genetic Algorithm (GA). By introducing a two-output NN architecture and exploiting geometric symmetries for data augmentation, we successfully reduce the trade-off between circular dichroism (CD) and reflectivity. Our comparative analysis on GaP and PMMA structures reveals complementary strengths: the GA excels in finding global optima for complex geometries, while the NN provides superior computational efficiency for large-scale screening. The optimized designs demonstrate a close to twofold increase in CD compared to Ref. [Mey & Rahimi-Iman, PSS-RRL 16, 2100571 (2022)]. We propose a hybrid workflow combining both methods to accelerate the design of effective chiral mirrors for polarization-selective light-matter interaction studies.

AKPIK 5.11 Thu 15:00 P5

Machine Learning for Tip Enhanced Raman Spectroscopy — •Harshit Sethi, Orlando Silveira, and Adam Foster — Aalto University, Espoo, Finland

Tip Enhanced Raman Spectroscopy (TERS) provides nanoscale chemical fingerprint alongside high-resolution topographic mapping of molecules, offering a powerful tool for materials discovery. However, TERS image datasets are challenging to interpret and typically demand time-consuming, computationally intensive quantum*chemistry calculations. To overcome this problem, we present an encoder-decoder model trained and evaluated on simulated TERS images of planar molecules, enabling direct prediction of molecular structures from spectral simulated data with high accuracy. Our approach demonstrates the feasibility of automating molecular structure identification from TERS images, bypassing traditional manual analysis. These findings provide a foundation for extending machine learning methods to experimental TERS datasets, potentially accelerating molecular discovery by integrating nanoscale spectroscopy with automated computational analysis.

AKPIK 5.12 Thu 15:00 P5

Non-unitary time evolution via the Chebyshev expansion method — •Aron Hollo[1,2], Daniel Varjas[3,4,5], Cosma Fulga[3,4], Laszlo Oroszlany[1,2], and Viktor Konye[3,4,6] — [1]Department of Physics of Complex Systems, Eötvös Loránd University, Budapest, Hungary — [2]Wigner Research Centre for Physics, Budapest, Hungary — [3]Institute for Theoretical Solid State Physics, IFW Dresden, Dresden, Germany — [4]Würzburg-Dresden Cluster of Excellence ct.qmat, Germany — [5]Department of Theoretical Physics, Budapest University of Technology and Economics, Budapest, Hungary — [6]Institute for Theoretical Physics Amsterdam, University of Amsterdam, Amsterdam, The Netherlands

The Chebyshev expansion method is a highly efficient technique for computing the time evolution of quantum states in Hermitian systems with bounded spectra. In the physics literature, its applicability is often assumed to be restricted to real spectra within the interval [-1,1], limiting its use for non-Hermitian dynamics.

Here, we show that this restriction is not fundamental. The Chebyshev expansion of the exponential function remains mathematically valid over the entire complex plane and can therefore be applied to arbitrary non-Hermitian matrices. The apparent breakdown of the method outside the conventional spectral bounds is traced back to numerical rounding errors rather than to a failure of the expansion. By deriving an analytic upper bound for the accumulated rounding error, we obtain a practical criterion for selecting safe time steps based on the spectral radius of the Hamiltonian.

AKPIK 5.13 Thu 15:00 P5

Nanomechanics-Driven Design of Flexible Textile-Based Metamaterials and Bio-Inspired Soft Composites — •Amine HAJ TAIEB — ISAMS, University of Sfax, Tunisia

Textiles, soft composites, and architectured metamaterials are emerging as key platforms for next-generation flexible systems in wearables, biomedical devices, adaptive structures, and energy-absorbing applications. Their unique mechanical performance*combining flexibility, stretchability, and durability*originates from complex interactions across multiple length scales, from fiber and yarn nanostructure to textile architecture and macroscopic response. Despite rapid progress, the lack of an integrated multiscale understanding still limits predictive design. This contribution explores how advanced nanomechanical characterization and multiscale modeling can accelerate the rational design of textile-based and bio-inspired flexible materials. Inspired by biological fibrous systems, we further discuss how hierarchical structuring and architectured textile geometries can be exploited to tune mechanical functionality. The integration of high-throughput testing and data-driven approaches, including machine learning, enables the identification of key design descriptors governing mechanical adaptability and robustness. By promoting interoperable experimental and simulation data, this work directly ontributes to a unified framework for the design of sustainable, high-performance textile-based flexible materials and metamaterial

AKPIK 5.14 Thu 15:00 P5

A Finite Element Homogenization Approach for Hollow Conductor Windings — •Shamim Aslam, Laura D'Angelo, and Herbert De Gersem — Institute for Accelerator Science and Electromagnetic Fields, TU Darmstadt, Germany

Future fast cycling synchrotrons require fast ramping dipole magnets. Due to high transients, eddy current and hysteresis effects become more pronounced in these magnets. Consequently, the associated thermal losses must be carefully considered in the overall magnet design. One key design solution to address this challenge is the use of hollow conductors. Hollow conductors facilitate the flow of electrical current while enabling efficient thermal cooling. Simulation-wise, hollow conductors are very challenging to compute as they impose a multi-scale problem, both geometrically and physically. The computational cost for multi-scale geometries can be potentially reduced by using homogenization technique. We present an advanced homogenization technique for the simulation of hollow conductor windings, tackling this multi-scale problem while maintaining a sufficient accuracy. In this homogenization technique, the fine model containing hollow conductor windings replaced with a bulk region with equivalent material properties. As a validation of the homogenization technique, the method applied on a dipole magnet with 16 hollow conductors windings. This application example demonstrate the high accuracy, reduced computation time and easy implementation of our homogenization technique as compared with the brute force finite element simulations.

AKPIK 5.15 Thu 15:00 P5

Digital-Analog Simulations of Schrödinger Cat states in the Dicke-Ising Model — •Dmitrii Shapiro[1], Yannik Weber[1], Tim Bode[1], Frank K. Wilhelm[1,2], and Dmitry Bagrets[1,3] — [1]Quantum Computing Analytics (PGI-12), Forschungszentrum Jülich, Germany — [2]Saarland University, Germany — [3]University of Cologne, Germany

We study the Dicke-Ising model: an Ising chain where all spins couple to a common bosonic mode. Due to competing spin-spin and spin-boson interactions, the phase diagram exhibits both second- and first-order superradiant quantum phase transitions (QPTs). At the QPT, the system evolves into an entangled superradiant state with a boson condensate. We discuss the free-energy landscape near the QPT, obtained by integrating out the spins. We then propose a digital-analog quantum simulator for the Dicke-Ising Hamiltonian based on interacting qubits coupled to a single-mode resonator. The many-body propagator is decomposed via Trotterization into layers of single- and two-qubit rotations alternating with Jaynes-Cummings (JC) gates that emulate spin-boson coupling. The JC gate is analog, as it exploits rotations in the resonator's native Hilbert space. We show that the superradiant state can be approximated by a quench protocol with a finite-depth circuit. Applying a selective measurement of global qubit parity yields a Schrödinger cat state in the photonic subspace—a hallmark of the superradiant ground state in finite-size systems. The cat state can be probed via Wigner tomography of the resonator field. For details, see [Shapiro et al., PRA 112, 042412 (2025)].

AKPIK 6: AI Methods for Physics and Materials Science

Time: Thursday 16:45–18:30 Location: BEY/0127

AKPIK 6.1 Thu 16:45 BEY/0127

Recycling resources from aborted quantum key distribution protocols — •Siyuan Qi[1] and Ramona Wolf[2] — [1]Universität Siegen, Siegen, Germany — [2]Universität Siegen, Siegen, Germany

In quantum key distribution protocols, abortion often occurs due to detected errors or leakages. A secure protocol must ensure that if abortion does not occur, the generated key is secure. However, when abortion happens, the resources used are lost and cannot be reused, leading to waste. A malicious party, Eve, can exploit this by intentionally interfering with the protocol, forcing an abortion every time it's run. While Eve cannot obtain the secret key or avoid detection, she can prevent key generation and cause significant resource waste, which is undesirable in practical scenarios. This issue can be addressed by implementing procedures that recycle resources from aborted protocols or by preventing Eve from interfering in such a way. A protocol is aborted when the minimum entropy of the key generated does not exceed the leakage. If an abortion is caused by large leakage, we can still generate certified private randomness from the minimum

entropy, provided it is not zero. Additionally, in specific scenarios where there is an identity designation process involved, we can move the identity designation to the last round so that Eve, not knowing she is a participant or not until the very end, will be discouraged from malicious behaviors.

AKPIK 6.2 Thu 17:00 BEY/0127

Causal–Physical Descriptor Discovery for Interpretable Materials Informatics — •Kanchan Sarkar and Axel Gross — Institute of Theoretical Chemistry, Ulm University, 89069 Ulm, Germany

Linking data-driven models to physically grounded behavior remains a key challenge in materials informatics. Data Nexus Vista (DNV1) is a causally informed framework that integrates domain knowledge with machine learning to identify interpretable descriptors. It provides standardized, configurable workflows spanning data preprocessing, feature construction, model training, and interpretation. DNV1 combines established feature-importance and descriptor-design tools with causal analyses, including counterfactual interventions, allowing for direct assessment of how model predictions respond to controlled changes. The framework supports both graphical and programmatic interfaces and provides descriptor-tracing utilities that map model features to physically meaningful variables. All workflows and outputs adhere to FAIR principles, ensuring reproducibility and transparency. The framework has been tested on multiple datasets and demonstrated with DFT-computed spinel cathodes. Rather than limiting ML models with fixed descriptors, DNV1 allows descriptors to emerge through causal interrogation of the data-physics nexus.

AKPIK 6.3 Thu 17:15 BEY/0127

Support for self-driving labs within the NOMAD ecosystem — •Sarthak Kapoor[1], Hampus Näsström[1], Ahmed Ilyas[1], Alvin N. Ladines[1], Alexander Fuchs[2], Joseph F. Rudzinski[1], Lauri Himanen[1], Sebastian Brückner[1], José A. Márquez[1], Martin Albrecht[3], and FAIRmat Team[1] — [1]Physics Department and CSMB, Humboldt-Universität zu Berlin, Germany — [2]Department Physik, FAU Erlangen-Nürnberg — [3]Department Materials Science, IKZ Berlin

Self-driving laboratories (SDLs) rely on robust digitization, structuring, and analysis of experimental data. We present NOMAD [nomad-lab.eu] [1] as a comprehensive research data management and workflow ecosystem that addresses the challenges inherent to emerging SDLs. The NOMAD ecosystem supports direct interfacing with lab instruments and addresses the transformation of instrument outputs into machine-actionable formats, a key requirement in SDLs, through a flexible schema system that allows researchers to represent raw data as standardized entries based on community-developed or laboratory-specific definitions. NOMAD Actions provide a robust framework for defining, executing, and monitoring sophisticated analysis and decision-making SDL workflows, such as ML pipelines and Bayesian optimization strategies. Moreover, NOMAD's workflow storage framework facilitates detailed provenance tracking, along with tools for navigating workflow graphs. Together, these capabilities position NOMAD as a foundational toolkit for realizing scalable, reliable, and FAIR SDLs.

[1] Scheidgen, M. et al., JOSS 8, 5388 (2023).

AKPIK 6.4 Thu 17:30 BEY/0127

Probabilistic greedy algorithm solver using magnetic tunneling junctions for traveling salesman problem — •Ran Zhang[1,2,3], Xiaohan Li[2], Caihua Wan[2,3,4], Raik Hoffmann[5], Meike Hindenberg[5], Yingqian Xu[2], Shiqiang Liu[2], Dehao Kong[2], Shilong Xiong[2], Shikun He[6], Alptekin Vardar[5], Qiang Dai[6], Junlu Gong[6], Yihui Sun[6], Zejie Zheng[6], Thomas Kämpfe[5,7], Guoqiang Yu[2,3,4], and Xiufeng Han[2,3,4] — [1]Present address: Max Planck Institute of Microstructure Physics, Halle (Saale), Germany — [2]Institute of Physics, Chinese Academy of Sciences, Beijing, China — [3]University of Chinese Academy of Sciences, Beijing, China — [4]Songshan Lake Materials Laboratory, Dongguan, China — [5]Fraunhofer IPMS, Dresden, Germany — [6]Zhejiang Hikstor Technology Co. Ltd, Hangzhou, China — [7]TU Braunschweig, Braunschweig, Germany

Combinatorial optimization is central to AI, logistics, and network design, yet classical methods often trade efficiency for solution quality. We introduce a probabilistic greedy solver that integrates spin-transfer-torque MTJ true random number generators with tunable switching statistics. A temperature parameter controls the balance between deterministic and stochastic choices. Applied to the traveling salesman problem, the framework achieves high-quality tours and surpasses simulated annealing and genetic algorithms in convergence speed, scalability, and computational cost.

AKPIK 6.5 Thu 17:45 BEY/0127

FAIR and Flexible Workflow Support within the NOMAD Infrastructure — •J.F. Rudzinski[1], T. Bereau[2], S. Botti[3], E.B. Boydas[1], N. Daelman[1], L. Himanen[1], S. Kapoor[1], A.N. Ladines[1], J.A. Márquez[1], B. Mohr[1], H. Näsström[1], and Fairmat Team[1] — [1]CSMB, HU Berlin — [2]ITP, Heidelberg Uni. — [3]RC-FEMS, Ruhr Uni. Bochum

NOMAD [nomad-lab.eu] [1, 2] is an open-source, community-driven research data infrastructure designed for modern physics. It provides FAIR-compliant storage, management, and analysis for diverse computational and experimental materials science data, and its modular, plugin-based architecture enables low-barrier extensions for adjacent and interdisciplinary domains. Here we present NOMAD*s workflow capabilities as a foundation for scalable and AI-ready data pipelines. A general workflow schema supports both standardized and custom workflows that record detailed provenance and link heterogeneous data streams. Standardized workflows enable powerful search, visualization, and automation features, while custom workflows support agile, project-specific digitalization. Workflow entries can be created via Python-based plugins, a YAML workflow specification, or the NOMAD ELN interface, ensuring accessibility for researchers with varying technical backgrounds. Combined with a toolkit for high-throughput interfacing, NOMAD provides a robust and sustainable digital infrastructure across physics subdisciplines.

[1] Scheidgen, M. *et al.*, JOSS **8**, 5388 (2023).
[2] Scheffler, M. *et al.*, Nature **604**, 635-642 (2022).

AKPIK 6.6 Thu 18:00 BEY/0127

Towards machine-learning-based on-the-fly analysis of neutron reflectometry — •Anne Rentzsch[1], Valentin Munteanu[1], Oliver Anyanor[2], Shreya Shah[1], Philipp Gutfreund[3], Rémi Perenon[3], Anthony Higgins[2], Vladimir Starostin[4], Alexander Hinderhofer[1], Dmitry Lapkin[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universistät Tübingen, 720726 Tügingen — [2]School of Engineering and Applied Science, Swansea University, Swansea SA1 8EN, Wales, United Kingdom — [3]Institut Laue-Langevin, 38000 Grenoble, France — [4]Cluster of Excellence 'Machine learning - new perspectives for science', Universität Tübingen, Maria-von-Linden-Straße 6, 72076 Tübingen, Germany

We present a real-time data analysis pipeline for neutron reflectometry that integrates `reflectorch`, a machine-learning-based software for reflectometry data analysis, into the IT infrastructure at the Institut Laue-Langevin. The workflow was tested during an experiment on the mixing behavior of bilayer thin films. Measured data are automatically reduced and analyzed, and the predicted sample parameters are returned to the instrument control system. The automated analysis can be triggered as frequently as every 10 seconds, enabling parameters and their uncertainties to be tracked with high temporal resolution and supporting continuous monitoring and data-driven adjustments. Compared to conventional software, `reflectorch` is up to two orders of magnitude faster. Together, these results pave the way for closed-loop experiments and demonstrate the potential of machine learning to enhance the efficiency of neutron reflectometry experiments.

AKPIK 6.7 Thu 18:15 BEY/0127

Multi-fidelity and -objective optimization of ONCV pseudopotentials — •Austin Zadoks[1], Cameron Hargreaves[2], Jusong Yu[1], Weiguo Jing[2], Matteo Giantomassi[2], Gian-Marco Rignanese[2], and Giovanni Pizzi[1] — [1]PSI Center for Scientific Computing, Theory and Data, 5232 Villigen PSI, Switzerland — [2]Institute of Condensed Matter and Nanosciences, UCLouvain, Louvain-la-Neuve, Belgium

The pseudopotential (PSP) approximation is essential to the tractability of many first-principles methods. However, it requires balancing the number of pseudized states, basis-set convergence, and accuracy w.r.t. all-electron (AE) results. One notable method for constructing soft, faithful, and widely-supported PSPs is the optimized norm-conserving Vanderbilt (ONCV) approach[1]. Various strategies have been proposed for generating meta-optimal tables of ONCVPSPs such as the SG-15[2], PseudoDojo[3], and SPMS[4]. Recent efforts to verify DFT codes have highlighted the importance of high-quality PSPs and expanded the necessary AE reference data, notably through $Z = 96$[5]. We present a fully-automated multi-fidelity multi-objective Bayesian optimization of ONCVPSPs targeting these reference data. This approach allows for the efficient mapping of the high-fidelity PW-DFT Pareto frontier by leveraging lower-fidelity intermediate radial- and PW-DFT results.

[1] D.R. Hamann. PRB, 88 (2013). [2] M. Schlipf & F. Gygi. Comp. Phys. Comms., 196 (2015). [3] M.J. van Setten, et al. Comp. Phys. Comms., 226 (2018). [4] M.F. Shojaei, et al. Comp. Phys. Comms., 283 (2023). [5] E. Bosoni, et al. Nat. Rev. Phys., 6 (2024).

Job Market (JOB)

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During the conference various companies and organisations will present their working fields and career opportunities to all interested participants.

Overview of Invited Talks and Sessions

(Lecture hall HSZ/0405)

Invited Talks

JOB 1.1	Tue	11:00–12:00	HSZ/0405	**d-fine GmbH: Entwicklung einer ERP-Software für Sanitätshäuser** — •Maximilian Sommer, •Philipp Banker-Busch
JOB 1.2	Tue	13:00–14:00	HSZ/0405	**Ritzenhoefer GmbH: Agentic Journey** — •Andreas Ringleb, •Alice von Bassewitz
JOB 2.1	Wed	11:00–12:00	HSZ/0405	**Data-Analytics in der HUK-COBURG – Wie Physiker den Weg in ein datengetriebenes Versicherungsunternehmen mitgestalten** — •Jannik Hofestädt, •Andreas Gleixner, •Goran Nakerst
JOB 2.2	Wed	13:00–14:00	HSZ/0405	**Basycon Unternehmensberatung GmbH: Aus der Wissenschaft in die Beratung** — •Tobias Weisrock, •Katharina Grässel
JOB 2.3	Wed	15:00–16:00	HSZ/0405	**Pädagogischen Hochschule Karlsruhe: Physik studiert – und jetzt? Dein Weg ins Lehramt.** — •Kay Burger, •Yvonne Ewen

Sessions

JOB 1.1–1.2	Tue	11:00–14:00	HSZ/0405	**Job Market I**
JOB 2.1–2.3	Wed	11:00–16:00	HSZ/0405	**Job Market II**

Sessions

– Invited Talks –

JOB 1: Job Market I

Time: Tuesday 11:00–14:00 Location: HSZ/0405

Invited Talk JOB 1.1 Tue 11:00 HSZ/0405

d-fine GmbH: Entwicklung einer ERP-Software für Sanitätshäuser — •Maximilian Sommer und •Philipp Banker-Busch — d-fine GmbH

Um die Herausforderungen des Digitalisierungstrends im Gesundheitssektor zu meistern, wurde ein Projekt zur Ablösung eines historisch gewachsenen Altsystems zugunsten einer cloudbasierten ERP-Software initiiert. d-fine übernahm die Gesamtprojektleitung, führte umfangreiche Business-Analysen und Requirements-Engineering durch und stellte sicher, dass das neue System optimal auf die Bedürfnisse des Kunden ausgerichtet ist. Zudem stellte d-fine auch einen Teil des Entwicklungsteams, um eine nahtlose Implementierung der Anforderungen zu gewährleisten.

60 min. break

Invited Talk JOB 1.2 Tue 13:00 HSZ/0405

Ritzenhoefer GmbH: Agentic Journey — •Andreas Ringleb und •Alice von Bassewitz — Ritzenhoefer GmbH, Düsseldorf

Raus aus der Umlaufbahn klassischer Transformation – auf Kurs Richtung Agentic Transformation, mit KI-Agenten und Multi-Agenten-Systemen.

JOB 2: Job Market II

Time: Wednesday 11:00–16:00 Location: HSZ/0405

Invited Talk JOB 2.1 Wed 11:00 HSZ/0405

Data-Analytics in der HUK-COBURG – Wie Physiker den Weg in ein datengetriebenes Versicherungsunternehmen mitgestalten — •Jannik Hofestädt, •Andreas Gleixner und •Goran Nakerst — HUK-COBURG

Ein Überblick über das Data-Analytics Programm bei der HUK-COBURG mit Fokus auf die typischen Aufgabenbereiche von Physikern.

Die Referenten berichten aus ihrem Arbeitsalltag in Forschung und Entwicklung in der Risikomodellierung und Telematik (auf Sensordaten basierende Bewertung von Unfallrisiken) sowie der Optimierung von internen Prozessen mit KI (speziell LLMs).

60 min. break

Invited Talk JOB 2.2 Wed 13:00 HSZ/0405

Basycon Unternehmensberatung GmbH: Aus der Wissenschaft in die Beratung — •Tobias Weisrock und •Katharina Grässel — Basycon Unternehmensberatung GmbH

Beratung bei Basycon heißt, die Vorteile von Forschung und klassischer Unternehmenskarriere zu verbinden. Insbesondere Naturwissenschaftler bringen aufgrund ihrer Ausbildung beste Voraussetzungen mit, um anspruchsvolle Fragestellungen zu lösen.

Die Veranstaltung richtet sich an Studierende der Naturwissenschaften, die nach Abschluss ihrer Hochschulausbildung eine Tätigkeit außerhalb der Universität anstreben und Beratung als Chance verstehen, vielfältige, herausfordernde Fragestellungen mit konkretem Praxisbezug zu bearbeiten und so intensive Einblicke in verschiedene Tätigkeiten / Rollen unterschiedlicher Unternehmen zu erhalten.

Konkret möchten wir Ihnen auf der Veranstaltung einen Einblick in folgende Themen geben:

- Welche Gemeinsamkeiten Forschungs- und Beratungsprojekte haben
- Wie sich Beratungstätigkeiten unterscheiden und welche Schwerpunkte Basycon setzt
- Welche Einstiegsmöglichkeiten und Perspektiven Basycon bietet

60 min. break

Invited Talk JOB 2.3 Wed 15:00 HSZ/0405

Pädagogischen Hochschule Karlsruhe: Physik studiert – und jetzt? Dein Weg ins Lehramt. — •Kay Burger und •Yvonne Ewen — Pädagogischen Hochschule Karlsruhe

Für alle, die einen Bachelorabschluss in Physik (o. ä.) erworben haben und neue Herausforderungen suchen: Informiere dich über den Dualen Masterstudiengang Lehramt Physik an der Pädagogischen Hochschule Karlsruhe und absolviere in nur drei Jahren den Master sowie das Referendariat und werde Lehrer:in für Physik und Mathe in der Sekundarstufe 1! Du bist dabei während des gesamten Studiums vergütet, hast eine sichere Standortperspektive und hervorragende Jobaussichten. Mehr Infos unter:

A. Berge, Siri ..... O 80.3
a. díaz, sebastián ..... MA 54.5
A. Helm, Christiane ..... CPP 13.7
A. Lemke, Edward ..... BP 4.5
A. Marques, Carolina ..... •O 80.3
A. Müller, Frank ..... DS 13.2
A. Rica, Raul .... CPP 10.12, DY 16.12
A. Ryndyk, Dmitry ..... O 6.5
A. Strassert, Cristian ..... FM 15.2
A.T.M. van Benthem, Rolf .. CPP 58.2
A. Traeger, Georg ..... MA 49.8
Aarts, Niek M. M. .... O 15.3, •O 89.4
Ababneh, Ewiese Mohammad MA 2.8
Abando Beldarrain, Nerea .... DS 16.1
Abart, Rainer ..... O 80.1
Abate, Antonio ..... HL 4.7
Abbasi, Fatemeh ..... •BP 27.4
Abbasi Taklimi, Neda ..... CPP 24.4, •CPP 29.5
Abbasi, Zahra ..... MM 34.1
Abdel, Dilara ..... HL 4.8
Abdelbarey, Doaa DS 20.21, HL 20.45, HL 55.10
Abdeldaim, Aly ..... MA 11.3, TT 21.3
Abdelghaffar, Yasmin ..... •BP 14.49
Abdelkawy, Ahmed . MM 39.7, O 13.3, O 65.7
Abdelrahman, Areeg ..... O 65.4
Abdel-Sattar, Adel ..... MA 7.24
Abdelwahab, Anas ..... •TT 94.7
Abdo, Mohamad ..... O 12.3
Abdoli, Iman ..... •DY 27.4
Abdolnezhad, Hossein .... CPP 17.51
Abdullayev, Azat ..... HL 40.5
Abe, Hiroko ..... O 42.5
Abedi, Ali ..... QI 16.7
Abedi, Mohammad . DY 14.13, •QI 6.7
Abedinnia, Atiye ..... •TT 51.6
Abele, Tobias ..... BP 7.37
Abeln, Andreas . TT 22.27, •TT 22.30, TT 82.2
Abert, Claas ..... MA 6.5, MA 7.41, MA 7.44, MA 9.9, MA 55.6, MA 58.2
Abetz, Volker ..... •BP 35.3, •CPP 51.3
Abilio, Ivan ..... O 47.1
Abkarian, Manouk .. BP 7.33, BP 41.1
Abouelela, Marwa ..... •TT 26.10
Abouhaidar, Rawan ..... UP 6.1
Abou-Hassan, Ali ..... CPP 46.23
Abouhasswa, Mennatallah . •MA 7.76
Abraham, Joyal J. ..... TT 79.5
Abram, Robin ..... MA 7.77
Abreu, E. ..... MA 25.6
Abril-Bermudez, Felipe ..... •DY 9.4
Abrosimov, N.V. ..... HL 38.10
Abrudan, Radu ..... MA 16.4
Abuawwad, Nihad ..... •MA 16.12
Abukaev, Ainur .. CPP 12.3, CPP 12.5
Acartürk, Tolga ..... O 19.1
Acevedo, Cristian . BP 26.1, CPP 43.1
Ach, Maximilian L. •MM 9.9, MM 13.7
Acharya, Manognya ..... TT 22.12
Achatz, Benjamin ..... •O 6.6
Achermann, Peter ..... SOE 12.3
Achilli, Beatrice ... DY 45.2, SOE 14.2
Achilli, Simona ..... TT 49.7
Acín, Antonio ..... QI 12.3
Ackermann, Kevin .. •TT 51.4, TT 71.6
Acosta Ramon, Jonathan Gustavo MA 7.6
Adabifiroozjaei, Esmaeil ..... DS 7.5, MA 50.4, MA 50.5
Adagideli, Inanc ..... TT 15.11
Adak, Subham ..... BP 14.45
Adakkattil, Ramesh ..... BP 27.11
Adam, Alaa ..... •FM 2.7
Adam, Assem ..... •TT 93.10
Adam, Torben ..... MA 36.10
Adam, Viktor ..... QI 14.24
Adame-Arana, Omar ..... BP 14.92, •BP 14.93
Adamyan, Grigor .... MA 19.1, TT 31.1
Adamyan, Zhirayr ..... •MA 36.2
Addayeva, Zeynab ..... •FM 11.1
Addison-Smith, Ian ..... BP 18.6
Adegboyega, S. ..... TT 5.9
Adel Aly, Mohammed ..... •HL 20.20
Adelmann, Christoph ..... MA 48.9
Adelung, Rainer . HL 20.23, HL 20.24, HL 26.23
Ademoglu, Ahmet Can ..... O 84.4, TT 84.4
Adhikari, Monoj . •CPP 35.3, •DY 37.3
Adibi, Elaheh ..... •TT 23.21
Adilbekova, Begimai ..... DS 14.9
Adlung, Louisa ..... DS 20.44
Ado, Ivan ..... O 89.7
Adrienko, Denis ..... •CPP 37.1
Adroja, D. T. ..... TT 62.5
Adroja, Devashibhai ..... TT 95.7
Adyemi, Shola ..... O 47.2
Aeberhard, Urs ..... CPP 40.6
Aebischer, Anton ..... BP 7.41
Aehle, Stefan ..... DD 7.1, •DD 20.4
Aeschbach, Werner ..... UP 7.3
Aeschlimann, Martin ..... MA 8.6, MA 38.7, MA 45.5, MA 47.3, MA 54.8, O 8.1, O 9.1, O 14.2, O 27.5, O 40.16, O 41.1, O 42.2, O 57.4, O 83.4, TT 37.16, TT 38.1, AKjDPG 1.1, AKjDPG 1.2
Afanasiev, Dmytro ..... •SYQF 1.5
Africh, Cristina ..... •O 33.1
Aftab, N. ..... BP 27.8, BP 37.2
Aftab, Namra ..... AKBP 3.4
Agarwal, Amit ... MM 19.35, TT 92.12
Agarwal, H. . O 19.10, O 59.2, TT 48.2
Agarwal, Harshit ..... TT 14.4
Agarwal, Mohit ..... •CPP 15.4
Agarwal, Tarushi .. TT 14.10, TT 64.3, •TT 93.16
Agarwalla, Vinit Kumar .... •MM 16.2
Agerbo Essendrop, Mikkel ... MM 8.4
Aggoune, Wahib ..... HL 40.10
Aghaei, Fatemeh ..... •SOE 4.9
Aghapour Ghourichay, Sahar •CPP 12.4
Aghashirinov, Farid ... •O 57.3, O 85.7
Aghvami, Banafsheh ..... •HL 20.56
Agirre, Andoni ..... •TT 26.6
Ağlarci, Furkan ..... HL 16.4
Agliari, Elena ..... DY 45.3, SOE 14.3
Agrait, Nicolas ..... O 87.8
Agrawal, Prarthana ..... •BP 21.3
Agterberg, Daniel ..... MA 33.3
Agudo-Canalejo, Jaime .... BP 10.10, CPP 18.10, DY 18.10
Aguilar, Javier ..... DY 33.10
Aguilar, Milton ..... O 99.8
Aguilar, Ritz ..... DS 20.34
Aguilar, Ritz Ann ..... •AKBP 8.8
Aguilar-Maldonado, Cintli .... TT 26.7
Aguilar-Trigueros, Carlos .... SOE 2.3
Aguirre García, Esteban ..... •TT 61.5
Aguliar, Milton ..... O 99.1
Agustí, Joan ..... QI 18.3
Aharonovich, Igor ..... HL 49.2
Aherns, Heiko ..... BP 5.4
Ahmad, Mashkoor ..... MM 4.9
Ahmadi, Majid .... FM 12.9, FM 12.10
Ahmadi, Mostafa ..... CPP 58.1
Ahmadiniaz, Naser ..... QI 17.2
Ahmed, Aamna ..... HL 31.1
Ahmed, Eslam ..... •TT 83.6
Ahmed, Shamail ... CPP 4.4, MM 4.6, O 70.1, O 95.12, TT 65.1, TT 96.12
Ahmed, Zehra ..... O 56.6
Ahmels, Pauline ..... •AKBP 3.3
Ahn, Kyo-Hoon ..... DS 7.5, MA 7.64, •MA 34.2
Ahsan, Umer ..... HL 35.6
Ahuja, Garima .... •MA 51.4, •TT 88.4
Aiello, Gaetano ..... •FM 7.2
Aimet, Stefan ..... •QI 3.3
Aizpurua, Javier ..... O 43.13
Ajay, Ajay ..... CPP 19.4, DY 20.4
Ajdari, Mohsen ..... •O 46.2
Ajeesh, Mukkattu O. ..... •TT 52.3
Akash, Ibnun Nur . BP 14.38, BP 14.38
Akashdeep, Akashdeep ..... MA 2.8, MA 47.3, •MA 51.2, •TT 88.2
Akbar, Muhammad Usama •MA 31.7, •TT 47.7
Akbari, Elahe ..... MM 19.20
Akbiyik, Alp ..... O 22.3, •O 86.2
Akhmadaliev, Shavkat ..... DS 20.12
Akhmerov, Anton ..... TT 74.8
Akhtar, Anas ..... O 94.9
AKPIK, DPG ..... TUT 3.1, AKPIK 1.1
Akram, Wasim ..... •FM 4.5
Akselrud, L. ..... TT 5.9
Aksoy, A. ..... BP 27.8, BP 37.2
Aktas, Oral Cenk ..... CPP 15.3
Akter, Moriom ..... DS 14.8
Akyüz, Okan ... AKPIK 4.4, AKPIK 5.8
Al Azar, Said ..... MM 16.5
Al Farsi, Basim ..... UP 8.1
Al Nachwati, Waafa ..... DS 11.7
Al Ruqaishi, Zainab ..... UP 8.1
Al Shahawy, Ahmed ..... MA 7.76
Al Shidhani, Hamood ..... •UP 8.1
Aladdin, Omar M. ..... TT 22.9
Alaeddini, Mobina ..... •MA 10.1
Alaei, Helya ..... MA 39.22
Alaei, Seyedeh Helya •O 70.4, O 70.5, •TT 65.4, TT 65.5
Alagia, Vincenzo ..... O 36.4
Alam, Shahidul ..... •CPP 57.5
Aland, Sebastian ... BP 1.5, BP 27.10, BP 37.3, •BP 37.8, CPP 1.5, DY 4.5
Alatas, Ahmet ..... TT 95.2
Alavi, Ali ..... DY 14.10
Alba Venero, Diego ..... MA 16.6
Albar, Esra Ilke ..... •O 49.1
Albe, Karsten ..... MM 7.3, MM 8.5
Albers, Tony .... DY 43.21, •DY 43.23
Albert, Carsten ..... •DD 40.1
Albert, Nico .... •DY 32.10, •TT 45.10
Albons, Llorenç ..... O 93.8
Albrecht, David ..... BP 33.4
Albrecht, Finn ..... •DY 44.12
Albrecht, Florian ..... O 3.2, O 9.12
Albrecht, Jan ..... DY 55.2
Albrecht, Manfred . DS 20.17, MA 7.7, MA 7.65, MA 7.70, MA 9.4, MA 12.1, MA 27.3, MA 37.8, MA 38.4, MA 39.17, MA 52.33, MA 55.6, TT 79.4
Albrecht, Martin ..... AKPIK 6.3
Albrecht, Theresa ..... •MA 38.12
Aldabag, Ahmed .. •DY 59.1, •TT 99.1
Aldag, Mandus ..... •BP 14.16
Aldamasy, Mahmoud Hussein HL 4.7
Aldarawsheh, Amal ..... •MA 55.10
Alderzy, Hanan ..... BP 14.29
Alebachew Seid, Biruk ..... HL 4.7
Alemani, Micol ..... TUT 2.1, DD 1.1, •DD 12.3
Alemansur, Hamed ..... O 44.11
Alert, Ricard ..... BP 3.11, BP 27.2
Al-Eryani, Aiman ..... TT 13.10
Aletsee, Clara ..... O 81.6
Aletsee, Clara C. ..... •O 88.4
Alexakis, Alexandros ..... DY 8.10
Alexander, Tristram ..... •SOE 11.2
Alexe, Marin ..... FM 12.3, FM 12.11, •MM 4.1
Alexiou, Terpsichori ..... BP 14.76
Alff, Lambert DS 7.5, DS 11.6, DS 13.3, TT 42.6, AKBP 9.3, AKBP 9.4
Alfonsov, Alexey ..... TT 79.5
Alhada-Lahbabi, Kevin ..... FM 4.1
Alhaj Ahmed, Hala ..... BP 14.58
Al-Hamad, Islam ..... •DS 20.12
Ali, Asif ..... MA 11.5, TT 21.5
Ali, Maryam ..... BP 14.29, BP 14.45, •BP 14.58, BP 33.7
Ali, Mazhar ..... O 76.4, TT 27.4
Ali, Muhammad ..... HL 20.12
Ali, Munawar ..... •O 7.7, •TT 9.7
Ali, Usman ..... •DY 59.8, •TT 99.8
Ali, Zayan A. ..... MA 36.13
Ali, Zayan Ahsan ..... •MA 42.1
alia, Ahmed ..... MA 55.10
Aliani, Linus ..... •TT 89.3
Aliberti, Raffaele ..... •O 21.1
Aliev, Farkhad G. ..... TT 73.9
Alim, Karen . BP 7.22, BP 7.23, BP 8.4, BP 14.19, BP 14.23
Alipour, Afshin ..... O 44.11
Alireza, Akbari ..... TT 93.9
Alkhezaim, Khawla ..... CPP 57.5
Al-Kuhaili, Mohammad ..... DS 20.12
Allan, Milan ..... TT 57.9, TT 73.1
Allan, Milan P. ..... TT 28.4, QI 20.8
Allegro, Isabel ..... HL 45.8
Allen, Jackson L. ..... TT 57.2
Allen, K ..... MA 19.7, TT 31.7
Allen, Kevin ..... MA 16.1
Alles, Martina ..... DD 26.4
Allington, Clifford ..... •MA 25.6
Almeida, Paulo ..... SYTP 1.4
AlMutairi, AbdulAziz ..... O 98.10
Aloi, Domitilla ..... O 80.1
Alokaidi, Samer ..... •BP 11.9
Alonso, Luis ..... BP 27.7
Alonso, Sergio ..... DY 22.5
Alonso-González, Pablo ..... O 96.4
Alonso-Mori, R. ..... MA 25.6
Alonso-Orts, Manuel ..... HL 9.1
Alqurashi, Maryam ..... CPP 57.5
Al-Reyahi, Anas ..... MM 16.5
Alshehri, Nisreen ..... CPP 57.5
Alsheika, Osama ..... CPP 17.14
Alsina, Adolfo .. BP 10.12, CPP 18.12, DY 18.12
Alston, Henry ..... •BP 32.5, DY 9.2, •DY 52.5
Altdorff, Daniel ..... UP 7.5
Altena, Marieke .... •TT 41.1, TT 57.9
Altendorf, Simone ..... HL 42.4
Altendorf, Simone G. ..... O 84.5, •TT 25.2, TT 84.5
Althammer, Matthias ..... MA 7.48, MA 30.5, MA 45.1, MA 51.8, MA 59.5, TT 22.33, TT 88.8
Althuon, Tim ..... TT 92.6, TT 92.7
Althüser, Joshua ..... •TT 56.5
Altin, Bilal ..... CPP 39.3
Altland, Alexander .. DY 13.9, TT 19.9
Altmann, Florian ..... •O 87.5
Altmann, Yannic ..... •TT 92.9
Alvarez Herrera, Pablo A. . CPP 46.12
Alvarez, Laura ..... •DY 55.1
Alvarez-Perez, G. ..... O 57.6
Alves Bastos, Vinicius ..... •HL 35.9
Alves, Frauke ..... AKPIK 2.3
Alves, Gabriel O. .... DY 32.5, TT 45.5
Amann, Andreas ..... O 44.11
Amann, Julia ..... HL 30.2, TT 59.2
Amann-Winkel, Katrin ..... CPP 19.3, CPP 27.4, CPP 46.1, CPP 46.2, CPP 58.1, DY 20.3, DY 26.4
Amano, Hiroshi ..... HL 57.1
Ambrogioni, Luca . DY 45.2, SOE 14.2
Ambrosio, Antonio ..... O 57.3
Ambure, Vidula ..... MM 35.4
Amelung, Robert ..... MM 25.4
Ameri, Tayebeh . CPP 15.3, CPP 17.48
Amersdorffer, Ines DS 21.8, HL 26.26
Amidani, L. ..... TT 5.9
Amin, Vivek ..... MA 2.8
Amini, Mohammad .. O 59.7, TT 48.7
Aminzadeh Gohari, S ..... BP 37.2
Aminzadeh, S. ..... BP 27.8
Amiraghyan, Lusik ..... TT 94.9
Amiri, Hesam ..... O 96.3
Amiridis, Vassilis ..... UP 3.3
Amirkhanyan, Z. .... BP 27.8, BP 37.2
Ammann, Markus CPP 19.5, DY 20.5, UP 6.1
Ammann, Max ..... •AKBP 1.3
Ammerman, Eve ..... •O 9.7
Ammon, Nico ..... •DD 36.2
Amrhein, Tim ..... MA 38.2
Amsharov, Konstantin Y. ..... O 69.5
An, Andy Disheng ..... •MA 7.32
An, Kang ..... CPP 17.19
An, Rong ..... O 87.4
An, Yanan ..... CPP 44.3
An, Yun ..... •FM 11.13
Anabaraonye, Chinwendu Nancy •CPP 17.34
Analytis, James ..... FM 10.5
Anampally, Aniketa ..... •HL 20.33
Anand, Amruthavarshini .. •MA 52.34
Anand, Amruthavsarshini . •MA 52.36
Anand, Gaurav ..... HL 12.5
Anand, Sriram ..... •MM 32.2
Anand, V. K. ..... TT 62.5
Anargirou, Eleni ..... DS 3.3, O 2.6
Anchamkudy, Sandhya ..... •O 31.3
Anchutkin, Gordei ..... DY 62.4
Andergassen, Sabine ..... TT 13.4, TT 13.10
Anders, Frithjof ..... O 84.4, TT 84.4
Anders, Janet ..... DY 43.3, DY 61.1, MA 7.39, MA 14.4
Andersen, Bent ..... FM 11.29
Andersen, Brian ..... TT 29.9
Andersen, Mie ..... •O 5.4
Andersen, Simon Guldager CPP 10.9, DY 16.9
Anderson, Eric ..... MA 43.6
Anderson, Harry L. ..... O 3.2, O 9.12
Andersson, Carl ..... MM 39.3
Ando, Yoichi O 63.9, TT 15.4, TT 15.5, TT 15.6, TT 55.9, TT 61.2, TT 74.2, TT 85.7, QI 11.8
Andolfatto, Maria ..... •MM 17.4
Andorfer, Fabian . MM 30.2, MM 30.3
Andrade, Ignacio ..... DY 19.1
Andrea Rozzi, Carlo ..... HL 1.8
Andreas, Heino ..... BP 12.9
Andres, Dieter ..... MA 6.2
Andricek, Laci ..... TT 22.32
Andrienko, Denis CPP 24.1, CPP 48.3, CPP 53.3, CPP 57.2, FM 10.4, HL 15.4
Andrieu, Stéphane ..... MA 48.1
Andriolo, Patrick ..... •QI 12.6
Andriushin, Nikita ..... •MA 17.2
Andriyakhina, Elizaveta .... •MA 35.2, •TT 60.2
Andriyanova, Iryna ..... QI 16.6

Androja, Devashibhai ..... MA 3.7
Andrzejewski, Tomasz ..... QI 13.8
Aneziris, Christos ..... FM 7.5
Anferov, Alexander ..... QI 3.4
Angane-Ambure, Vidula .. •MM 19.45
Angelika, Kühnle ..... O 5.2
Angelini, Maria Chiara ..... DY 33.12
Anger, Felix ..... TT 93.10
Anggara, Kelvin ..... O 9.8, O 35.7
Anghel, Roxana ..... HL 20.26
Angloher, Godehard ..... TT 22.32
Angnes, Lucio ..... FM 2.6
Angrick, Christoph . •O 84.6, •TT 84.6
Angster, David ..... •MA 48.6
Anić, Daniel ..... MA 38.8
Aniculaesei, Constantin .... BP 14.47
Anis, Geraldine ..... •MM 27.5
Anisimov, Andrey N. HL 18.7, TT 32.7
Anja, Wolter-Giraud ..... TT 94.4
Ankerhold, Joachim DY 40.3, TT 62.9, TT 73.2, TT 82.5, TT 82.6, TT 85.4, TT 89.4, QI 14.4, QI 20.2
Annesi, Brandon Livio .... •AKPIK 2.2
Annweiler, Caja ..... •MM 37.1
Anooz, Saud Bin ..... DS 9.5
Ansari, Jaafar ..... •MA 54.10
Ansari, Lida ..... HL 24.11
Ansari, Mohammad ... QI 2.2, QI 3.12, QI 8.1
Ansari, Mohammad H. ..... QI 14.15, QI 16.2
Anselmi, Fabio ..... QI 16.8
Anson, Christoper E. ..... MA 36.13
Anson, Christopher ..... MA 7.75
Anstett, Martin ..... O 8.1, •O 83.4
Antalicz, Balázs ..... •DS 20.13
Antczak, Maciej ..... BP 14.54
Anthofer, David .. •MA 36.9, MA 39.3
Anthuparambil, Nimmi Das . BP 14.44
Antila, Hanne ..... DY 54.4
Antonija Grubisic-Cabo, Antonija HL 48.5
Antonov, Alexander CPP 11.5, DY 17.5, DY 27.3
Antonov, Alexander P. ..... DY 49.10
Antonowicz, Jerzy ..... MM 19.3, MM 19.22
Antrack, Tobias ..... CPP 17.24
Antunes, Gonçalo ..... •DY 62.8
Anufriev, Ilya ..... •AKPIK 5.1
Anyanor, Oliver ..... AKPIK 6.6
Aolita, Leandro ..... DY 28.2, QI 5.6
Apellaniz, Iagoba ..... •QI 14.11
Apfelbeck, Fabian CPP 4.6, CPP 17.27
Apfelbeck, Fabian A.C. ..... CPP 16.2
Appel, Heiko ..... O 49.1
Appelfeller, Stephan ..... O 81.1
Appleford, Thomas ..... •CPP 10.6, •DY 16.6
Apseros, Andreas ..... MA 6.10
Aqeel, Aisha ..... PSV VI, MA 16.4, MA 29.11, •MA 37.7, MA 51.6, TT 46.11, TT 79.4, TT 88.6
Aqeel, Musfira ..... TT 81.5
Aquaro, Miriam ... DY 45.3, SOE 14.3
Aquilanti, Giuliana ..... MA 7.76, MM 19.28
aquino, rui ..... MA 20.4
Aranzadi, Juan ..... O 98.5
Aranzadi, Juan I. ..... •O 14.9, O 38.8
Araspin, Estéban ..... •BP 14.96
Arat, Kerim ..... O 44.11
Arauz-Moreno, Carlos ..... •CPP 58.4
Aravinda, S. ..... DY 47.8
Araya Day, Isidora ..... TT 74.8
Arbel, Eden ..... •HL 34.5
Arbel-Goren, Rinat ... BP 1.9, CPP 1.9, DY 4.9
Arbor, Nicolas ..... HL 26.2
Archambault, Aubin ..... DY 19.1
Archer, Emily ..... AKBP 8.4
Ardenghi, A. ..... O 57.6
Ardyaneira, Aristo ..... •TT 92.10
Arefi, Hadi ..... O 61.10
Aremanda, Sudeepthi ..... O 13.5
Arend, Germaine ..... QI 2.6
Aretz, Joost ..... •TT 27.4
Aretz, Joost aretz ..... O 76.4
Arhangelskis, M. .. CPP 32.3, DY 35.3
Ari, Metehan ..... •DS 20.14
Arian Zad, Hamid ..... MA 36.2
Ariani, Bianca .... •BP 36.8, •DY 57.8
arima, taka-hisa ..... O 95.9, TT 96.9
Arita, Ryotaro ..... TT 56.10, TT 91.1
Arndt, Mira Sophie ..... •O 69.6
Arneth, Jan ..... MA 7.74, MA 7.75, •MA 42.6
Arnold, Andre ... AKBP 2.1, AKBP 2.2, AKBP 2.5
Arnold, Jonas . O 15.4, O 17.7, O 17.11, O 89.3, •O 99.2, O 99.10, TT 13.12, •TT 13.13
Arnold, Lisa ..... O 8.7
Arnold, M. ..... AKBP 1.1
Arnold, Michaela ..... AKBP 4.4, AKBP 9.3, AKBP 9.4
Arnold, Otto ..... DS 16.7, •DS 20.8
Arora, Abeer ..... MA 27.2, •O 40.11, •TT 37.11
Arora, Ankur ..... •HL 20.30
Arora, Ashish ..... •HL 35.3
Arora, Raagya ..... DS 7.4
Arora, Shivang ..... QI 2.1
Arregi, Jon Ander ..... O 98.3
Arribas, Daniel •O 9.8, O 12.6, O 95.6, TT 96.6
Arribas, Irene Sánchez ..... HL 18.8, TT 32.8
Arrieta, Xabier ..... O 43.13
Arsatiants, Oleksandr ..... •O 78.2
Arshad, Atiqa ..... MA 7.46, O 41.3, TT 38.3
Arshad, Saba ..... •DS 18.6
Arslan, Büsra Gamze O 59.7, TT 48.7
Arslan, Cazibe ..... CPP 22.5
ARSU, Nergis ... CPP 17.30, MM 16.4
Artemov, Vasily ..... •CPP 6.3
Artiaco, Claudia ..... •QI 15.4
Artiglia, Luca ..... UP 6.1
Artyukhin, Sergey .. •MA 4.2, MA 4.5, MA 4.6, MA 16.2, MA 17.2, MA 17.9, MA 27.6, MA 30.3, MA 30.10, MA 37.7
Arushi, Arushi ..... TT 14.9
Aryasetiawan, Ferdi ..... TT 44.10
Arzumanov, Alexey ..... AKBP 9.3, AKBP 9.4
Asa Rajan, Sruthy ..... •CPP 48.5
Asboth, Janos ..... QI 21.9
Asboth, Janos Karoly ..... QI 14.18
Aschenbrenner, Michael .... MA 12.2
Asfia, Shima ..... BP 14.26
Ash, Soumen ..... •TT 5.7
Ashok, Sanjay ..... •MA 37.4
Ashtiani Abdi, Ali •CPP 19.4, •DY 20.4
Ashtiani, Ali ..... CPP 27.2, DY 26.2
Asirim, Özüm Emre ..... •CPP 46.24
Asl Soleimani, Yahya ..... •CPP 57.1
Aslam, Shamim ..... •AKPIK 5.14
Aslanidis, Theodoros ..... •DD 27.5
Aso, Hinata ..... O 61.11
Assaad, Fakher ..... TT 10.1, TT 26.4, TT 86.4, TT 90.3
Assaad, Fakher F. ..... TT 92.13
Assenbaum, Stefan ..... •AKBP 6.1, AKBP 6.2, AKBP 6.3, AKBP 6.5
Assi, Issam ..... •BP 5.4, CPP 46.29
Ast, Christian ..... O 44.16, O 44.17, TT 62.9
Ast, Christian R. ... TT 73.2, •TT 73.4
Astakhov, Georgy V. . HL 18.7, TT 32.7
Aswartham, Saicharan .... MM 40.4, TT 4.9, TT 5.7, TT 11.4, TT 23.9
Atabay, Azra ..... CPP 54.4
Atalay, Seyma Esra ..... •HL 54.8
Atencia, Rhonald Burgos .... HL 23.1
Ateş, Serkan ..... •HL 16.4
Athanasopoulou, Angeliki ... O 83.10
Athanassiadis, Athanasios .. BP 7.56, BP 30.2, CPP 47.2
Athanassiadis, Athanasios G. BP 7.55
Atodiresei, Nicolae ... O 10.1, TT 16.1
Atoufi Kashani, Maedeh . •CPP 46.41
Atris, Zeynep ..... BP 14.81
Attanasio, Carmine ..... TT 5.4
Atxitia, Unai ..... MA 38.4
Aubert, A. MA 23.5, MA 50.3, TT 35.5
Aubert, Alex ..... MA 50.4, MA 50.6, MA 50.7, MA 52.23, MA 52.27
Audinot, Jean-Nicolas ..... HL 11.6
Auer, Andrea ..... •O 13.10, O 39.1
Auer, Naomi ..... DY 33.8
Auerbach, Daniel ..... O 34.7
Auernhammer, Günter ..... BP 7.8, CPP 17.50, DD 42.3
Auernhammer, Günter K. .. •CPP 41.7, CPP 60.2
Auffray, E. ..... O 85.2
Auffray, Elisa ..... MM 40.5, •TT 29.3
Augusiak, Remigiusz ..... QI 12.3
Aulagnet, Corentin ..... MA 27.11
Aulbach, Julian ..... O 8.5
Auras, Sabine ..... •O 4.5
Aussillous, Pascale . DY 19.2, DY 19.5, DY 19.6
Autieri, Carmine .... MA 44.7, TT 76.7
Au-Yeung, Kwan Ho ... O 6.2, •O 15.4, O 17.7, O 17.9, O 89.12, O 99.2, O 99.10
Auzelle, Thomas .... FM 7.8, HL 57.5
Auzély, Rachel ..... CPP 31.6
Auzuma, Hikaru ..... FM 18.4
Avarvari, Narcis ..... O 46.1, O 69.10
Avdeev, Julia ..... HL 20.36
Avdeev, Maxim ..... MA 31.8, TT 47.8
Avdoshenko, Stanislav .... MA 36.12, MA 49.1
Avetisyan, Diana ..... •DS 20.25
Avila, Karina ..... DD 9.2
Avila, Mishai ..... O 81.7
Avitabile, Francesco ..... TT 5.4
Avtarovski, Juliana ..... •MA 7.3
Awsaf, Chowdhury S. ..... MA 38.4, MA 38.6
Awsiuk, Kamil ..... O 87.4
Axmann, Thomas ..... •CPP 20.10, •DY 23.10
Ayache, Mohamed ..... AKBP 8.7
Ayari, Sourour ..... •O 21.2, O 93.6
Ayeni, Olugbenga ..... •CPP 15.3
Azab, Abdelrahman ..... •TT 23.35
Azad, Fariha ..... •QI 3.7
Azam, Sikander ..... •HL 1.10
Azarov, Alexander ..... HL 40.5
Azevedo, Tamara ..... •MA 48.7
Azhar, Maria ..... •PRV VI, MA 7.71, MA 7.72, MA 37.3, TT 6.6
Azimi Mousolou, Vahid .... •MA 59.3
Azizmalayeri, Reza ..... •CPP 17.50
Azuma, Hikaru ..... FM 15.3
B. Braz, Lauro ..... •TT 69.10
B. Iyer, R. ..... O 57.6
B. Martins, George ..... TT 69.10
B. Sousa, Frederico ..... HL 47.2
B, Vaishnav ..... CPP 41.4
Baabe, Dirk ..... TT 81.5
Baba, Yuriko ..... TT 6.2, •TT 15.8
Babeva, Tsvetanka ..... DS 20.3
Babić, Luka ..... •O 23.8
Babij, Michał ..... MA 7.27
Babin, Hans Georg ..... HL 26.31
Babla, Harsh K. ..... QI 6.10
Bacani, Mirko ..... •MA 6.2
Bacellar, Camila ..... BP 9.6
Bach, Nora ..... O 79.7
Bach, Thi Phuong Anh ..... •HL 36.4
Bacher, Andreas ..... QI 11.4, QI 11.5
Bachmaier, Andrea ..... •MM 24.1
Bachmann, Lydia J. ..... •O 34.6
Bachtold, Adrian .... HL 10.1, TT 20.1
Bačić, Iva ..... •DY 8.2
Back, Christian ... DS 20.17, MA 16.4, MA 37.7, TT 74.12
Back, Christian H. ..... TT 97.1
Bäcker, Arnd ..... DY 32.4, DY 32.7, TT 45.4, TT 45.7
Bäcker, Charlotte .... QI 9.5, •QI 10.3, QI 10.5
Backes, Claudia ..... O 70.5, TT 65.5
Backes, Dirk ..... MA 37.2
Backes, Juri ..... •SOE 10.1
Backus, Ellen H.G. ..... CPP 19.2, CPP 46.3, DY 20.2, O 36.5, O 87.5
Bácsi, Ádám ..... •TT 22.6
Baczewski, Lech Thomas .. DS 20.48
Baczewski, Lech Tomasz .... DS 18.2
Badala Viswanatha, Chetana ... O 9.1
Badalov, Sabuhi . •HL 24.7, •MM 12.4
Badenhorst, Chris ..... MA 39.7
Bäder, Alexander .... O 86.5, •O 95.8, •TT 96.8
Bader, Vera P. ..... QI 11.6, QI 11.9
Badola, Shalini .... DS 12.8, MA 19.9, MM 21.7, TT 31.9
Badragheh, Mohammad A. . MM 14.5
Badura, Phil ..... HL 20.47
Badura, Phil Julien ..... •HL 20.41, HL 26.31
Bae, Jin Hee ..... QI 6.9
Bae, Yujeong ..... O 17.1
Baek, Insu ..... MA 29.4, TT 46.4
Baek, Jinhyun ..... MA 52.12
Baenitz, M. ..... TT 62.5
Baenitz, Michael .... TT 61.3, TT 94.3
Baenke, Franziska ..... BP 37.7
Baeumer, Christoph ..... DS 6.6
Bag, Poulami ..... •DY 44.1
Bagaglini, Michele ..... •HL 36.2
Bagger, Alexander ..... O 13.7
Bagnich, Sergey ..... CPP 48.5
Bagrets, Dmitry ..... QI 3.2, QI 3.9, AKPIK 5.15
Bähr, Mario ..... FM 7.1, HL 31.3
Bahrami, Amin ..... FM 11.14
Bahubalindruni, Pydi Ganga MA 49.9
Bai, Mei ..... CPP 23.1, DY 24.1
Bai, Shaoling ..... DS 13.1
Bai, X. ..... MA 3.8
Baier, Thomas .. CPP 12.4, CPP 44.2, CPP 46.48, CPP 48.2, CPP 53.6, •CPP 59.3
Baigol, Alexandre ..... SYBT 1.2
Bailey-Darland, Sully ..... BP 20.6
Bailles, Anais ..... •BP 12.9
Bajpai, Nandita ..... •HL 52.3
Bäker, E. ..... •HL 37.6
Bakhshinezhad, Pharnam ... TT 17.9, QI 4.9, •QI 7.2, QI 21.5
Bakin, Andrey ..... O 95.1, TT 96.1
Bakis, Eduards ..... CPP 21.1
Bakkers, Erik ..... HL 20.40
Bakkers, Erik P.A.M. ..... HL 17.1
Balajka, Jan ..... O 5.6, •O 55.4
Balakrishnan, Geetha ..... TT 33.3
Balan, Aravind ..... MA 43.4
Balashov, Timofey .... O 41.4, O 54.3, TT 38.4
Balayeva, Narmina . DS 20.19, O 74.9, TT 68.9
Baláž, Damián ..... •DY 14.5
Baldassarre, Leonetta ..... •SYQF 1.4
Baldauf, Julia ..... •DS 20.49
Baldini, Edoardo ..... O 49.5
Baldo, Anthony ..... O 36.1
Baldofski, Matthias ..... MM 32.5
Balducci, Federico •DY 53.3, •TT 87.3
Balduque, José ... •HL 29.3, •TT 58.3
Baldwin, Ash ..... •O 86.3
Balents, Leon ..... TT 86.3
Baljozović, Miloš ..... O 9.11
Balland, Theo ..... •MA 7.66
Ballauff, Matthias ..... •BP 35.2, •CPP 51.2
Ballone, Pietro ..... DY 54.5
Balodhi, Ashiwini ... TT 5.6, TT 23.10, •TT 26.9, TT 81.8
Balodhi, Ashwini ..... TT 23.9
Baltisberger, Timon L. ..... HL 55.4
Baltrusch, Florian ..... •HL 26.52
Baltz, Vincent ..... MA 7.52
Bampoulis, Pantelis ..... TT 41.1
Bamrah, Navjot ..... DS 20.30
Bandyopadhyay, Malay ..... TT 92.11
Bandyopadhyay, Sayam ... •CPP 54.3
Bandyopadhyay, Subhadeep •MA 20.3
Banerjee, Arnab .... O 69.4, •O 89.11, TT 72.4
Banerjee, Eshan ..... O 84.4, TT 84.4
Banerjee, Tirthankar ..... DY 49.3
Banerjee, Varsha ..... DY 15.6
Banerji, Natalie ..... CPP 57.6
Bang, Junho ..... TT 4.10, TT 78.5
Bange, Jan Philipp ... O 14.3, O 14.10, O 38.1, O 40.18, O 40.19, O 40.20, O 40.21, •O 66.1, O 66.9, O 98.10, TT 37.18, TT 37.19, TT 37.20, TT 37.21, TT 44.9
Banisch, Sven ... SOE 10.3, •SOE 11.1
Banker-Busch, Philipp ..... •JOB 1.1
Banov, Krum ..... FM 5.11
Banterle, Niccolò ..... BP 12.10
Banys, Juras ..... FM 4.4
Bao, Changhua ..... •O 38.6
Bao, Ruicheng ..... DY 21.5
Bapat, Nikhil ..... O 13.1
Baptist, Anna ..... BP 20.8
Bär, Christian ..... BP 16.11
Bär, Marcus ..... •CPP 12.6
Bär, Markus ..... •DY 22.5
Bar, Michael ..... HL 26.44
Baraban, Larysa ..... FM 6.11
Baradyn, Maciej ..... •O 34.3
Baraldo, Luis M. ..... O 87.1
Baranda Pellejero, Lorena .. BP 14.27
Baranov, Dmitry ..... HL 4.1
Baranov, Fedor ..... •TT 40.4
Baranowski, Daniel ..... O 9.1, O 69.2
Baranowski, M. ..... HL 54.10
Barbier, Jean ..... DY 45.5, DY 58.9, SOE 14.5, SOE 17.9
Barbosa, Matheus ..... •MA 36.12, TT 40.3
Barcikowski, Stephan ..... MA 13.7,

MA 50.5
Barcons Ruiz, David . HL 10.1, TT 20.1
Bard, Matthieu ..... TT 74.7
Bardarson, Jens H. . DY 42.1, TT 63.1
Bardazzi, Alessia .... O 95.3, TT 96.3
Barducci, Alessandro ..... BP 15.2, BP 32.4, DY 52.4
Barends, Rami TT 93.6, QI 6.9, QI 8.5
Barentin, Catherine .....CPP 20.9, DY 23.9
Barfuss, Wolfram ..... SOE 2.9
Barghathi, Hatem .....TT 64.1
Bargheer, Matias .HL 26.52, MA 7.39, MA 14.4, MA 38.9, O 40.15, TT 37.15
Barik, Bikash ..... HL 29.2, TT 58.2
Barke, Ingo BP 14.25, BP 33.9, O 27.2, O 44.13, O 46.9, O 68.6
Barner, Jörg .....•BP 14.43
Barnett, Julian ..... O 79.4
Barnowsky, Tom ....FM 6.2, •FM 6.3, MM 11.6, O 18.6, O 95.4, TT 96.4
Baron, Joseph W. .....DY 8.8
Baroncha, Georgiy .....•CPP 6.2, CPP 46.8
Baronio, Stefania .....DS 6.2
Barragan, Selena ... HL 29.5, TT 58.5
Barrera, Eduardo ..... O 56.6
Barrera Ramirez, Eduardo .... O 56.5
Barreto, Rafael R. .... O 95.2, TT 96.2
Barrier, Julien ..... HL 10.1, TT 20.1
Barriet, David ..... MA 6.11
Barriga, Elias .....•BP 27.1
Bärschneider, Toni ..... HL 26.16
Bart, Nikolai ..... HL 20.35
Bartels, Frederik .....•HL 20.54
Bartels-Rausch, Thorsten ....•UP 6.1
Barth, Johannes ..... O 69.10
Barth, Johannes V. .... O 9.4, O 45.4, O 78.3, O 83.1
Barth, Michael .....TT 74.12, TT 97.2
Barth, Stephan .....MA 52.11
Barth, Valentin ....•HL 18.2, •TT 32.2
Barthe, Marie-France ..... FM 11.17
Barthlott, Dominic .....•QI 14.24
Bärtl, F. .....•TT 80.6, TT 93.7
Bartley, Tim .....QI 5.9
Bartnick, Lara .....•CPP 40.5
Barton, Brandon ... DY 58.1, SOE 17.1
Bartosch, Sascha ..... CPP 13.3, •CPP 17.9
Bartsch, Tim ..... •DS 7.4, DS 20.24
Barua, Avijit ..... HL 13.1
Baruah, Tushar .....•MA 27.5
Barutel, Cedrik ....•BP 36.3, •DY 57.3
Barysch, Vera ..... FM 5.5
Barzola Quiquia, J. ..... TT 74.5
Basaric, Farah .....•TT 73.6
Basavarajappa, Manasa Gattavadi •MM 8.6
Baše, Tomáš ..... O 72.4, TT 67.4
Bashaish, Saleh .....•MM 16.5
Basini, M. ..... MA 25.6
Basini, Martina ...•MA 14.2, MA 25.8
BAŞKAN, Taylan .. FM 19.6, •QI 14.12
Basov, Dmitri .....•PLV I
Bassanoni, Alberto ..... •DY 7.2
Bassi, Marion ..... QI 2.10
Bässler, Heinz .... CPP 57.2, HL 53.3
Bassoli, Riccardo .. HL 55.7, HL 56.4, HL 56.5
Bastard, Gerald .....HL 29.5, TT 58.5
Basu, Abhik ..... DY 43.13, DY 43.14
Basu, Urna ..... DY 44.2
Bate, Teagan .....BP 20.6
Bat-Erdene, Bat-Amalgam ... DY 43.7
Bat-Erdene, Bat-Amgalan ...•DY 43.4
Bathen, Nicolai Leonid ..... HL 20.17
Bathiany, Sebastian .....•SYTP 1.3
Batle, Josep ..... DY 22.9
Batsuuri, Urantuya .....•DY 41.5
Battistelli, Riccardo .....MA 37.8
Battiston, Luca .....•BP 14.46
Baù, Enrico .....O 85.7
Bauch, Chris .....•SYTP 1.2
Bauden, Cecilia ..... FM 11.24
Bauer, Andreas .... MA 7.5, MA 7.33, MA 37.7, TT 23.3, TT 41.6, TT 61.6, TT 61.7, TT 62.1
Bauer, Antonia .....•DD 20.3
Bauer, Daniela ..... CPP 21.4
Bauer, Eric D. .....TT 52.3
Bauer, Ferdinand ..... O 26.2, •O 27.6
Bauer, Frederik ..... O 89.6
Bauer, Jan .....DD 16.1
Bauer, Jens .....O 68.3, O 68.5
Bauer, Lukas .....TT 23.3, TT 62.1
Bauer, Marianne .....•BP 32.10, •DY 52.10, SOE 2.10
Bauer, Martin ..... HL 56.4
Bauer, Michael .....O 14.4, O 66.4, O 84.11, TT 84.11
Bauer, Robert P.C. ..... CPP 46.5
Bauer, Tobias .....HL 34.1, QI 18.6
Bauer, Wolfgang .....•DY 47.6
Baumann, Aljoscha F. •MM 3.7, QI 1.8
Baumann, Danny ..... TT 11.4
Baumann, Michael ..... HL 45.5
Baumann, Susanne ... O 12.3, O 15.7, O 43.11, O 89.1, O 89.5, O 99.1, O 99.8
Bäumchen, Oliver .. BP 1.10, BP 7.28, BP 7.29, BP 14.5, CPP 1.10, DY 4.10
Baumert, Thomas . MA 39.22, O 70.4, O 70.5, TT 65.4, TT 65.5
Baumgarten, Gerd .....UP 3.5
Baumgarten, L. .....DS 3.4
Baumgarten, Lutz .... FM 4.2, O 19.2, O 93.2
Baumgarten, Robert .....O 23.4
Baumsteiger, Jakob .....•MA 3.2
Baunthiyal, Aman .....•HL 20.66
Bauriedl, Lorenz ..... TT 97.1
Bausch, Andreas ..... BP 12.8
Bavisotto, Robert .....•O 78.4
Baweja, Kriti .....•TT 53.6
Bayat Nejad, Farahnaz .....•MM 18.6
Bayat Nejad, Farzaneh ..... MM 18.6
Bayer, Johannes C. .HL 17.6, •HL 25.1
Bayer, Johannes Christian ... HL 17.2
Bayer, Maximilian .....•TT 94.8
Baykal, Doruk ..... BP 14.27
Bayraktar, Ömer ..... QI 14.1
Bazarnik, Maciej .... MA 5.3, O 40.14, O 71.22, •O 71.23, O 72.3, TT 7.3, TT 37.14, TT 66.22, •TT 66.23, TT 67.3
Bazazzadeh, Nasim ..... MA 58.7
Bazulin, Daniil .....•TT 28.7
Beale, Emma ..... BP 9.6
Beanland, Richard ..... FM 12.3
Beaulieu, N. .....MA 52.8, MA 59.8
Beaulieu, Nathan .....MA 52.10
Beaulieu, Samuel .... MA 7.18, O 76.2
Beauvois, Ketty ..... TT 57.2
Bebelman, Maarten P. ..... BP 27.3
Bebon, Robin .....•DY 9.3
Becca, Federico .. MA 19.11, TT 31.11, TT 95.5
Bechberger, Moritz .....•MA 9.12, MA 48.1, MA 52.19
Becher, Christoph ... HL 34.1, QI 18.6
Becher, Simon .....•DD 21.2
Bechinger, Clemens ..... CPP 10.11, DY 6.1, DY 16.11, DY 21.10, DY 21.11, DY 54.3
Bechler, Nicolai Timon .....•MA 33.2
Bechstein, Ralf . O 5.3, O 36.3, O 36.6, O 39.2
Beck, Janic .....•QI 11.4, QI 11.5
Beck, Mathias ..... MA 27.10
Beck, Timon ..... BP 27.10
Beckemeyer, Laurenz ..... DY 46.3, TT 75.3
Becker, Eleonore .....•DD 13.1
Becker, Gabriele .....•AIW 2.1
Becker, Janne Oskar .....•CPP 17.46
Becker, Karoline ..... HL 20.25
Becker, Khang Vi ..... MA 37.2
Becker, Klaus.-D. ..... FM 11.30
Becker, Leon ..... O 84.4, TT 84.4
Becker, Martin DS 8.2, DS 9.1, DS 11.7, MM 35.7
Becker, Maximilian .....CPP 23.3, DY 24.3, DY 54.4
Becker, Maximilian R. .....O 87.7
Becker, Paula ....•DD 39.2, •AKC 1.3
Becker, Petra ..... FM 18.8
Becker, Wanja .....•DY 43.1
Becker-Bohatý, Petra ..... TT 23.18
Beckert, Sebastian FM 19.1, MA 7.52, MA 7.61, •MA 7.65
Beckmann, Benedikt .....•MA 10.3, MA 13.2, MA 50.8, MA 52.23
Beckmann, Detlef ..... TT 73.10
Bédard, Charles Alexandre ..DY 47.11
Bedirkhanov, Gusein .....•TT 53.1
Bednarz, Beatrice ..... DS 6.5
Bedoya-Pinto, Amilcar O 64.5, TT 41.2
Beeks, Kjeld .....MA 39.25
Beenakker, Carlo W. J. ..... O 63.6, TT 55.6
beenken, Wichard .....•HL 26.4
Beer, Leonie .....•CPP 46.18
Beest, Bas ter ..... CPP 17.49
Bégon-Lours, Laura ..... •SYBT 1.2
Begur Prakash, Sumanasa ... O 71.8, TT 66.8
Behera, Akash Chandra .....•O 85.4
Behera, Lipsa .....•TT 94.5
Behler, Jörg .... CPP 9.4, CPP 46.54, MA 36.1, MM 19.1, O 18.3, O 24.4, O 24.5, O 24.6, O 24.7, O 39.5, O 97.6
Behn, Wyatt .....•O 33.2
Behnami, Mahdi ..... TT 11.1
Behnisch, Thomas ..... FM 19.4
Behnken, Christian .....DY 15.11
Behr, Ralf .....TT 22.7, TT 28.10
Behrends, Robert B. ..... QI 18.7
Behrendt, Drew ..... MA 4.1
Behrendt, Florian ..... FM 4.9
Behrens, Malte ..... O 34.8
Behrens, Silke ..... O 23.2
Beier, Sönke .....•BP 11.8
Beiersdorfer, Anton .....•MM 19.12
Beignon, Roméo .....•MA 59.7
Bein, Thomas ..... CPP 59.3, HL 15.1
Beinortaite, Judita .....•AKBP 12.4, AKBP 13.2
Beisler, Franziska .... O 48.5, DD 14.3
Bejas, Matias ..... TT 39.7
Beka, Fatime ..... DD 31.1
Beke, Bálint .....•MA 17.7
Bekir, Marek .....MM 19.41
Bektas, Onurcan .....•BP 10.12, •CPP 18.12, •DY 18.12
Bektas, Umutcan .....HL 40.5
Belashchenko, Kirill D. .....MA 30.8
Belbase, Bishnu Prasad ..... TT 72.4
Belik, Andrei A. ..... MA 17.3
Belinchón, David Muradas . MA 24.4, TT 36.4
Belissimo, Alessandra ..... O 93.1
Beljonne, David ..... CPP 17.9
Belke, Christopher ..... HL 20.10
Bellersen, Hilde .....•HL 26.25
Belousov, Roman .....•DY 47.1
Belozertsev, Mikhail ..... O 65.5
Belyaeva, Tatyana ..... DY 44.11
Belz, Juergen ..... O 10.9, TT 16.9
Belz, Jürgen CPP 4.4, O 70.1, O 95.12, TT 65.1, TT 96.12
Belzig, Wolfgang . MA 52.4, MA 54.5, TT 22.1, TT 29.10, TT 61.13, TT 90.1, TT 98.6
Ben Amor, Nada .....•CPP 21.4
Ben Tanfous, Zeineb ..... O 44.12
Ben Youssef, Jamal ..... MA 52.10
Benali, Dalal ..... QI 20.8
Ben-Ami, Tom .....•DY 13.7, •TT 19.7
Benatti, Fabio ..... QI 16.8
Benavente, Diego ..... CPP 41.5
Benckiser, Eva .....•TT 39.2
Ben-David, Uri .....BP 32.11, DY 52.11
Bendin, Hannah .....•HL 57.1
Benduhn, Johannes ..... CPP 15.6, CPP 17.20, CPP 17.24, CPP 22.3, CPP 25.5, CPP 40.1, CPP 40.4, CPP 40.6, CPP 57.1, CPP 57.3, CPP 57.6, DS 16.5, HL 1.12, HL 22.6, •HL 25.5
Benedičič, Izidor ..... O 80.3
Benedikt, Jan ..... O 7.5, TT 9.5
Beneke, Charlotte .....•TT 2.2
Beneke, Grischa .. MA 55.2, MA 55.3, •MA 55.9
Benetatos, Panayotis ..... DY 40.2, •DY 44.18
Bengaard Hansen, Ursula .... MA 3.7
Benhabib, Siham . MM 40.5, TT 29.3, TT 29.11
Benini, Mattia ..... MA 30.9, •O 64.4
Benito, César .....QI 3.1
Benito, Mónica .... •HL 31.1, HL 31.2, HL 38.8, MA 7.29, TT 78.2, TT 78.7, QI 3.5
Benito, Santiago ..... MM 34.6
Benjamin, Claire ..... QI 2.8
Benke, D. ..... MA 18.1, TT 30.1
Benke, Magnus ..... •QI 20.1
Bennecke, Wiebke ... O 14.3, O 14.10, O 38.1, O 40.18, O 40.19, O 40.20, O 40.21, •O 66.9, O 98.10, TT 37.18, TT 37.19, TT 37.20, TT 37.21, TT 44.9
Benneka, Leo-Malik •O 74.6, •TT 68.6
Bennemann, Benjamin ..... HL 12.1, QI 6.9, QI 14.26
Bennenhei, C. .... HL 54.10, HL 54.12
Bennett, Philipp ....TT 92.6, •TT 92.7
Bensemhoun, Adrien ..... QI 18.1
Bensmann, Jannis MA 7.7, •MA 9.13, MA 12.1, MA 52.5, MA 52.14
Benson, Luke .....DS 4.2
Benthin, Frederik .HL 20.49, HL 55.10
Bentmann, Hendrik MA 3.4, MA 24.3, O 2.1, O 2.5, O 76.6, TT 25.11, TT 36.3
Benzi, Roberto ..... DY 62.9
Ben-Zvi, Ilan .....AKBP 14.3
Bera, Anup Kumar ..MA 19.9, TT 31.9
Bera, Palash .....•DY 62.2
Bera, Soumya .... DY 13.3, MA 34.12, TT 19.3
Berchialla, Luca ....MA 44.2, TT 76.2
Berciaud, Stéphane .....O 12.9
Bercioux, Dario .....•TT 4.4
Bercoff, P. .....TT 74.5
Bercx, Marnik .....MM 13.9
Berdermann, Jens .....O 68.6
Bereau, T. .....AKPIK 6.5
Berecová, Valentína .....•MM 19.26
Berekovic, Laris .....•DY 49.11
Berencén, Yonder ..•HL 11.4, HL 56.1
Berenschot, Erwin ..... TT 28.5
Berg, Aleksey .....•MA 30.7
Berg, Erez ..... TT 4.5
Berg, Lukas .....HL 20.35
Berg, Nikita .....•HL 20.26
Bergamasco, Enrico .....TT 23.18
Bergbauer, Valentin .....•O 12.5
Berge, Siri A. .....•TT 5.10
Berger, Andreas .....•DY 60.4
Berger, Christoph .....•HL 37.5
Berger, Florian .....DY 47.1
Berger, Johanna .... TT 73.7, TT 97.1
Berger, Lucas ..... TT 23.14
Berger, Lukas .....•TT 62.12
Berger, Richard .....O 6.8
Berger, Roland .....•DD 27.1
Berger, Rüdiger .... CPP 5.1, CPP 8.5
Bergerot, Clémence .....SOE 9.5
Berges, Jürgen .....DY 42.2, TT 63.2
Bergman, Anders ..... MA 34.1
Bergmann, David .....•HL 20.60
Bergmann, Max .....O 70.1, •O 95.12, TT 65.1, •TT 96.12
Bergmann, Nicolas .....•O 97.10
Bergmeier, Franziska ..... O 66.2
Bergmeier, Tim .....•O 14.6
Beringuier, Maurice .•O 71.5, •TT 66.5
Berkel, Leon L. ..... DY 28.3
Berkovich, Ronen .....O 87.4
Berland, Kristian ..... MM 37.4
Berlitz, Benedikt .....TT 22.13
Bermudez, Alejandro .....QI 3.1
Bernard, Alexandre .....TT 74.4
Bernard, Mark .....O 34.7
Bernd, Büchner ..... TT 94.4
Berndt, Richard ... O 6.4, O 6.4, O 6.4, O 6.4, •O 6.4, O 17.10, O 45.7, O 69.4, O 83.8, O 89.9, O 89.11
Berner, Fiona ....•CPP 8.5, CPP 27.4, DY 26.4
Bernert, Constantin .....AKBP 6.2
Bernevig, B. Andrei ..... TT 74.1
Bernhard, Nicolas .....MM 32.5
Bernhard, Nils .....HL 40.6
Bernhardt, Birgitta ..... O 43.7
Bernhardt, Nils ..... HL 55.11
Bernheim, Anne ...BP 10.2, CPP 18.2, DY 18.2
Bernien, Hannes ..... QI 3.10
Bernien, Matthias .....•O 78.5
Bernlochner, Florian ..... DD 19.1
Bernstein, Fabian .....•DD 17.3
Bernstroff, Sigrid CPP 44.2, CPP 53.2
Berry, Joseph ..... HL 46.1
Berryman, Joshua T. ..... BP 15.6
Bert, Fabrice .....TT 57.2, TT 57.3
Berth, Gerhard ....HL 20.33, HL 49.3, HL 54.4
Berthelette, Sophie .....•DY 47.11
Berthier, Ludovic ..... DY 62.7
Bertini, Bruno ..... TT 70.5
Bertolotti, Micol .....HL 20.15
Bertram, F. ..... HL 37.2, HL 37.6
Bertram, Florian ...CPP 19.4, DY 20.4
Bertram, Paul ..... FM 19.4
Bertrand, Benoit ..... QI 2.10
Bertrand, Thibault ..CPP 11.9, DY 9.2, DY 17.9
Bertrang, Kevin ..... O 78.2
Bertschi, Hannah .....•O 14.7
Berwagner, Kevin .....•HL 26.50
Beschoten, Bernd ...HL 3.3, MA 43.2
Besenius, Pol ..... CPP 14.7
Besproswanny, Julia . O 63.2, TT 11.3,

•TT 11.4, TT 55.2
Bessarab, Pavel ..... MA 21.5
Bester, Gabriel ..... HL 3.4, HL 13.6
Beta, Carsten ..... BP 11.8, DY 33.5, DY 55.2
Bethune, Julia ..... MA 39.7
Betker, Marie ... CPP 25.4, CPP 32.4, DY 35.4
Betz, Nicolaj ... O 15.7, O 89.1, O 89.5, •O 99.1, O 99.8
Betz, Timo BP 7.10, BP 7.25, BP 7.27, BP 7.30, BP 7.31, BP 7.32, BP 7.39, BP 7.43, BP 7.48, BP 7.49, BP 27.4, BP 37.1, DY 43.5, DY 43.18
Betzold, Simon .... HL 1.12, HL 20.30
Beu, Julian ..... TT 62.2, TT 62.3
Bewersdorff, Arne ..... •DD 11.1
Beye, M. ..... O 19.10
Beye, Martin ..... TT 14.4
Beyer, Bjarne ..... •MA 21.5
Beyer, David ..... CPP 46.25
Beyer, Hauke ..... O 66.4
Beyer, Jörn TT 22.7, TT 28.3, TT 82.3
Beyer, L. MA 18.4, MA 52.22, TT 30.4
Beyreuther, Elke ..... FM 12.2
Bezjak, Dragica ..... CPP 41.3
Bezmaternykh, L. N. ..... MA 17.7
Bezsmertna, Olha •MA 44.6, MA 49.5, •TT 76.6
Bezvershenko, Alla MA 23.6, TT 35.6
Bhandari, Bashudev ..... •CPP 17.41
Bhandari, Tika Ram ..... •BP 4.4
Bhandarkar, Sanjay ..... •DY 44.20
Bhar, Rajdwip ..... FM 11.31
Bharadwaj, Mukund ..... TT 22.32
Bharadwaj, Venkata K. ..... MA 47.6
Bharadwaj, Venkata Krishna . MA 8.5
Bharati, Ritadip ..... MA 49.2
Bhardwaj, Atmika ..... CPP 59.5
Bhardwaj, Harsh ..... QI 8.5
Bhardwaj, Richa . MA 9.13, •MA 52.5, MA 52.14
Bhasker, Arjun ..•TT 22.25, TT 22.26, QI 14.21
Bhasme, Sarang ..... •DS 21.6
Bhat, Bhoomika R ..... •TT 28.6
Bhat, Vinayak Shantaram .... MA 6.1
Bhateja, Moksh ... •DY 53.6, •TT 87.6
Bhatt, Neeraj ..... MA 11.5, TT 21.5
Bhattacharjee, Anirban •QI 8.3, QI 11.6
Bhattacharjee, Paromita ... HL 20.19, •HL 48.4
Bhattacharjee, Somasree .•MA 16.10, MA 45.2
Bhattacharya, Aranya ..... QI 21.2
Bhattacharya, Khokan ..... MA 31.2, TT 47.2
Bhattacharyya, Komal ..... BP 7.15, BP 7.16, •BP 12.4, DD 24.4
Bhayani, Ghata ..... HL 34.1
Bhobe, Preeti A. .... HL 10.4, TT 20.4
Bian, Guodong ..... QI 13.5
Bianchi, Andrea D. ..... TT 52.5
Bianchi, Marco ..... O 76.4, TT 27.4
Biasiol, Giorgio .... TT 22.24, TT 73.7
Bibes, M. ..... TT 69.6
Bibes, Manuel ..... FM 18.6, •O 75.1, TT 69.4, TT 69.5, •TT 77.1, TT 81.1
Bick, Christian ..... •FM 19.8
Bickermann, Matthias ..... FM 14.3
Biderang, Mehdi ..... TT 93.9
Biedenweg, Doreen BP 7.34, BP 7.35, BP 7.36, BP 7.38, BP 7.40
Biedermann, Jan ..... •TT 27.3
Biedinger, Jan ..... CPP 3.4
Biedron, Aleksandra ..... TT 43.8
Biehle, Martin ..... TT 70.2
Biel, Katharina ..... •O 17.8
Bieler, Mark ..... TT 22.7, TT 22.12, TT 28.3, TT 28.6, TT 28.9, TT 28.10, TT 43.5
Bielfeldt, Meike ..... BP 33.9
Bieling, Jan ..... •O 67.2
Bienau, Alexandra ... •BP 5.1, BP 8.4, BP 14.23
Bienek, David ..... •CPP 13.5
Bieniek, Przemyslaw ..... •MA 58.8
Bienvenu, Baptiste •MM 9.1, MM 15.4
Bier, Markus ..... •MM 31.7
Bierbach, David ..... BP 14.90
Bieringer, Malte •MA 31.12, •TT 47.12
Biermann, Klaus ..... HL 55.2
Biermann, Silke .....•O 37.4, TT 13.6, TT 13.9, TT 23.16, TT 81.4
Biersack, Matthias .. DY 19.9, DY 41.2
Bierwagen, O. ..... O 57.6
Bierwagen, Oliver ... HL 40.1, HL 40.8
Bietz, Finn .....•FM 11.21
Biggs, M. ..... MA 25.6
Bigi, Chiara ..... MA 33.12
Bigi, Filippo ..... MM 9.8
Bihlmayer, G .....MA 19.7, TT 31.7
Bihlmayer, Gustav . MA 5.8, MM 27.4, O 2.2, O 37.3, O 50.1, •O 64.3, O 71.6, TT 7.8, TT 66.6
Bijalwan, Viranchika ..... CPP 41.4
Biktagirov, Timur •FM 11.12, FM 11.20, HL 26.24, MA 13.8
Biletter, Emanuel ..... O 88.4
Bilous, Oksana .... DY 19.9, •DY 25.2, DY 41.2
Bilous, Pavlo ..... TT 51.5, •QI 14.20
bin Ali, Annas ..... O 78.5
Bincoletto, Davide ..... QI 3.5
Binder, Johannes . HL 26.37, HL 35.7
Binek, Christian ..... O 60.6
Bing, Wu ..... O 76.5
Binger, Hayden ... MA 58.2, •TT 40.1, TT 40.3, TT 92.3
Biniskos, Nikolaos ..... MA 47.6
Binninger, Tobias ..... MM 25.5
Binysh, Jack ..... SYBS 1.5
Bippus, Frederic ..... TT 10.1
Biquet-Bisquert, Anaïs ..... BP 41.1
Birch, Max ..... MA 16.6
Birk Hellenes, Anna ..... MA 20.6
Birkel, Christina ..... MA 52.26
Birkhan, J. ..... AKBP 1.1
Birla, Hariom .....O 9.6, O 48.4
Birol, Turan ..... MA 8.8
Biroli, Giulio ..... •DY 45.1, •SOE 14.1
Bischof, Lars ..... BP 14.64
Bischof, Luca ... MA 52.38, MM 19.13
Bischoff, Markus .... BP 7.41, BP 11.9
Bischoff, Rasmus ..... O 23.9
Bischopink, Tom ..... BP 33.6
Bisht, Neeta ..... •MA 5.4, •TT 7.4
Biskupek, Johannes .. O 10.6, TT 16.6
Bisset, Rebecca ... TT 5.10, •TT 29.2
Biswal, Ayusa Aparupa ..... •DS 4.1
Biswas, Arpan ..... TT 64.1
Biswas, D. ..... O 93.9
Biswas, Deepnarayan ..... HL 48.5
Biswas, Madhurima MA 31.2, TT 47.2
Biswas, Manas Pratim ..... •O 12.9
Biswas, Samanwita •TT 78.6, TT 90.1
Biswas, Santu ..... O 81.2
Biswas, Shuvrodev ..... CPP 16.3, •CPP 16.6, CPP 17.39
Biswas, Subhadip ..... •BP 15.1
Biswas, Subham ..... BP 12.3
Bittihn, Philip ..... BP 7.48, BP 7.54, BP 10.6, BP 37.9, CPP 18.6, DY 18.6, •DY 33.2, DY 44.12
Bittrich, Eva ..... CPP 17.9
Bitzek, Erik ..... •MM 7.4, MM 32.2
Bitzenbauer, Philipp DD 13.1, DD 25.2, DD 27.4, •DD 30.3
Bitzer, Paul ..... •DY 41.14
Bizot, Quentin ..... •MM 3.8
Björklund Svensson, Jonas AKBP 12.4
Black, Maximilian ..... O 27.4
Blackburn, Tom ..... AKBP 4.5
Black-Schaffer, Annica M. ... TT 56.4
Blanchet, Sandra ..... BP 9.2
Blanco Canosa, Santiago .... DS 12.6
Blanco Peces, Alejandro .... TT 14.10
Blanco-Canosa, S. ..... MA 7.85
Blank, Kerstin G. .. •BP 7.12, BP 14.81
Bläsing, Jürgen .... DS 11.4, HL 33.2, HL 33.3, HL 34.3
Blatnik, Matthias ..... O 58.7
Blatt, Rainer ..... QI 15.2
Blázquez Martínez, Alfredo .•HL 25.3
Blech, Alexander ..... HL 8.12
Blick, Robert ..... BP 26.8, BP 26.10, CPP 43.8, CPP 43.10, DS 16.3, FM 11.29, MA 39.7
Blick, Robert H. .. DS 20.10, FM 11.26, O 71.19, TT 66.19
Blickberndt, Jan . TT 22.18, •TT 22.19
Bliem, Roland DS 20.13, O 4.5, O 11.7, O 23.8, O 28.1
Bligaard, Thomas ..... O 18.1
Blinov, Lara ..... HL 3.6, HL 20.17
Blinzer, Tim ..... •CPP 5.3
Blödorn, Felix ..... O 93.1
Blom, Kristian .... DY 41.10, •SOE 9.3
Blom, Paul ..... HL 15.6
Blom, Paul W.M. .... FM 10.4, HL 15.4
Blom, Tycho ..... •TT 57.9, QI 20.8
Blom, Tycho J. ..... TT 28.4
Blonski, Markus A. ..... •DS 11.3
Blue, Brandon ..... O 56.6
Blügel, Stefan ... MA 16.12, •MA 19.7, MA 34.7, MA 40.2, MA 51.4, MA 51.7, MA 55.4, MA 55.10, O 37.3, O 37.6, O 50.1, O 64.3, O 71.6, •TT 31.7, TT 66.6, TT 88.4, TT 88.7
Bluhm, Hendrik . CPP 19.5, CPP 23.2, CPP 27.3, DY 20.5, DY 24.2, DY 26.3
Blukis, Roberts ..... FM 14.3
Blum, Christian G. F. ..... MA 7.37
Blum, Jonas ..... •HL 3.3
Blum, Peter ..... •AKBP 8.4
Blum, Tobias ..... •TT 70.3
Blumberger, Jochen CPP 25.1, O 97.2
Blumenthal, David B. ..... BP 14.50
Blümler, Peter .. MA 46.3, •MA 52.30
Blythe, Richard A. ..... DY 7.7
Boariu, Florin ..... HL 26.52
Boban, Honey ..... O 2.2
Bobrova, Ekaterina ..... MA 38.2
Bocaniciu, Camil ..... O 30.3
Bocchi, Dario ..... AKPIK 2.2
Bocchini, Adriana ... •HL 49.3, O 16.1
Bochkarev, Anton ..... MM 19.10
Bock, Antonia Joëlle ..... •DY 42.7, •TT 63.7
Bock, Stefan ... AKBP 11.3, AKBP 11.4
Bockhorn, Lina .... DS 14.6, HL 20.10, •HL 29.4, HL 30.5, •TT 58.4, TT 59.5
Böckmann, Hannes FM 11.33, O 22.2, O 86.2, •O 86.7
Böckmann, Rainer ..... •BP 4.1
Bocquet, François C. . O 45.9, O 67.9, O 83.2
Bocquet, Marie-Laure ..... O 83.8
Bode, Matthias ... MA 5.5, MA 39.20, O 31.6, O 44.2, O 56.4, O 60.4, O 63.2, O 63.3, TT 7.5, TT 11.3, TT 55.2, TT 55.3, TT 85.2
Bode, Simeon ..... •O 73.3
Bode, Tim . QI 3.2, QI 3.9, AKPIK 5.15
Bodenschatz, Eberhard ..... •DY 22.1
Bodesheim, David ..... CPP 26.3
Bodewei, Paul ..... •TT 91.3
Bodini-Lefranc, Quentin ..... BP 29.3, CPP 45.3
Bodnar, Andrii ..... •HL 20.7
Bodnarchuk, Maryna ..... HL 45.4
Boehrer, Bertram ..... UP 7.1, UP 7.2, UP 7.3
Boer, Lotte ..... MA 58.2, TT 40.1, •TT 40.3, TT 92.3
Boers, Niklas ..... SYTP 1.3
Boesenberg, Ulrike .O 40.15, TT 37.15
Bogdanoff, Nils ..... O 80.4
Boghiu, Emanuel-Cristian .... QI 12.3
Bogner, Christina ..... CPP 41.7
Bogucki, Aleksander .....•O 56.3
Bogush, Igor ..... •TT 97.8
Bohamud, Tamam ..... O 11.4
Bohatý, Ladislav ..... FM 18.8
Bohaty, Petra Becker ..... MA 23.6, TT 35.6
Bohl, Sonja ..... •O 8.7
Bohlemann, Chris Yanic ..... O 54.2
Bohlemann, Chris Yannic •CPP 46.43
Böhm, Lukas ..... O 40.8, TT 37.8
Böhm, Maite .....O 24.4, •O 24.5
Böhm, Thomas ..... MA 33.8
Böhme, Florian ..... •BP 14.5
Böhme, Lucas ..... HL 16.7
Böhmer, Anna ..... MA 33.4
Böhmer, Anna E. .•FM 6.8, MM 19.42, TT 5.6, TT 23.9, TT 23.10, TT 26.9, TT 81.7, TT 81.8
Böhmer, Jan ..... •HL 16.7, HL 56.3
Bohn, Benjamin ..... HL 55.10
Böhnert, Tim ..... MA 39.12
Böhnke, Jan ..... O 42.4
Bohrdt, Annabelle .... TT 51.6, QI 5.9
Boian, Vladimir ..... •DS 20.29
Boison, Urs ..... •O 44.9
Bojunga, Leon ..... O 28.3, •O 44.14
Bokemeyer, Paul . HL 26.22, •HL 40.9
Boky, Mohammed .....•TT 23.25
Bolat, Rustem ..... O 61.10
Boldt, Regine .. •CPP 46.19, CPP 59.1
Bolhuis, Peter ..... DY 7.8
Bolielyi, Oleksandr .....•TT 25.8
Bolio, Jorge Esteban .....•TT 15.6, TT 74.2
Boll, Torben ..... MM 30.3
Bolle, Frederik ..... •TT 5.2
Bollenbach, Tobias ..... BP 11.10
Bollmann, Steffen TT 64.5, •TT 83.12
Bolotova, Daria ..... BP 33.6
Boltje, Daan B. ..... TT 28.4, •QI 20.8
Boltje, Raluca ..... HL 38.8, MA 37.8
Boltz, Horst-Holger DY 44.4, DY 44.8, •DY 55.7
Bölükbaşi, Ismail ..... HL 20.41
Bolz, Lukas ..... •O 88.5
Bomers, Mario ..... PSV IV
Bonacci, Miki ..... •MM 17.5
Bonafé, Franco ..... O 49.1
Bonanni, Alberta ..... HL 54.4
Boneberg, Johannes ..... MA 52.33
Boneß, Daniel K. J. ..... MA 52.4
Bonetti, Gaetano ..... FM 23.6
Bonetti, Pietro ..... TT 13.4, TT 94.1
Bonetti, Stefano ..... MA 14.4
Bonfà, Pietro ..... MM 13.9
Bongardt, Lukas ... •O 84.3, •TT 84.3
Bonifer, Markus .... •O 40.5, •TT 37.5
Bonitz, Michael ... DY 42.3, MA 7.59, TT 63.3
Bonivardi, Adrian ..... O 88.5
Bonmassar, Nicolas ..... •DS 6.2
Bonn, Mischa ..... CPP 13.2, •O 51.1
Bonneau, Klara ..... •BP 15.7
Bonnes, U. ..... AKBP 1.1
Bonnet, Nicéphore . MM 41.5, O 97.10
Bontke, Florian ..... O 96.9
borah, hrishikesh .. TT 5.3, •TT 22.23
Boraley, X. ..... TT 25.9
Boras, Dominik .... FM 5.3, •FM 19.7
Borcherding, Daniel ..... QI 16.3
Borchers, Christopher .... •HL 20.49, HL 20.51
Borchert, Martin ..... MA 38.3
Bordács, Sándor .. MA 16.8, MA 17.7, MA 23.2, MA 37.9, MA 54.2, TT 35.2
Bordet, Alexis ..... CPP 46.42
Bordin, Alberto ..... TT 15.3
Borhade, Poonam ..... HL 20.16
Borić, Tina ..... •BP 7.46
Borisenko, Sergey ..... O 2.3, TT 5.7
Borisov, Vladislav •MA 34.11, MA 58.9
Bork, Sophie ..... MA 30.9
Börner, Georg ..... SOE 16.1
Börner, Richard .. BP 14.54, BP 14.79, BP 18.2
Börner, Tom C. D. ..... CPP 41.7
Bornhake, Thomas ... O 37.3, •O 50.1
Bornmann, Benjamin ..... MM 19.44
Bornschein, Jens ..... DS 21.4
Bornscheuer, Uwe T. ..... MA 39.7
Borodavka, Fedir ..... MA 17.3
Borodin, Dmitriy ..... O 11.5, O 15.11, O 17.1, O 17.4, O 34.7, O 77.6, •O 99.11
Borondics, Ferenc ..... CPP 46.17
Borriello, Mattia ..... •CPP 21.6
Borrmann, Stephan ..... UP 6.3
Borsch, Markus ..... HL 8.1
Borysenko, Yelyzaveta A. . •MA 39.11
Bosak, Alexei ..... TT 95.2
Bosch, Felix ..... BP 11.1
Bosche, Jonas ..... BP 14.6
Boscher, Nicolas D. ..... CPP 17.11
Boschetto, Gabriele ..... QI 2.10
Bosco, Stefano ..... HL 38.4
Bose, Roni ..... •TT 57.1
Bose, Subhaya .... BP 10.2, CPP 18.2, DY 18.2
Bossert, Marine ..... •MM 15.7
Bostan, Yusuf Kerem ..... HL 24.4
Bostwick, Aaron ..... MA 5.8, TT 7.8
Bothe, Dieter ..... DY 28.3
Bothe, Lucas ..... •DS 20.38
Bothe, Marc ..... •O 95.1, •TT 96.1
Böttcher, Andreas ..... BP 11.1
Böttcher, Artur ..... O 23.2
Böttcher, Florian ..... •DD 30.2
Böttcher, Lukas ..... •O 44.13
Botti, Ermanno ..... •MM 41.5
Botti, S. ..... AKPIK 6.5
Botti, Silvana ..... •MM 5.1, MM 22.3, O 59.6, TT 48.6
Bottomley, Adam ..... O 56.6
Bötzel, Steffen ..... TT 69.7, •TT 69.9
Bouajhine, Mohamed ..... CPP 17.9
Bouatou, Mehdi ..... O 83.6
Bouaziz, J ..... MA 19.7, TT 31.7
Bouaziz, Jordan ..... FM 4.1
Bouaziz, Juba ..... •MA 55.4, O 21.1
Bouaziz, M. ..... O 85.2
Boucher, Richard ..... •MA 39.10
Bouck, Ryan ..... HL 8.6
Boudjenane, Meriem ..... CPP 46.45
Bougammoura, Yasmin ..... •QI 16.8

Bougeard, Dominique ..... TT 73.7
Bouhet, Baptiste .....•BP 9.2
Boukany, Pouyan E. ..... BP 27.7
Boulton, Lewis ..... AKBP 12.4
Bourel, Hippolyte Raymond ... O 85.3
Bourgett, Mirjam .....•UP 2.2
Bournel, F. ..... O 85.2
Bourret, Edith ..... FM 11.34, FM 18.7
Bouss, Peter ..... DY 58.7, SOE 17.7
Bovensiepen, U. ..... MA 7.14
Bovensiepen, Uwe FM 11.31, MA 42.3, •O 16.2, O 59.5, O 71.1, O 71.18, O 84.8, O 98.4, TT 48.5, TT 66.1, TT 66.18, TT 84.8
Bovyn, Matthew J. .....•BP 27.3
Boydas, E.B. ..... AKPIK 6.5
Boydas, Esma ..... MM 22.3
Boyer, Finn Marten .....•AKPIK 5.4
Boyle, Greg .....AKBP 12.4
Bozkurt, A. Mert .....HL 17.4
Bozkurt, Ata .....HL 4.1
Bozkurt, Mert ..... TT 15.3, TT 15.11
Braakman, Floris ..... QI 14.25
Brabec, Christoph .....HL 23.4
Bracht, Hartmut .....MM 35.6
Brackertz, Stefan ..... DD 18.1
Braconnier, Benjamin ..... CPP 21.4
Braden, Markus ..... MA 3.6, MA 3.7, TT 23.13
Bradford, Jonathan .. O 95.6, TT 96.6
Bradforth, Stephen CPP 19.5, DY 20.5
Braicovich, Lucio ..... O 67.10
Braithwaite, Daniel .....TT 2.1
Brambilla, Alberto ..... MA 30.9
Brancolini, Giorgia ..... CPP 29.6
Brand, Christian ..... O 72.1, O 85.5, •O 98.4, TT 2.5, TT 67.1
Brand, Paul ..... DY 28.3
Brandbyge, Mads .... O 74.7, TT 68.7
Brandenbourger, Martin ..... DY 62.8
Brandhoff, Jonas ..... •O 6.8, O 10.7, O 28.3, O 30.2, O 44.14, O 45.3, O 45.8, O 45.11, O 83.2, TT 16.7
Brando, M. ..... TT 5.9
Brando, Manuel .... TT 29.5, TT 52.5
Brandstetter, Dominik ..... •O 69.2
Brandt, Julia .....CPP 3.5
Brandt, Kenneth .....•HL 40.2
Brandt, Martin S. .. HL 26.34, QI 14.10
Brandt, Mike ..... CPP 11.4, DY 17.4, •DY 44.5
Brandt, Oliver ..... DS 4.5, FM 7.8, HL 23.10, HL 24.6, HL 33.4, HL 57.2, HL 57.5
Brandt-Talbot, Agnieszka .. CPP 26.1
Braner, Simon .....•AKBP 4.2
Braniste, Tudor ..HL 20.23, HL 20.24, •HL 26.23
Braß, Martin .....TT 71.6
Brataas, Arne ..... MA 51.5, TT 88.5
Bratschitsch, Rudolf .....CPP 17.46, FM 15.2, HL 20.59, MA 7.7, MA 9.13, MA 12.1, MA 52.5, MA 52.14
Bräu, Susanna .....•QI 21.7
Brauburger, Simon ... BP 7.37, O 13.9
Brauch, A. ..... AKBP 1.1
Bräuer, Torsten ..... O 78.1
Braun, Dieter .....BP 14.19
Braun, Franziska M. ..... CPP 28.3, DY 29.3
Braun, Josephine ..... •HL 26.15
Braun, Matthias .....•CPP 17.40
Brauner, Markus .....•TT 62.1
Brauns, Fridtjof .....•BP 37.10
Brauns, Leon .....HL 8.5, O 40.13, TT 37.13
Braunschweig, Björn ..... CPP 5.3, CPP 17.49, CPP 41.6, CPP 46.32, CPP 46.36, O 25.1
Bravo, Luciano .....DY 60.4
Bréchet, Yves .....•PLV VI
Brede, Jens .....•TT 85.7
Brede, Mariana .....MM 21.8
Bredol, Philipp .....HL 18.4, HL 18.6, •HL 18.7, TT 32.4, TT 32.6, •TT 32.7
Brehm, Lucas ..... BP 14.4
Brehm, Verena .. MA 40.3, •MA 40.4, MA 48.6
Brehms, Xaver ..... CPP 46.45
Breiholz, Benjamin .....•QI 18.6
Breitbach, David ..... MA 9.12
Breitkreiz, Maxim . MA 35.2, TT 40.4, TT 41.10, TT 60.2
Brem, Matthias .....HL 3.8
Brem, Samuel ..... HL 3.7
Bremer, Alice ..... O 34.7
Bremer, Lara .....•TT 23.24
Bremerich, Alice ..... O 71.8, TT 66.8
Brems, Maarten ..... MA 55.8
Brems, Maarten A. ..... MA 21.1
Brendel, Johannes .....FM 4.9
Brendel, Johannes C. .....CPP 46.27
Brendel, Lothar ..... O 33.6
Brenig, Wolfram .....•TT 33.1
Brenneis, Luisa .....•HL 46.4
Brennfleck, Ellen .....•O 27.5
Brenninger, Thomas ..... QI 11.9
Bresges, André ... •DD 28.2, DD 28.4, DD 38.1, DD 41.2
Bressler, Christian . CPP 23.1, DY 24.1
Bresteau, David ..... O 14.1
Brett, C.J. .....MA 7.21
Breuer, Daniel .....•DS 20.32
Breuer, Heinz-Peter .. •TT 18.1, QI 7.6
Breunig, Oliver ..... O 63.9, TT 55.9
Brezina, Krystof ..... •O 9.2, O 61.5
Brida, Daniele .....HL 20.15
Briesenick, Simon .. O 33.2, •O 40.13, •TT 37.13
Brighi, Pietro .....•DY 53.4, •TT 87.4
Brihuega, Iván ..... O 15.1
Brill, Lorenz .. O 6.8, •O 30.2, O 44.14
Brink, Tobias .....•MM 15.5
Brinkamn, Alexander .....TT 6.1
Brinker, Manuel .....•CPP 6.5
Brinker, Theresa ..... MA 39.7
Brinkman, Alexander ..... TT 15.11, TT 41.1, DD 36.3
Brinkman, Stefanie S. ..... MA 24.3, TT 36.3
Brinkman, Stefanie Suzanne ... O 2.1, •O 2.5, O 76.6
Brinkmann, Martin ..... •CPP 17.51
Brinster, Raphael .....•QI 15.2
Brison, J.-P. ..... TT 29.1
Brito, Hermi Felinto ..... BP 33.12
Britton, Callum .....•DY 9.2
Brixner, Tobias .....HL 8.8, HL 26.55, HL 46.4
Brizolla, Gusthavo .....MA 7.45, •MA 35.9, •TT 60.9
Brockmann, Dirk ..... BP 2.6, BP 8.1, BP 8.6, BP 14.69, DY 48.1, SOE 2.3, SOE 2.6, SOE 4.5, •SOE 7.1
Brocorens, Patrick ..... CPP 17.9
Brödner, Kerstin .....CPP 17.6
Broedersz, Chase .....•DY 40.1
Brommer, Peter .....MM 27.5
Bronsch, Wibke ... •CPP 37.5, O 66.7
Brookes, Nicholas B. .....MA 33.11
Brookes, Nick .....MA 52.27
Brooks, Henry .....SOE 2.5
Brosda, Nico Frédéric .....HL 20.41, •HL 26.2
Brosi, Miriam .....AKBP 7.1
Brösigke, Georg ..... DY 41.15
Brouwer, Benedict .....HL 3.9
Brouwer, Piet ..... MA 35.2, TT 41.10, •TT 50.5, TT 60.2
Brouwer, Piet W. ..... MA 27.1
Browne, Leon .....•O 62.9, •TT 54.9
Brucas, Rimantas .....MA 12.6
Bruckhoff, Mike J. MA 13.5, MM 21.8
Bruckmann, Christian .....•DS 11.4
Bruckmeier, L. ..... O 19.10
Bruckmeier, Lukas . O 71.17, TT 66.17
Bruckmoser, Niklas .. TT 28.7, QI 8.3, QI 11.6, •QI 11.9
Bruckner, Florian .. MA 7.41, MA 7.44, MA 55.6, MA 58.2
Brückner, Max .....•TT 5.6
Brückner, Sebastian ..... AKPIK 6.3
Bruder, Enrico .... MA 50.5, MM 23.5
Bruggesser, Tobias .....•HL 20.37, HL 20.42
Brugues, Jan .....•SYGF 1.2, BP 10.3, BP 10.4, CPP 18.3, CPP 18.4, DY 18.3, DY 18.4
Brummel, Olaf ..... O 13.12, O 65.12
Brun, Boris ..... TT 82.1, QI 2.10
Brunander, Hampus .....•QI 14.14
Bründermann, Erik ..... AKBP 4.2, •AKBP 12.1
Brune, Harald .....O 99.11
Brune, Oliver .....HL 33.5, •HL 42.3, HL 42.5
Brünig, Florian .....•CPP 9.3
Brunkhorst, Nora .....MM 39.2
Brunner, Daniel ..... AKPIK 3.4
Brunner, Dominik .....•UP 3.1
Brunner, Michael ..... BP 18.3
Bruno, Alessandro ..... QI 20.8
Bruno, Vincenzo ..•DY 59.9, •TT 99.9
Bruß, Dagmar ..... QI 10.10, QI 14.9, QI 15.2, QI 18.4, QI 18.8
Bruschi, David Edward .....•QI 10.1
Brütting, Fabian .. HL 26.50, HL 45.4, HL 45.5
Brütting, Wolfgang .....CPP 48.3
Buba, Jonas .....•CPP 11.3, •DY 17.3
Bubis, Anton V. ..... TT 28.11
Bucci, Giada .....HL 20.34
Buchberger, Sebastian .....O 76.7
Bucher, Dominik .....•BP 33.11
Bucher, Dominik B. .....HL 26.34
Bucher, Jean-Pierre .....O 9.4
Bucher, Tobias .....•DS 16.7, DS 20.8
Buchhold, Michael . DY 42.5, DY 46.1, DY 46.2, TT 63.5, TT 75.1, TT 75.2
Buchholtz, Stephanie ..... CPP 57.1
Buchhorn, Jonas .....•TT 74.3
Buchleitner, Andreas .....DD 17.1
Büchner, Bernd .... MA 6.3, MA 7.28, MA 7.37, MA 13.1, MA 17.4, MA 33.8, MA 36.12, MM 40.4, O 2.3, O 63.2, TT 4.9, TT 5.7, TT 11.1, TT 11.2, TT 11.3, TT 11.4, TT 40.3, TT 55.2, TT 57.1, TT 79.5, TT 92.3, TT 93.3, TT 93.5, TT 93.10, TT 93.14
Buchner, Carlotta ..... MM 40.7
Buchta, Maximilian ..... DS 20.38
Buck, Jens .. MA 24.3, O 7.5, O 71.17, TT 9.5, TT 36.3, TT 66.17
Budaraju, Sasank •MA 19.11, •TT 31.11
Budde, Thea ..... QI 3.4
Budhiraja, Amarjit ..... DY 7.3
Budich, Jan .....DY 47.7, TT 10.4
Budich, Jan Carl ... DY 46.8, TT 75.8, TT 83.7, QI 9.1
Budnyk, Andriy .....FM 19.3
Bueble, Joschua .....DS 20.44
Bugase, Jonas .. CPP 30.2, •MA 36.5
Buhot, Jonathan ..... TT 80.3
Bui Thi, Yana .....•CPP 37.3
Buiarelli, Luca ..... MA 8.8
Bukas, Vanessa J. .... O 13.2, O 24.3, O 81.3, •O 97.1, O 97.11
Bukov, Marin ..... TT 51.2
Bulchandani, Vir B. ... TT 17.6, QI 4.6
Bulgakov, Michael ..... CPP 57.5
Büll, Alexander Kai ..... DY 44.19
Bull, C. L. ..... CPP 32.3, DY 35.3
Bullinger, Thomas .....•CPP 17.31
Bulsara, Yashvi .•HL 20.21, •HL 26.47
Bulut, Nebahat ... MM 3.9, MM 19.33, •MM 19.34, MM 19.46, O 74.2, O 74.3, TT 68.2, TT 68.3
Bulut, Yusuf ..... CPP 46.17
Bunch, David .. QI 8.3, QI 11.6, QI 11.9
Bünermann, Oliver ..... O 11.2
Bunney, Matthew .•TT 29.7, TT 56.12
Bünte, Judith .. •CPP 46.14, MA 7.62, MA 7.63
Bunz, Uwe H. F. ..... CPP 17.6
Buonemani, Francesco ..... •TT 15.7
Burde, Jan-Philipp .. DD 13.2, DD 19.1, DD 24.1, DD 27.7
Burdinski, Angelique .....•BP 2.6
Burduli, Luka ..... DY 62.5
Bureau, Lionel .... BP 11.6, CPP 26.5, CPP 31.6
Bureau, Matilde ...CPP 20.9, DY 23.9
Burgdörfer, Joachim ..... O 93.1
Bürgel, Jan Lukas .....•FM 6.7
Bürger, Justin .....AKPIK 5.5
Burger, Kay .....•JOB 2.3
Burger, Ludwig ... BP 14.53, •BP 15.8
Burghammer, Manfred ..... BP 14.30
Burgholzer, Katharina ..... HL 54.4
Burgstaller, Anna ... BP 16.4, BP 40.2
Burgwal, Roel ..... O 89.4
Buriks, Manuel ..... O 86.7
Burioni, Raffaella .....•DY 7.1, DY 7.2
Burkard, Guido .....•TT 24.4, QI 6.6, QI 6.8, QI 8.4, QI 9.6
Burkard, Ruben .....•TT 33.6
Burkhardt, Lea Mareike ..... DD 31.1
Burkhardt, U. ..... TT 5.9
Burkhardt, Ulrich .. MA 2.6, MM 40.3, O 84.5, TT 5.8, TT 42.12, TT 84.5
Burkholz, Rebekka DY 45.4, SOE 14.4
Burla, Aditya .....•MM 35.6
Burnet, Anton .....DY 43.16
Burnet, Anton Francis .....•DY 43.17
Burrello, Michele ..... TT 73.12
Burset, Pablo .....TT 6.2, TT 15.8, TT 42.11
Burshtein, Amir ..... QI 2.3
Buß, Lars ... •O 10.3, O 84.6, O 88.10, •TT 16.3, TT 84.6
Busby, Oliver ..... TT 62.7
Busch, Kurt ..... O 44.12
Busch, Oliver ..... MA 38.11
Busch, Wibke ..... BP 7.34
Buschbeck, Robin .•FM 14.1, FM 18.3
Büscher, Florian ..... MA 40.8
Bushev, Pavel ..... TT 93.6, QI 8.5
Bushev, Pavel A. ..... QI 6.9
Busse, Arne .....HL 33.2, HL 33.3
Busse, Carsten ..... O 71.8, •O 95.3, TT 66.8, •TT 96.3
Busse, Lena .....•DD 24.2
Bussetti, Gianlorenzo ..... O 60.3
Bussmann, Michael .....AKBP 6.5, AKBP 7.3, AKBP 8.8, AKBP 10.1, AKBP 10.3, AKBP 11.3, AKBP 12.5
Bustamante Lopez, Daniel •MA 40.3, MA 40.4
But, Dmytro B. ..... HL 52.2
Butcher, Tim .....MA 7.67
Butcher, Tim A. .....•DS 6.1, MA 7.81
Butler, Paul .....•DS 11.1
Butscher, Julian F. .....HL 15.7
Butt, Friederike .....•QI 16.1
Butt, Hans-Jürgen . CPP 5.1, CPP 8.5, CPP 27.4, DY 26.4
Butterling, Maik .....DS 20.22
Buttersack, Tillmann ..... •CPP 19.5, CPP 23.2, CPP 27.3, •DY 20.5, DY 24.2, DY 26.3
Büttgen, Norbert ... MA 31.2, TT 47.2
Buttinoni, Ivo .....DY 62.3
Buttkus, Paul .....•BP 14.69
Büttner, Felix ..... HL 38.8, MA 7.35, MA 7.40, MA 16.3, MA 37.8
Büttner, Simon .....HL 26.55
Butz, Vera .....•TT 23.32
Butzke, Julia ..... •BP 7.45, BP 7.46
Buyan-Arivjikh, Altantulga •CPP 44.3, CPP 48.2, CPP 59.3
Buzdakov, Aleksandr ..... MA 27.6, •MA 30.3
Buzzi, Alessandro .....HL 34.4
Byczuk, Krzysztof ..... DY 47.9
Bykov, E. ..MA 18.1, MA 18.5, TT 30.1, TT 30.5
C. Althorpe, Stuart .....DY 14.10
C.Ganguli, Somesh ..... TT 56.13
C. Gerber, Iann ..... DS 12.8
C. Hövelmann, Svenja ..... CPP 27.2, DY 26.2
C. Inácio, João .....•TT 86.4
C. Rhodes, Luke .....O 80.3
Cabala, Andrej ..... TT 93.17
Cabrera Aguilar, Ariel Moises •HL 49.4
Caceres, Joan ..... TT 50.6
Caetano, Frédérick CPP 20.9, DY 23.9
Caglieris, Federico ..... MM 40.4
Cahen, D. ..... HL 54.12
Cahen, David .....HL 46.2
Cahlik, Ales .....O 59.7, TT 48.7
Cakaj, Albin ..... CPP 48.3
Calabrese, Justin .. BP 32.9, DY 52.9
Calandra Buonaura, Matteo MM 15.2
Calandra, Matteo ...HL 8.2, •HL 46.7, MA 33.12, TT 49.4
Calarco, Tommaso ...QI 10.6, QI 16.5
Calcinelli, Fabio ..... O 58.7
Caldwell, J. D. ..... O 57.6
Callahan-Coray, Kevin ..... MA 30.2
Calloni, Alberto .....•O 60.3
Călugăru, Dumitru ..... TT 74.1
Calzado, Carmen J. ..... O 9.4
Camacho, Daniela .....MM 3.6
Camacho, Gonzalo ....•QI 3.6, QI 3.8
Camarasa-Gómez, María ... HL 24.8, HL 39.10, •O 47.4
Camerano, Luigi .....•MA 17.5
Camilli, Francesco DY 58.9, SOE 17.9
Cammann, Jan .....•DY 62.5
Cammarota, Chiara ..... AKPIK 2.2
Camp, Philip J. ..... CPP 24.3
Campbell, Aidan ...•TUT 1.3, •FM 1.3, HL 33.4, HL 40.8, HL 57.5
Campbell, Aidan F. ... TUT 1.1, FM 1.1
Campbell, Steven ..... TT 90.5
Campi, Davide .... MM 17.4, MM 41.5
Campos, Leonardo .....HL 47.2
Campos, Leonardo C. O 95.2, TT 96.2
Campos, Luis M. ..... TT 90.6
Campos, Warlley ..... MA 47.6
Campos, Warlley H. .....•MA 54.6
Camposs Jara, Sergi ..... O 34.5

Camps, A. ..... MA 25.6
Camsari, Kerem Y. ..... MA 30.2
Camuti Borani, Alessia ..... •QI 10.6
Cancado, Luiz G. .... O 95.2, TT 96.2
Canero Infante, Ingrid ..... FM 4.1
Caneva, Sabina ..... BP 9.1
Canfield, Paul ..... TT 95.6
Cangi, Attila ..... FM 11.10, MM 22.7
Canhassi, Carlos ..... MA 13.8
Cano Gutiérrez, Carlos ..... QI 14.19
Canola, Sofia ..... O 12.6, O 43.13
Cañón Bermúdez, Gilbert Santiago MA 49.1
Cantarella, Arianna ..... MM 13.9
Cantele, Giovanni ..... O 7.7, TT 9.7
Cao, H ..... MA 19.7, TT 31.7
Cao, L. ..... MA 3.8
Cao, Shixun ..... MA 47.9
Cao, Tianyi ..... •BP 14.31, BP 37.4
Cao, Xiao-Yu ..... HL 31.4
Cao, Xin ..... DS 20.21
Cao, Yunjun ..... •O 8.3
Capa Salinas, Andrea ..... TT 57.9
Capalbo, D. ..... DS 3.4
Capalbo, David ..... •O 19.2, O 93.2
Capista, Daniele ..... HL 23.3
Capone, Massimo .. TT 10.2, TT 13.2, TT 13.9, TT 95.5
Capotondi, F. ..... MA 25.6
Caprini, Lorenzo ... CPP 11.5, DY 17.5, DY 49.9
Car, Diana ..... HL 20.40
Caracciolo di Torella, Pietro . DY 33.6
Caratti, Davide ..... HL 46.2
Carbogno, C. ..... O 57.6
Carbogno, Christian . DY 14.8, FM 5.7, MM 5.4, •MM 12.5, MM 13.7, O 96.8
Carbonell, Carmen Gómez .. MA 7.46
Carde, Leon ..... •QI 17.7
Cardenas-Gamboa, Jorge .. •HL 8.11, O 63.4, TT 55.4
Cárdenas-López, Francisco ... QI 8.2, QI 8.5, QI 8.6, QI 11.3, •QI 13.4, QI 16.5, QI 17.6
Cárdenas-López, Francisco Andrés QI 13.10
Cardoletti, Juliette .. DS 11.6, DS 13.3
Cardoso, Claudia .. •MM 37.4, O 84.7, TT 84.7
Cardoso-Gil, Raul ..... MM 19.46
Caretta, Lucas ..... MA 16.3
Carini, G. ..... •O 57.6
Carini, Giulia ..... O 96.8
Cario, Laurent ..... TT 49.4
Carlson, Shane ..... O 87.3
Carmesin, Hans-Otto ..... •DY 60.9, •DD 5.2
Carmona Almazán, Juan Pablo •BP 11.4
Caroca-Canales, Nubia ..... TT 25.7
Carpene, Ettore ..... TT 49.7
Carpenter, Michael ..... FM 12.10
Carrasco, Rigo A. ..... DS 21.3
Carrasco, Roberto ..... O 15.1
Carrasco Salas, Yeraldinne .. BP 11.6
Carrasquilla, Juan . DY 58.1, SOE 17.1
Carreck, Amber ..... TT 22.17
Carrez, Philippe ..... MM 23.5
Carrillo-Aravena, Eduardo .. FM 22.5, MA 7.2
Carrio, Baptiste ..... BP 41.1
Carro, Pilar ..... O 96.10
Carstens, Finn-Ole ..... AKBP 10.1, AKBP 10.2, AKBP 10.3, •AKBP 12.5
Carstens, Frederik Leon ... •MA 31.5, •TT 47.5
Cartarius, Holger .... DD 7.3, DD 17.2, DD 20.4, DD 21.2, DD 30.9
Cartwright, Elin ..... DS 3.3
Caruso, Fabio ..... HL 8.9, HL 46.5, O 84.11, •O 98.1, O 98.2, TT 84.11
Carva, Karel ..... HL 39.1
Carvalho, Miguel M. F. ..... •MA 19.5, •TT 31.5
Carvallo, Claire .... CPP 20.7, DY 23.7
Casadiego, Jose .. DY 51.4, SOE 15.4
Casagrande, Luca ..... •DY 49.4
Caselle, Michele ..... AKBP 4.2
Casey, Andrew ..... TT 22.17
Caspari, Verena ..... •TT 73.3
Cassabois, Guillaume O 95.6, TT 96.6
Cassina, Silvia ..... QI 18.1
Cassol, Francesco TT 23.16, •TT 81.4
Castellanos-Reyes, Jose Angel MA 30.6
Castelli, Ivano E. ..... MM 5.2
Castelli, Ivano Eligio ..... MM 8.4
Castelnovo, Claudio ..... MA 31.12, TT 47.12
Castillo Robles, José Maria . MM 8.4
Castro, Jorge ..... •O 61.5
Castro, Túlio de .... MA 27.2, O 40.11, TT 37.11
Castro, Túlio H. L. G. ..... O 38.4
Casu, M. Benedetta ..... O 6.7
Catalan, Gustau ..... FM 18.2
Catalan, Rodrigo ... BP 7.28, BP 7.29
Catarina, Gonçalo .... MA 5.9, TT 7.9
Catelani, Gianluigi ..... QI 11.8
Cates, Michael ..... DY 15.7
Caupin, Frédéric •CPP 27.5, •DY 26.5
Cavagna, Andrea ..... •SOE 2.2
Cavalcanti-Adam, Ada ..... BP 7.29
Cavalleri, A. ..... MA 4.4
Cavalleri, Andrea ..... •PRV I, MA 4.3
Cavanaugh, Kate E. ..... BP 3.11
Ćavar, Lukas D. ..... •MA 37.2
Caviezel, Andrin . MA 7.32, •MA 27.9, O 98.2
Cayao, Jorge ..... TT 56.4, •TT 98.5
Ceccardi, Michele . •MM 40.4, TT 11.1
Čechal, Jan O 6.1, O 6.3, O 8.2, O 69.1
Celebi, Alper T. ..... O 22.4, O 87.5
Celebi, Alper Tunga ..... O 30.3
Çelik, Hüseyin ..... FM 15.1
Cerchez, Mihai ..... HL 20.54
Cerchez, Mirela ..... BP 14.47
Cerdin, Tristan ... •CPP 11.6, •DY 17.6
Ceriotti, Michele ... CPP 9.7, MM 9.2, MM 9.8, MM 17.3
Černý, Miroslav .. MM 16.6, •MM 16.7
Cerqueira, Tiago F. T. ..... FM 6.6
Cerullo, Giulio ..... HL 20.15
Cervantes Villanueva, Jorge . •HL 8.3
Cervantes-Villanueva, Jorge .. O 59.3, TT 48.3
Cervellera, Luca ..... •TT 42.3
Cesa, Francesco ..... QI 3.10
Çetin, Mahmut ..... TT 22.12
Çeven, Kadir ..... •TT 23.29
Cezar De Campos Ferreira, Rodrigo O 43.17
Chabaud, Baptiste ..... CPP 31.6
Chae, Jungseok ..... O 15.11
Chagas, Thais ..... O 95.3, TT 96.3
Chagua Encarnacion, Kennedy BP 11.6
Chahar, Preeti ..... O 58.3
Chahine, Karim ..... DY 46.1, TT 75.1
Chahshouri, Fatemeh ..... •QI 2.5
Chai, De Min ..... TT 69.1
Chai, Misha ..... •DY 48.2
Chaitram, Aparna ..... •O 23.7
Chajewski, Grzegorz ..... TT 29.5
Chakrabarti, Amitabha ..... DY 60.1
Chakrabarti, Rajarshi ..... BP 20.5
Chakrabartty, Dola MA 7.35, •MA 16.5
Chakraborti, Neelanjan ..... MA 2.2
Chakraborti, Subhadip ..... •DY 33.3
Chakraborty, Ahana ..... TT 43.12
Chakraborty, Arijit ..... DS 20.21, HL 20.45, HL 20.51, HL 55.10
Chakraborty, Atasi ..... •MA 20.6
Chakraborty, Nilotpal •DY 2.3, •TT 1.3
Chakraborty, Papri ..... O 23.2
Chakraborty, Sourav ..... MA 7.84
Chakraborty, Subhadip ..... •DY 42.9, •TT 63.9
Chakraborty, Sudip . MM 8.6, MM 12.1
Chalker, John ..... DY 46.7, TT 75.7
Champain, Victor ..... QI 2.10
Chan, Brian ..... BP 35.1, CPP 51.1
Chan, Edmond ..... TT 57.2
chan, yute ..... MM 19.11
Chandola, Sandhya . •O 13.11, O 58.3, O 86.6, O 86.8
Chandra, Manabendra .... CPP 17.47, O 10.4, TT 16.4
Chandra, Sushmita ..... •MM 30.6, TT 49.2, TT 57.10, TT 93.15
Chandrakant Palekar, Chirag . HL 55.1
Chandran, Anushya •DY 2.2, DY 53.3, •TT 1.2, TT 87.3, QI 3.11
Chandran, Hrisheekesh Thachoth CPP 40.6
Chandrashekhar, Prathibha •MM 37.5
Chandratre, Chinmay Pradeep •DY 7.9
Chandratre, Prerana ..... •AKPIK 5.5
Chaney, Daniel ..... FM 12.11
Chang, Ching-Hao ..... HL 20.55, •HL 29.1, •TT 58.1
Chang, Chun F. ..... MA 19.5, TT 31.5
Chang, Chun-Fu ..... O 84.5, TT 3.2, TT 3.3, TT 25.2, TT 84.5
Chang, Hung-Tzu ..... MA 27.3
Chang, Li-Wei ..... TT 22.12, •TT 43.5
Chang, Shan-Fu ..... TT 93.8
Chang, Wei-Che ..... •MM 3.2
Chang, Yen-Yu AKBP 10.1, AKBP 11.3, AKBP 11.4, AKBP 13.3
Chang, Young Jun ... •O 71.9, O 71.15, •TT 66.9, TT 66.15
Chang, Yu-Chuan ..... BP 14.38
Changdar, Susmita ..... O 2.3, TT 5.7
Changiarath, Arya ..... CPP 17.4
Chaou, Adam ..... TT 50.5
Chaou, Adam Yanis TT 41.10, TT 74.8
Chaoui, Ziad ..... •QI 18.9
Chapoulie, Rémy ..... MM 18.6
Chaput, Laurent ..... HL 23.9
Charilaou, Michalis ..... MA 38.10
Charlafti, Evgenia ..... O 88.9
Charry, Jorge ..... BP 2.10
Charyton, Marek K ..... CPP 17.11
Chassot, Frédéric ..... O 67.6
Chaté, Hugues ..... •PLV VII
Chatterjee, Pallabi ..... •DY 47.8
Chatterjee, Ratnamala ..... MA 7.26
Chatterjee, Sangam DS 11.7, HL 23.8, HL 26.3, HL 26.28, HL 42.2, HL 45.3
Chatterjee, Sidhartha ..... •MA 52.15
Chatterjee, Snehashish ..... TT 49.5
Chatterjee, Sreya ..... •BP 14.9
Chatterjee, Swarnajit ..... CPP 11.1, DY 17.1
Chatterji, Apratim ..... BP 2.1
Chattopadhyay, Jayeeta .. •CPP 10.9, •DY 16.9
Chattopadhyay, S. ..... TT 24.7
Chattopadhyay, Shirsopratim •TT 40.2
Chaturvedi, Raghav ..... •TT 83.3
Chaturvedi, Shaswat ..... TT 22.4
Chatzichrysafis, Dimos ... •MA 39.23
Chatzieleftheriou, Maria .... •TT 98.3
Chatzigiannakis, Georgios .. •DS 16.2
Chatzittofi, Michalis ..... •DY 15.7
Chaudhary, Shivam ..... BP 15.9
Chaudhary, Vikrant ..... •FM 6.4
Chaudhry, Nishtha ..... •TT 22.9
Chauhan, Amit ..... •TT 13.5
Chauhan, Deepanshu ..... MA 42.6
Chauveau, Jean-michel ..... HL 55.11
Chavarría-Vidal, Martín .... •CPP 41.3
Chaves, Rafael ..... QI 12.6
Chavez, Elvia ..... FM 11.4
Che Abdullah, Che Azurahanim BP 7.1
Cheeran, Sheba ..... BP 2.3
Chekhonin, Paul ... HL 40.5, MM 11.2
Chen, Caiyun ..... •O 12.11
Chen, Chien-Te ..... TT 25.2
Chen, Dong ..... TT 57.7
Chen, Guangze ..... MA 5.9, TT 7.9
Chen, Hao ..... •MM 26.3
Chen, Hongxuan ..... MM 31.2
Chen, Hsiao-Yi ..... O 7.2, TT 9.2
Chen, Hua ..... MA 23.2, TT 35.2
Chen, Jianhan ..... BP 39.1, CPP 55.1
Chen, Jiasheng .... TT 29.11, TT 95.7
Chen, Kaiwen ..... •MM 19.49
Chen, Kaiyuan ..... HL 13.5
Chen, Letien ..... CPP 11.9, DY 17.9
Chen, Li ..... •CPP 7.1, O 12.3
Chen, Lin ..... DS 20.17, TT 74.12
Chen, Rong ..... TT 61.4
Chen, Sheng H. ..... MA 19.5, TT 31.5
Chen, Sheng-Huai ... O 84.5, •TT 3.3, TT 84.5
Chen, Shouzheng ..... •CPP 58.2
Chen, Shuai ..... MM 19.16
Chen, Shuang ..... O 55.6
Chen, Shuxia ..... •O 43.5
Chen, Tawat ..... •HL 20.16
Chen, Tianzhe ..... O 84.9, TT 84.9
Chen, Wei ..... TT 29.12, TT 95.3
Chen, Wei-Tin .... MA 31.10, TT 47.10
Chen, Wenhan ..... •MA 58.6
Chen, Xi ..... •BP 29.5, •CPP 45.5, TT 95.3, QI 13.4
Chen, Xiang ..... AKBP 10.4
Chen, Xiao ..... HL 35.5
Chen, Xiaowen ..... MA 16.9
Chen, Xingsen ..... •TT 85.1
Chen, Xinren ..... MA 50.4
Chen, Xinxiang ..... •CPP 58.3
Chen, Yi-Hsun ..... O 48.6
Chen, Ying-Jiun ..... MA 5.7, TT 7.7
Chen, Yitong ..... HL 42.4
Chen, Yong P. ..... TT 72.8
Chen, Z. ..... HL 37.2
Chen, Zekai ..... MA 24.2, •TT 25.3, TT 33.3, TT 36.2
Chen, Zhuo ..... CPP 46.42
Chen, Zhuohui ..... HL 57.2
Cheng, Bowen ..... •CPP 46.66
Cheng, Jinguang ..... TT 93.11
Cheng, Li ..... •MA 39.4
Cheng, Lyuyang .. CPP 4.6, CPP 12.4, CPP 16.2, CPP 17.15, •CPP 17.27, CPP 17.42
Cheng, Po-Yuan ..... TT 2.1, •TT 93.8
Cheng, Shangjun •BP 14.33, BP 14.37, BP 14.45
Cheng, Xinle ..... •O 49.5, O 79.1
Cheng, Yajun .... CPP 4.6, CPP 17.26, CPP 17.27, CPP 17.32
Cheng, Yu-An ..... HL 20.55
Chennur, Madhuri HL 20.46, •HL 47.3
Cheong, Kijoon ..... DS 20.24
Cheong, S-W ..... MA 19.7, TT 31.7
Cherepanov, Vasily ... O 41.4, O 54.3, TT 38.4
Chergui, Majed ..... HL 8.10
Cherif, Chokri ..... FM 19.4
Cherifi-Hertel, Salia ..... •FM 12.1
Cherkasskii, Mikhail ..... MA 12.3
Cherkouk, Charaf ..... CPP 17.36
Chernikov, Alexey ..... HL 3.7
Cherniukh, Ihor ..... HL 20.49
Chernov, S. .. O 19.10, O 59.2, TT 48.2
Chernov, Sergii ..... DS 20.41, O 42.9, TT 14.4, QI 6.5
Cheruvary, Karthik ..... DY 7.10
Chervanyov, Alexander .... •CPP 39.6
Chervinskaya, Anastasia .. •BP 36.11, •DY 57.11
Cheung, Cheuk Kit .. •QI 13.5, QI 20.3, QI 20.4
Cheung, Christopher Tat Shun •O 95.10, •TT 96.10
Chhallare, Piyush ..... TT 72.4
Chiang, Cheng-Tien .. O 40.9, TT 37.9
Chiang, Wanchung ..... CPP 26.5, CPP 31.6
Chiappisi, Leonardo ..... CPP 46.31
Chiatti, Olivio ..... HL 23.6, •TT 5.5
Chigrin, Dmitry ..... O 26.1
Chikita, Kazuhisa A. ..... UP 7.1
Chilakalapudi, Prabhath ... •MM 13.4
Chinnakanna Muruga, Lokesh •DY 21.11
Chiodo, Letizia ..... O 58.3
Chioncel, Liviu .... MM 41.8, •TT 81.2
Chiravuri, A. ..... BP 27.8, BP 37.2
Chirkov, Valerii ..... SOE 9.5
Chishti, Shahrukh ..... •QI 17.6
Chitra, Rama ..... DY 60.6
Chiu, Chi-cheng ..... BP 14.60
Chiu, Ching-Hung ..... •DS 14.7
Chiu, Wei-Sheng .... •MA 5.7, •TT 7.7
Chlan, Vojtěch ..... MA 7.30
Chmeruk, Artem ..... •MM 41.8
Cho, Doohee ..... TT 4.10, TT 78.5
Cho, Franklin H. ..... O 89.10
Cho, H.K. ..... HL 37.6
Cho, Hyeyeon ..... •FM 11.3
Cho, Po-Yu ... O 84.5, TT 3.3, TT 84.5
Cho, Sangeun ..... HL 36.4
Cho, Woonghee ..... MA 43.5
Cho, Yongjin ..... HL 33.1
Chobanyan, Ani ..... MA 36.2
Chodkiewicz, M. .. CPP 32.3, DY 35.3
Chodyra, Paulina ... •O 71.7, •TT 66.7
Choi, Dasom ..... •O 15.6, O 15.9
Choi, Duk-Yong ..... DS 16.8
Choi, Eun Sang ..... TT 72.4
Choi, Hyeji ..... •O 45.7
Choi, Jiwon .... •CPP 11.12, •DY 17.12
Choi, Kwang-Yong ..... TT 72.7
Choi, Luca ..... HL 35.1
Choi, Luca S. M. ..... HL 40.6
Choi, Luca Sung-Min ..... HL 55.11
Choi, Myunil ..... MA 20.5
Choi, Pyuck-Pa ..... MM 36.1
Choi, Wonjune ..... TT 33.5
choi, woojae ..... TT 25.11
Choi, Yoonji ..... MM 15.5
Choi, Young-Gwan MA 6.12, MA 58.2, TT 40.1, TT 40.3, TT 92.3
Chong, Yan Meng ..... DY 6.6
Chong, Yan-Meng ..... •FM 12.4
Choorikkat, Sreehari ..... •BP 14.6
Chopdekar, Rajesh V. ..... HL 8.10

Chorkendorff, Ib ..... O 88.4
Choubey, Peayush ..... TT 22.4
Choudhary, Ankita ..... DS 20.21, •HL 20.50, HL 20.51
Choudhary, Monika .....•DS 14.8
Choudhary, Shraddha ..... MA 9.13, MA 52.5, MA 52.14
Choudhury, Asha Rani .....•BP 20.5
Choudhury, Tanushree ..... HL 24.4
Chow, Weng .....HL 54.11
Chowdhury, Awsaf .....MA 7.47
Chowdhury, Rajeswari Roy .. MA 11.5, TT 21.5
Chowdhury, Sourav ..... DS 20.41, •MA 7.67, MA 39.18
Christ, Lisa-Marie ..... DD 15.3
Christen, J. .....HL 37.2, HL 37.6
Christensen, Oliver ..... O 88.8
Christian, Dickel .....•QI 11.8
Christianen, Arthur ..... HL 13.4
Christis, Maximilian .....•HL 12.2
Christodoulides, Demetrios N. DY 48.6
Christova, Darinka ..... DS 20.3
Chrysostomou, Varvara .. CPP 46.26
Chryssos, Leon .....MM 7.7
Chshiev, Mairbek ... MA 51.3, TT 88.3
Chu, Hao .....TT 14.8
Chu, Hyunwon ..... FM 10.3
Chu, Yiwen .....QI 3.4
Chuang, Feng-Chuan . MA 5.7, TT 7.7
Chudak, Maciej ..... DY 9.1, •DY 27.5
Chudzinski, Piotr ..... O 8.5
Chulist, Robert ..... MM 7.9
Chulkov, Ruslan ... MA 24.4, TT 36.4
Chulliparambil Shaju, Sandra •MA 37.3
Chumak, Andrii ..... MA 9.9
Chumak, Andrii V. ..... MA 48.2
Chumakov, Andrei ..... CPP 46.64, •MA 7.21
Churkin, Lev .....•HL 20.62
Chusnutdinow, Sergij ..... HL 26.45
Ci, Xiaojing ..... CPP 44.2, CPP 44.5, •CPP 48.2, CPP 53.6, CPP 59.3
Ciandrini, Luca ..... BP 15.2, BP 32.4, DY 52.4
Ciani, Alessandro .... QI 3.9, •QI 13.6, QI 16.4
Ciccacci, Franco ..... O 60.3
Cichocki, Bogdan ..... CPP 10.10, DY 16.10, DY 34.4, DY 34.5
Cichoň, Stanislav .....DS 7.5
Cichos, Frank ..... BP 14.46, BP 33.8, CPP 10.13, DY 14.7, DY 16.13, DY 44.19, DY 62.4, O 13.9, O 22.6
Cicuta, Pietro ..... BP 5.2
Cigarini, Luigi .....•DS 7.2
Cihan, Ebru .... O 6.5, O 45.5, O 58.4, •O 87.4
Cilento, Federico ... CPP 37.5, O 66.7
Cimbir, Cătălin .....DS 20.29
Cinchetti, Mirko .... MA 30.9, O 64.4, O 69.6, O 71.3, O 83.6, O 84.4, TT 66.3, TT 84.4
Cindrak, Saud .....•QI 10.4
Ciobanu, Alexandru ..... •DY 43.9
Ciobanu, Vladimir ..... •HL 20.23, •HL 20.24, HL 26.23
Ciola, Riccardo .....•MA 9.1
Čípek, Petr ..... MM 8.10
Cipelletti, Luca .... CPP 35.2, DY 37.2
Cipriano Marcos, Luis Antonio O 88.8
Cirelli, Claudio .....BP 9.6
Cirillo, Carla ..... TT 5.4
Cirkel, Jasper ..... DD 25.3
Cisternas, Marcelo ..... BP 5.3
Citro, Roberta ..... DY 59.9, TT 99.9
Ciubotaru, Florin ..... MA 48.9
Claessen, R. ..... O 59.2, TT 48.2
Claessen, Ralph .. DS 14.3, DS 20.43, O 8.5, O 63.5, O 63.8, O 74.4, TT 55.5, TT 55.8, TT 68.4
Claeys, Pieter ..... DY 46.6, TT 75.6, QI 3.11
Claeys, Pieter W. ... DY 32.5, TT 45.5
Classen, Laura TT 2.7, TT 2.8, TT 41.3
Clausen, Kai Uwe ..... O 83.8
Claussen, Jens Christian ... •SOE 2.5
Clémence, Maël .....TT 62.6
Clemens, Helmut ..... MM 17.1
Clowes, Steven K. ..... HL 11.6
Coasne, Benoit ...•CPP 3.1, CPP 21.4
Cobet, Christoph .....MM 19.20
Cobos, Jesús ..... QI 3.1
Cocchi, Caterina CPP 22.4, CPP 26.2, HL 1.6, HL 1.8, HL 20.14, HL 26.25, HL 54.1, O 10.6, O 98.7, TT 16.6
Cochi, Caterina ..... CPP 22.2
Coehoorn, Reinder ..... HL 15.5
Coghi, Francesco .....•DY 7.3
Cohen, Joachim .....QI 17.7
Cohen Miles, Adam .....•FM 5.8
Cohen, Reuven ..... DY 47.2
Cohen, Ronald E. .....FM 4.3
Coiteux-Roy, Xavier ..... DY 47.11
Cojocariu, Iulia . O 9.1, O 10.3, O 83.6, O 88.10, TT 16.3
Colangelo, Francesco ..... TT 5.4
Colazzo, Luciano .....O 89.10
Colell, Noah .....•MM 19.29
Coletti, Camilla .....O 98.9
Colina Araujo, Enrique .....•BP 12.6
Colire, Owen .....•TT 23.16
Colla, Alessandra .....•QI 7.4, QI 7.6
Collazo, Luciano .....MA 49.8
Colling, Maurice .....•MA 37.6
Colnaghi, Timoteo ..... MA 58.1
Colombi Manzi, Emanuel ..... O 34.1, •O 81.3
Colonna, Nicola ..... MM 17.5
Comin, Riccardo ..... HL 24.10
Comizzoli, Samuele ..... O 67.10
Commeto, F. ..... TT 74.5
Compagnie, Arnaud .....•DY 62.3
Conboy, James P. .....•BP 27.7
Confalone, Tommaso ..... TT 4.11, •TT 73.11
Cong, Zugeng .....•CPP 46.36
Connolly, Malcolm R. ..... QI 11.7
Connolly, Thomas .....QI 6.10
Conquest, Oliver .....•MM 14.1
Conquest, Oliver J. ..... FM 23.2
Conradi, Maximilian .....•CPP 38.6
Conrads, Lukas .....O 26.5, O 57.5, O 96.4, •O 96.9, O 96.11
Consiglio, Armando ..... •MA 47.2
Constantino, Sara .....•SYTP 1.1
Constantinou, Anna P. .... CPP 46.12
Constantinou, Procopios C. .. O 42.9
Constien, Leonard .....•BP 14.68
Conti, Andrea ... O 5.6, O 55.4, O 80.1
Contreras, Max .....•SOE 8.2
Contreras-Payares, Alexander O 23.3
Coogan, Katrina .....FM 15.1
Coolen, Anthony .. DY 45.3, SOE 14.3
Coquinot, Baptiste ..... O 54.4
Cora, Ildikó .....DS 6.4
Cordes, Thorben ..... BP 20.8
Cordier, Andreas .....•DS 20.48
Cordier, Patrick ..... MM 23.3
Cordiez, Justine .....TT 49.4
Corona, Domenico ..... O 58.3
Corral Sertal, Javier ..... DS 12.6, •MA 7.85
Corrales, Tomas .. BP 26.1, CPP 43.1
Corrales, Tomas P. ..... •CPP 33.4, CPP 41.3, CPP 41.5, O 56.7
Correa, Victor Felix ..... TT 11.3
Correa-Puerta, Jonathan ..... O 67.3
Corredor, Laura T. •MA 3.3, MA 39.19, MA 52.35, TT 5.7
Corsaletti Filho, José Claudio MA 6.12, MA 7.79, •MA 42.11
Cortés, Diego .....CPP 33.4
Cortes, Emiliano .... DS 12.3, O 96.10
Cortés-del Río, Eva ..... O 15.1
Cortes-Huerto, Robinson .. DY 43.10, DY 54.5
Cosco, Francesco ..... MA 12.6
Cosma Fulga, Ion ..... TT 83.3
Costa, Andreas ....•TT 73.9, TT 97.2
Costa, Antonio C. ..... BP 14.68
Costa, Antonio Carlos ..... •TUT 4.2, •SOE 1.2
Costa, Antonio T. ..... O 15.1
Costa, Fábio J. R. .....O 12.9
Costa Gomes, Margarida ...CPP 21.1
Costa, Natanael .....TT 26.4
Costi, Theo A. ..... O 89.8, TT 90.6
Costi, Theodoulos .....•TT 90.5
Cotelli, Giacomo .....•HL 15.5
Coto, Pedro B. .....CPP 53.5
Coulais, Corentin ..SYBS 1.5, TT 98.4
Couperus Cabadağ, Jurjen AKBP 10.1
Courtois, Hervé .....TT 78.1
Courtois, Theo ..... TT 14.12
Cowan, Thomas .....AKBP 8.8
Cox, Horatio ..... FM 12.10
Cozar, Abel De ..... CPP 13.4
Cranston, Rosemary .....•O 56.6
Crassous, Jerome ..... DY 19.1
Crauste-Thibierge, Caroline .. DY 21.2
Crawford, Daniel .... O 15.8, TT 22.24
Crawford, Ethan .....•MA 42.7
Cremer, Julian ..... CPP 7.5
Cremer, Nils ..... O 40.5, TT 37.5
Cremonesi, Llorenc .....•CPP 46.6
Cren, Tristan ..... DS 12.4, TT 49.4
Crepaldi, Alberto ..... TT 49.7
Crespi, Vincent H. ..... O 33.3
Creutzburg, Carl Nelson ....•HL 17.8
Creutzburg, Sascha .....•DS 21.4
Crippa, Jacopo Simone ..... DS 16.1
Crippa, Lorenzo ... TT 10.4, TT 23.24
Crisafulli, Paride .....•SOE 10.2
Crispin, Hebrew .....•O 37.2
Crispino, Matteo .....•TT 95.8
Crommelin, Daan .....DY 7.8
Crosato, Alice ..... O 38.2
Cross, Graham ..... O 78.6
Cross, Sam ..... TT 80.3
Crossley, Joe .....•TT 70.5
Croy, Alexander ... CPP 21.5, •HL 1.11
Crudden, Cathleen ..... O 11.8
Cruz Hidalgo, Raúl . DY 25.3, DY 25.5
Csonka, Szabolcs .. HL 30.2, TT 59.2
Cubaynes, Tino ..... TT 92.6, TT 92.7
Cubitt, Robert .....CPP 31.4
Cubuk, Ekin Dogus ..... FM 6.6
Cucini, Riccardo ..... O 38.2
Cudazzo, Pierluigi ..... HL 46.7
Cuesta, Angel ..... O 25.1
Cuevas, Juan C. ..... TT 22.1
Cuevas, Juan Carlos MM 31.2, O 87.8, TT 73.2, TT 73.4
Cugliandolo, Leticia ..... DY 60.3
Cui, Longji ..... MM 31.2
Cui, Qirui .....•MA 59.2
Cui, Yangzhe ..... AKBP 8.8
Cui, Yinan .....MM 23.5
Cula, Beatrice ..... CPP 22.2
Cunibert, Gianaurelio .....CPP 7.1
Cuniberti, Gianaurelio .....CPP 7.3, CPP 7.5, CPP 26.3, MM 7.1, O 94.6
Cunningham, Arvin ..... MM 12.7
Cunningham, Oliver .....•CPP 14.1
Curcio, Davide ..... O 85.3, TT 22.24, TT 73.7
Currle, Marc .....•TT 23.4
Curson, Neil J. ..... O 42.9
Custers, Jeroen .....•TT 52.5
Czerner, Michael ... HL 37.1, HL 48.2, MA 39.16
Czibula, Caterina ..... MM 41.1
Czora, Pauline .....DD 6.1
Czyszanowski, Tomasz ... AKPIK 3.4
D. Lorincz, Balázs ..... BP 2.10
D. Natterer, Fabian ..... O 44.9
D. Soares, Rafael . •MA 11.9, •TT 21.9
Da, Binbin ..... MA 5.4, TT 7.4
Da Costa Jesus, José .....QI 8.5
Da Costa Jesus, José Diogo . •QI 8.6
da Costa, Pedro F. G. M. ..... DS 20.7
Da Roit, Nicola ..... O 23.2
da Silva Borges, Danilo .....•UP 3.2
Da Vela, Stefano ..... CPP 46.26
Dabkowski, Patryk ..... QI 2.1
Dadgar, Armin .....DS 11.4, HL 33.2, HL 33.3, HL 34.3, HL 37.5
Dadhich, Priyal .....•HL 38.3, QI 2.9
Daelman, N. ..... AKPIK 6.5
Daelman, Nathan . FM 6.4, •MM 22.3
Daetwyler, Stephan ..... BP 14.38
Dagand, Leo .....CPP 13.6
Daghofer, Maria . •MA 47.1, TT 92.16, TT 92.17, TT 93.19
D'Agosto, Franck ..... DY 62.5
Dahan, Daniel ..... QI 11.7
Dahdoul, Remah ..... SOE 11.3
Dahl Pinholt, Henrik ..... BP 27.11
Dahler, Katharina . HL 20.38, HL 34.2
dahliah, Diana ..... •MA 7.42
Dahmen, David .... DY 43.9, DY 58.7, DY 58.8, SOE 4.8, SOE 17.7, SOE 17.8
Dähn, Christoph .....•MM 5.4
Dähne, Mario ..... O 58.2, O 58.3
Dai, Dinghe .....O 96.5
Dai, Qiang ..... AKPIK 6.4
Dai, Wei .....QI 6.10
Dai, Xi ..... QI 16.10
Dajka, Bence ..... CPP 17.43
Dake, Jules M. ... MM 30.2, MM 30.3
Dakovski, Georgi L. ..... MA 33.11
Dal Conte, Stefano ..... HL 20.15
Dalcea, Michaela ..... MA 39.7
D'Alessio, Matteo .....•TT 10.6
Dall'Ara, Marco .....QI 13.3
Dallera, Claudia ..... TT 49.7
Dalwadi, Mohit .....BP 3.8
Dalzell, James ..... FM 12.5
Damerow, Sarah .....•MA 45.6
Damiani, Elisa .....•DS 13.4
Damião, Iris .....SYTP 1.4
D'Amico, Pino ..... O 84.7, TT 84.7
Damilano, Benjamin ..... HL 55.11
Damköhler, Jens ..... DD 24.3
Dammak, Yosra .....•FM 5.10
Dan, Shachar ..... CPP 15.1
Dan, Zhiying •HL 48.5, O 76.4, TT 27.4
d'Andrea, Giovanni ..... DS 7.5
Danel, Zoriana .....•CPP 56.2
Dang, Nguyen-Hoang ..... O 71.14, •O 71.15, TT 66.14, •TT 66.15
Dang, Toan .....MA 7.30
D'Angelo, Laura .....AKPIK 5.14
Dani, Olfa ..... •HL 17.6
Daniel Hanke, Kai ..... HL 48.3
Danielsson, Elsa .....•TT 53.2
Danilov, Alexey .....HL 55.7
Danneau, Romain ..... TT 73.10
Dannegger, Tobias .....•MA 38.7, MA 48.6
Dannenberg, Simon ..... CPP 17.3
Danner, Lukas .....TT 82.5
Dantas, Renato M. A. ..... TT 41.2
Dany, Leonie-Charlotte .....•MA 55.8
Dänzer, Laureen ...•DD 21.1, DD 30.7, DD 30.8
Danzglock, Maria .....DD 27.1
Danziger, Jakob ..... CPP 59.2
Darahan, Serhii ..... HL 12.1
Darbois Texier, Baptiste .... •DY 25.1
D'Arcy, Richard ..... AKBP 12.4
Dargasz, Michelle BP 14.24, BP 14.72
Darius, Pohl .....•MA 7.61
Darmawan, Andri .....•MA 38.1
Darras, Alexis ..... BP 14.41, BP 36.7, DY 57.7
Dartige, Thomas ..... •CPP 46.23
Darwin, Emily .... •MA 44.2, •TT 76.2
Das, Anindit .....•MA 7.82
Das, Anirban .....•HL 38.6
Das, Ankita .....O 58.3
Das, Arkaprava .....•O 6.7
Das, Arpan .....•TT 93.13
Das, Arunima .....•UP 7.4
Das, Chandan K. .•BP 2.8, CPP 46.42
Das, Debankur .. CPP 10.11, DY 16.11, DY 54.3
Das Mohapatra, Bikash ..... MA 9.8
Das, Mowpriya ..... O 58.3
Das, Pallabi •BP 1.2, •CPP 1.2, •DY 4.2
Das, Proloy T. ..... HL 23.1, MA 49.5
Das, Proloy Taran MA 49.6, •MA 49.7
Das, Risov ..... MM 5.4
Das, Sambunath ..•DY 53.5, •TT 87.5
Das, Souvik .....•O 84.9, •TT 84.9
Das, Subhadip ..... TT 72.8
Das, Sudipto ..... QI 6.4, •QI 20.7
Das, Sunit .....•TT 92.12
Das, Tanmoy .....MM 31.6
Dasari, Durga ..... •QI 7.5, QI 13.5
Dasari, Nagamalleswararao . TT 53.1, TT 53.5
Dasbiswas, Kinjal .....•BP 10.2, •CPP 18.2, •DY 18.2
Dasgupta, Writu .....•DY 14.6
Dašić, Miljan .....•BP 2.5, MM 32.5
Daskalakis, Konstantinos C. . HL 15.3
Das-Mohapatra, Bikash ..... MA 7.8
Datta, Agniva ..... BP 11.8, •DY 33.5
Datta, Sawani .....•O 33.3, O 62.6, TT 54.6
Daudin, Remi .....MM 14.4
Dauer, Christoph ..... TT 44.8
Daum, Etienne .....•TT 22.13
Daum, Winfried ..... O 58.6, O 83.9
Daurer, Benedikt J. ..... MA 6.10
D'Auria, Virginia .....•QI 18.1
Dautzenberg, Lara S. ..... DY 55.2
Dauwe, Tim .....•O 79.7
Davenport, Henry .....TT 61.12
David, Christin ...BP 33.7, CPP 46.65
David, Felix HL 18.4, •HL 18.6, HL 18.7, HL 31.5, TT 32.4, •TT 32.6, TT 32.7
David Gonzalez, Carlos ... CPP 10.12, DY 16.12
Davidkova, Kristyna .....MA 9.9
Davidson, Bruce .....DS 6.2
Davidsson, Joel ..... O 59.4, TT 48.4
Davies, Francis H. ... O 95.3, TT 96.3
Davis, Tim ..... O 26.4
Davis, Timothy J. ..... O 79.5

Davitti, Niccolò .... MA 29.3, TT 46.3
Davoodabadifarahani, Azam •CPP 46.48
Davydok, Anton .. CPP 4.6, CPP 16.2, CPP 17.27
Dawid, Anna ..... DY 58.1, SOE 17.1
Day, Matthew ..... O 98.5
Day, Peter K. ..... QI 11.8
de Almeida Marques, Carolina O 93.7, TT 5.10
De, Anulekha ..... MA 45.5
De Bacco, Caterina ..... SOE 4.5
de Barros Righes, Gabriel ... BP 7.29
de Bruyn, Emile ..... BP 14.57
de Camargo, Andrea S. S. ... DS 20.7
de Castro, Tulio ..... •MA 7.18
De Chavez, Danjo ..... •O 50.6
De Feyter, Steven ..... O 69.11
De Franceschi, Silvano ..... QI 2.10
De Franco, Francesca ..... •DY 32.1, •TT 45.1
De Gersem, Herbert ..... AKPIK 5.14
De Giovannini, Umberto ..... O 61.1
de Gois, Carlos ..... QI 12.7
de Graaf, Sebastian ..... TT 22.12, TT 22.17
De Jong, Jarn ..... QI 18.9
de Juan, Fernando ..... TT 14.10
De la Barrera, Gaspar ..... •MA 7.58
de la Torre, Bruno ..... O 69.13
De Los Rios, Paolo BP 39.5, CPP 55.5
De Luca, Filippo ..... BP 12.5
de' Medici, Luca ..... TT 95.8
de Oliveria, Geovane Arruda . FM 6.10
de Pablo, Pedro J. ..... BP 2.4
De Pas, Marco ..... O 85.4
de Podesta, Christian ..... TT 62.7
De Santis, Duilio ..... TT 71.3
De Sio, Antonietta . HL 46.2, •HL 46.3
De Tomasi, Giuseppe ..... MA 34.12
de Vasconcellos, Steffen Michaelis MA 52.14
De Vita, Alessandro ..... •MA 33.12, O 38.4, O 38.7, O 71.10, O 98.7, TT 66.10
de Vos, Erik ..... MA 7.32
de Vos, Erik W. ... •MA 24.2, TT 25.3, TT 33.3, •TT 36.2
de Vries, Insa F. ..... •MM 19.37
de Wiljes, Jana ..... DS 20.35
de Wit, Stijn ..... •TT 15.11
Deb, Shamarita ..... •TT 93.15
Deb, Swarup ..... HL 24.9
Débarre, Delphine BP 11.6, •CPP 26.5, CPP 31.6
Debbontridder, François ..... TT 49.4
Debertolis, Maxime ..... DY 42.1, •DY 46.11, TT 63.1, •TT 75.11
Debnath, Sayan ... •O 10.11, •TT 16.11
Debus, Alexander ..... •AKBP 10.1, AKBP 10.2, AKBP 10.3, AKBP 12.5
Debus, Jörg ..... MM 21.6
Decitre, Hugo ..... TT 29.2
Deckers, Carolin ..... •QI 10.10
Deckert, Thomas ..... HL 20.15
DeCock, Mieke ..... DD 14.1
Dediu, Valentin Alek ..... O 64.4
Dednam, Wynand ..... MM 40.8
Deffner, Michael ..... TT 90.6
DeFreitas, Luke .... MA 23.2, TT 35.2
Degen, Christian L. ..... FM 23.5
Dehm, Gerhard ..... FM 2.1, MM 15.5
Dehnert, Martin ... •BP 7.3, BP 14.34, BP 26.6, CPP 43.6
Dehnhardt-Fehst, Natalie ... HL 26.28
Deilmann, Thorsten ..... HL 20.17, HL 25.2, MA 52.1, O 7.3, O 60.7, O 71.23, O 72.3, TT 9.3, TT 66.23, TT 67.3
Deinert, Jan ..... MA 7.46, MA 12.4
Deinert, Jan-C ..... O 41.3, TT 38.3
Deinert, Jan-Christoph ..... MA 25.8, MA 35.6, TT 14.8, TT 60.6
Deinhart, Victor ... FM 11.28, MA 7.67
Deiringer, Nora .... •BP 7.22, BP 14.51
Deisenhofer, Joachim ..... MA 7.50, •MA 8.9, MA 54.2
Deka, Jitul ..... MA 35.4, TT 60.4
Del Bufalo, Giovanni ..... •MA 52.18
del Campo, Valeria .... O 56.7, O 67.3
Del Maestro, Adrian ..... TT 64.1
del Pino, Javier ..... DY 8.7
Del Pozo, Frederick . •TT 17.4, •QI 4.4
Del Re, Lorenzo ..... •MA 33.9
Delan, Annekatrin ..... CPP 17.36
Delan, Arthur ..... •AKBP 8.2
Delcea, Mihaela ..... BP 14.25
Deleruyelle, Damien ..... FM 4.1
Delesma, Antonio F. ..... O 37.5
Delfino, Francesco ..... BP 15.2
Delgado, Fernando .... O 15.7, O 89.1, O 89.5
Delgado, Frederico ..... HL 40.3
Delgado, Frederico P. ..... MM 9.3
DELight Collaboration, for the TT 22.37
Delin, A. ..... MA 7.14
Delin, Anna ..... MA 34.1, MA 34.11, MA 58.9
Della Valle, Enrico G. ..... O 42.9
Dellevoet, Jolijn ..... •HL 38.12
Delobbe, Anne ..... HL 38.11
Deluca, Marco ..... MM 4.4
Demel, Johann ..... •CPP 17.24
Demidov, V. E. ..... MA 48.11
Demidov, Vladislav E. ..... MA 9.13, MA 52.14
Demir, Kubilay T. ..... UP 5.4
Demir, Merve ..... DS 8.5
Demiralp, Berke ..... HL 31.5
Demler, Eugene ..... TT 56.3, TT 71.3
Demokritov, S. O. ..... MA 48.11
Demokritov, Sergej O. ..... MA 9.13, MA 48.2, MA 52.14
Dempsey, Nora ..... •FM 9.1, MA 58.1
Dempwolf, Wibke ..... FM 5.11
Demsar, J ..... O 59.2, TT 48.2
Demsar, Jure .... MA 27.10, TT 23.31, TT 57.6, TT 71.1
Demuth, Thomas ..... •MM 4.6
Dendzik, Maciej ..... MA 7.18
Deneke, Kristian .. DS 16.3, DS 20.10, FM 11.26, •FM 11.29
Denell, Thea ..... FM 6.5
Dénes, Gergo ..... •TT 17.7, •QI 4.7
Deng, Shibin ..... TT 44.4
Deng, ZhiYuan ..... O 66.4
Denizer, Florian ..... O 16.2, •O 84.8, •TT 84.8
Denk, Mariella ..... DS 21.6
Denker, Andrea .... •AIW 1.2, •AIW 1.5
Denker, Christian ..... MA 39.7
Denker, Sophia ..... •QI 21.4
denligner, jonathan ..... TT 25.11
Denlinger, Jonathan . MA 5.8, TT 3.2, TT 7.8
Denneulin, Thibaud ..... MA 43.4
Denysov, Sergiy ..... QI 9.4
Deodhar, Mrunmayee ..... •HL 20.38
Derenek, Maike ..... BP 7.41
Derewjanko, Dennis ..... CPP 37.2
Derla, Mishael ..... •DY 43.6
Desaleux, Thibault ..... DY 49.3
Desch, Klaus ..... DD 16.3, AKBP 1.2, AKBP 1.3, AKBP 2.4, AKBP 3.5, AKBP 7.2, AKBP 7.6, AKBP 14.2
Deschler, Felix ..... MM 4.2
Deshpande, Aniruddha ..... TT 14.1
Desmedt, Arnaud ..... •CPP 36.1
Desort, Thibaut ..... •TT 83.13
Despoja, Vito ..... O 71.8, TT 66.8
Desroche, Emmett ..... O 11.8
Detemple, Ralf ..... DD 23.1, DD 30.6
Dethloff, Christiane ..... •HL 26.21
Dette, Holger ..... MM 19.25
Dette, Ulrike ..... •MM 3.4
Dettmar, Ralf-Jürgen ..... •DD 22.1
Deussen, Andreas ..... BP 14.10
Deutsch, Andreas ..... DY 33.9
Devda, Harshita ..... •MA 12.5
Devi, Anjana ..... FM 11.24
Devi, Parul ..... MA 39.3
DeVine, Jessalyn ..... O 34.7, QI 20.8
Devolder, Thibaut ..... MA 9.3
Devoret, Michel H. ..... QI 6.10
Dewage, Nipun T. S. K. ..... O 81.2
Dewhurst, John ..... MA 14.1
Dewhurst, John Kay ..... MA 35.10, MA 58.6, TT 60.10
Dextre, Aaron ..... •MA 50.6
Dey, J. K. ..... O 19.10
Dey, Jayjit ..... MA 7.67, TT 14.4
Dey, Jyotirban ..... CPP 17.47
Dey, Manoj ..... •HL 47.4
Dhakal, Ramesh ..... TT 72.9
Dhar, Jayabrata .... BP 1.11, CPP 1.11, DY 4.11
Dhard, Chandra Prakash ..... O 78.1
Dharmaraj, Karuppasamy .... O 13.11
Dhawan, Prerak ..... CPP 46.9
Dhont, Jan ..... BP 39.4, CPP 55.4
Dhurjati, Abhishikth ..... •HL 56.4
Dhurjati, Sai A ..... HL 56.5
Dhurjati, Sai Abhishikth ..... HL 55.7
Di Benedetto, Enrico ..... TT 43.11
Di Bernardo, Angelo ..... TT 28.1, TT 28.12, TT 29.10, TT 81.3
Di Castro, Daniele ..... TT 14.5
di Fini, Andrea ..... QI 3.10
Di Gianluca, Gabriele ..... TT 43.8
Di Giulio, Valerio .. O 49.3, •AKBP 4.3
di Marcantonio, Francesco .... QI 3.1
Di Martino, Giuliana ..... FM 18.5
Di Michele, Lorenzo ..... BP 5.2
Di Nunzio, Marnin ..... •MA 8.12
Di Sante, Domenico MA 47.2, O 63.8, TT 29.7, TT 55.8
Di Trelizzi, Ivan ... •BP 32.7, •DY 52.7
di Vora, Robert ..... O 43.7
Dianat, Arezoo ..... O 94.6
Dias, Manuel dos Santos ..... O 17.1
Díaz Duque, Álvaro ..... O 51.2
Diaz Hernandez Rojas, Rafael •DY 7.10
Díaz, Juan Pablo ..... •AKBP 13.2
Diaz Lopez, Carlos Alberto . •TT 82.6
Diaz-Granados, K. ..... O 57.6
Díaz-Palacio, Isabel ..... AKBP 9.2
Díaz-Palacio, Isabel González FM 11.29
Diaz-Pardo, Rebeca ..... TT 74.12
Dichelle, Hannah ..... •HL 9.6
dichtl, valentin ..... DY 19.3, O 27.6, •O 57.2
Dick, Anneli ..... •AKBP 11.2
Dick, Daniel ..... •HL 48.8
Dickbreder, Tobias .... O 5.3, •O 36.5
Dickel, Christian .... TT 15.6, TT 74.2
Diddens, Diddo . CPP 14.4, CPP 17.34, CPP 17.35, CPP 46.50
Didier, Nicolas ..... QI 17.7
Didiş Körhasan, Nilüfer ..... •DD 3.2, DD 3.3
Dieball, Cai ..... •SYSD 1.1
Diebell, Ella ..... CPP 27.2, DY 26.2
Diebold, Ulrike . O 5.6, O 55.4, O 58.7, O 80.1, O 94.5
Diederich, Geoffrey M. .... •SYQF 1.1, •HL 20.63
Diederichs, Jost ..... O 44.11
Diedrich, Cornelius ..... HL 47.1
Diedrich, Johannes .... •O 4.3, O 88.2
Diego López, Josu ..... •MM 15.2
Diehl, Douglas ..... BP 32.6, DY 52.6
Diehl, Sebastian ..... DY 9.8, DY 46.8, TT 75.8
Diekmann, Florian ... O 59.5, TT 48.5
Diekmann, Florian K. ... O 7.5, O 71.1, O 71.16, TT 9.5, TT 66.1, TT 66.16
Diekmann, Florian Konstantin O 71.18, TT 66.18
Diekmann, Jan ..... DY 44.15
Dienelt, Laura ..... DS 4.6
Dieplinger, Johannes ..... TT 93.13
Diercks, Alexander ..... HL 4.5
Diesen, Elias . •O 13.2, O 24.3, O 97.11
Dieterich, Peter ..... BP 14.10
Dietrich, Alina ..... TT 5.5
Dietrich, C. ..... HL 20.27
Dietrich, Fabia ..... AKBP 12.5
Dietrich, Jana ..... O 58.8
Dietrich, Peter ..... UP 7.5
Dietz, Elena ..... O 65.6
Dieval, Lucie ..... CPP 26.1
Dil, Hugo ..... O 67.6
Dil, J. Hugo ..... O 66.5
Dilhaire, Stefan ..... FM 4.5
Dillenz, Manuel .... MM 8.2, •MM 8.4
Dilling, J. ..... O 19.10
Dilling, Jakob ..... O 70.3, O 71.17, TT 65.3, TT 66.17
Dimakis, Emmanouil ..... HL 17.5
Dimić, Vjeko ..... •TT 22.24, TT 73.7
Ding, Andy Z. ..... QI 6.10
Ding, Chenrui ..... •CPP 46.39
Ding, Fei ..... DS 20.21, HL 20.45, HL 20.49, HL 20.50, HL 20.51, HL 26.30, HL 31.4, HL 55.8, HL 55.10
Ding, Jiaqi ..... •CPP 17.28
Ding, Jinxue ..... MM 23.5
Ding, Kuan ..... •MM 23.3
Ding, Shilei ..... •MA 29.3, •TT 46.3
Ding, Yuxiao ..... O 59.7, TT 48.7
Dingel, Kristina .... DY 41.13, MA 7.23
Dingeldein, L. B. ..... AKBP 1.1
Dingeldein, Lisa ..... AKBP 14.1
Dingeldein, Lisa B. ..... •AKBP 4.4
Dinh, Duc V. ..... HL 57.2
Dinh, Thi Lan ..... O 14.10, O 40.19, TT 37.19
Dinnebier, Robert E. ..... TT 49.8
Dinter, Julius K. ..... •DS 20.20
Diona, Pietro ..... •MA 30.10
Diotallevi, Francesco ..... QI 3.5
Dirba, Imants ..... DS 7.5, MA 50.9, MA 52.31, MA 57.5
Dirnberger, Florian ..... •SYQF 1.3, HL 39.8, MA 7.48
Disa, A. ..... MA 4.4
Disch, Sabrina . •CPP 33.1, •CPP 36.1
Dissayanake, Rasika ..... O 88.2
Ditter, A. ..... MA 50.3
Dittloff, Johannes .... HL 1.1, HL 12.7, MM 4.2, MM 4.3
Dittmann, Regina ..... DS 6.6
Dittmar, Marco ..... MA 47.5, •O 48.5
Dittrich, Thomas ..... HL 23.4
Divinski, Sergiy ..... MM 19.4
Divinski, Sergiy V . MM 11.5, MM 35.6
Diwan, Parisha ..... •MM 19.32
Dixer, Fabian ..... •O 45.9
Dixit, S. ..... O 57.6
Diz-Muñoz, Alba ..... •SYGF 1.4
Djurdjevac Conrad, Natasa . •SOE 8.1, SOE 8.3
Dmytro, Skachko ..... •FM 9.3
Dmytruk, Olesia .... •TT 15.2, TT 15.7, TT 74.9
Dobariya, Krupali ..... •HL 20.45
Dobiasch, Martin ..... MA 34.4
Döbler, Katarina ..... •CPP 46.12
Döblinger, Markus ..... CPP 59.3
Dobrautz, Werner . •TT 17.1, TT 23.19, TT 23.20, TT 23.22, TT 23.25, •QI 4.1, QI 5.1, QI 14.14
Dobroserdova, Alla ..... •DY 44.21
Dobrovolskiy, Oleksandr ..... TT 5.4, TT 14.12, •TT 97.6, TT 97.7, TT 97.8, TT 97.9
Docheva, Martina ..... DS 20.3
Dočkalová, Kateřina MM 8.10, •O 50.4
Doerr, Mark ..... MA 39.7
Doerr, Mathias . MA 55.11, •MA 55.12
Doert, Thomas ..... MA 7.2, TT 61.3, TT 72.3
Dogadov, Oleg ..... •HL 20.15
Dogan, Ismet N. ..... •DD 30.1
Dogra, Nishant ..... •DD 7.2
Döhn, Johannes ..... •FM 5.6
Dolay, Pritha ..... BP 14.64
Dolchinkova, Trayana ..... •HL 20.64
Doležal, Jiří ..... O 43.17
Dolgirev, Pavel ..... TT 12.3
Doling, Daniel ..... TT 22.17
Doll, Andrin ..... TT 52.1, TT 57.3
Doll, Simon ..... BP 31.2, CPP 50.2
Doll, Sven ..... •HL 12.6
Dollmann, Antje ..... •MM 7.10
Dolmantas, Paulius ..... •TT 3.2
Doltsinis, Nikos L. ..... MM 19.37
Dolynchuk, Oleksandr .... CPP 46.49, CPP 59.2, CPP 59.4, •CPP 59.6, MA 39.15
Domaradzki, Jarosław ..... DS 11.5
Domingo, Marina Isabel de la Higuera O 23.10
Domínguez Arca, Vicente ... CPP 7.4, •DY 60.8
Dominguez, Fernando ..... O 63.8, TT 15.10, TT 55.8
Dominguez Flores, Fabiola ... •O 13.4
Dominguez-Calderon, Sebastian TT 22.26, •QI 14.21
Dominko Kobilica, Natan .. •BP 14.51
Domnick, Joscha .... QI 6.9, QI 14.26
Donarini, Andrea ..... O 99.12
Donath, Markus ..... •O 60.2, O 60.4, O 60.5, O 60.7, O 63.5, O 67.2, O 67.5, O 67.8, O 84.6, TT 55.5, TT 84.6
Donati, Fabio ... O 8.6, O 15.6, O 15.9, O 15.11, O 64.2, O 77.6, •O 89.10, O 99.11
Dong, Chengye ..... O 66.4
Dong, Shuo ..... MA 7.18
Dong, Xiaochen ..... DY 33.1
Donnelly, C. ..... MA 50.3
Donnelly, Claire .... •FM 23.1, MA 6.4, MA 6.10, MA 6.12, MA 7.36, MA 7.61, MA 7.79, MA 8.13, MA 42.11, MA 58.2, TT 40.1
Donner, Reik V. ..... •DY 8.9
Doostani, Reza ..... •MA 7.69
Doostmohammadi, Amin .. CPP 10.9, DY 16.9

Döpp, Andreas ..... AKBP 8.7
Dora, Balazs ..... DY 46.10, TT 75.10
Dörfler, Magdalena ..... •HL 53.3
Dörfler, Maximilian ..... •HL 4.3
Dörflinger, Patrick ..... CPP 17.10
Dorfner, Maximilian F. X. ... CPP 15.6, CPP 17.23, •CPP 40.3, CPP 53.4, DS 20.45
Doria, Elena ..... BP 2.3
Döring, A. ..... MA 18.1, TT 30.1
Döring, Allan ..... •MA 18.2, •TT 30.2
Dormann, Dorothee ..... BP 29.6, CPP 45.6
Dormann, Kay-Robert ..... •DY 44.3
Dorn, Anton Emil ..... •BP 14.57
Dorn, Franziska .. BP 14.25, •BP 33.9, O 44.13
Dornhege, Ruth ..... DD 9.1
Dornquast, Niklas ..... •MA 39.12, MA 54.11
Dornseifer, Jan L. ..... •DS 8.2
Dörr, Kathrin .... MA 30.12, MA 39.15, O 38.3
Dorsel, Dominik ... •DD 25.1, DD 36.1
Dorst, Arved ..... O 4.3, O 88.2
Dörstel, Tobias ... •DY 46.2, •TT 75.2
dos Santos Dias, Manuel ..... O 64.9
Dou, Jie ..... TT 69.1
Douarche, Carine .. CPP 11.6, DY 17.6
Dourdent, Hippolyte ..... QI 12.3
Douvis, Kostas ..... UP 5.2
Dowben, Peter ..... O 60.6
Downer, Michael ..... AKBP 10.1
Doyle, Spencer ..... MA 27.7
Dragland, Ruben .. •FM 4.6, FM 11.34, FM 18.7
Drautz, Ralf TUT 6.1, MM 1.1, MM 3.8, MM 5.7, MM 7.2, MM 9.1, MM 9.7, MM 11.4, MM 19.10, MM 19.17
Drawer, J.-C. ..... HL 54.12
Draxl, Claudia ..... FM 6.5, MM 9.6, MM 37.1, O 66.9, AKjDPG 1.1, AKjDPG 1.2, AKjDPG 1.4
Draxler, Till ..... •HL 20.36
Drechsler, Alina .. •O 71.22, •TT 66.22
Drechsler, Felix .... FM 7.5, •MM 13.3
Drechsler, Stefan-Ludwig ... •TT 94.4
Dreckhoff, Johannes ..... •BP 14.67
Dreher, Pascal O 26.4, •O 57.1, O 85.5, O 96.2, TT 6.6
Dreier, Kim Noelle ..... •O 36.3
Dreiner, Herbi ..... •DD 35.1
Dreßler, Christian •CPP 9.6, MM 26.2
Dressel, Martin . CPP 17.45, MA 7.34, MA 33.4, TT 5.2, •TT 12.6, TT 14.1, TT 14.2
Dressler, Fabienne ..... CPP 20.12, DY 23.12
Dreuw, Andreas ..... CPP 17.6
Drevelow, Tim ..... MA 39.21
Dreyer, N. ..... •HL 37.2, HL 37.6
Dreyer, Rouven .... •MA 9.8, MA 35.3, MA 52.16, MA 52.21, MA 59.7, TT 60.3
Drichko, Natalia ..... TT 41.4
Drieb-Schön, Maike ..... QI 3.2
Driouech, Mustapha ..... •HL 1.6
Drobinski, Barbara . •O 40.9, •TT 37.9
Droghetti, Andrea ..... O 64.4, O 83.6
Drost, Robert ..... •O 59.7, •TT 48.7
Drozdowski, Oliver M. ..... •BP 3.10
Dsouza, Reuel ..... MA 33.3
D'Souza, Sunil ..... TT 62.11
DSouza, Sunil Wilfred ..... •MA 13.6
Du, Ao ..... MA 39.1
Du, K ..... MA 19.7, TT 31.7
Du, Shilling ..... TT 43.8
Du, Xin ..... •HL 33.1
Duan, Juanmei ..... O 44.6, O 79.2
Duan, Sisheng ..... •TT 49.6
Duan, Siyu ..... •TT 71.2
Duarte, Maria Jazmin ..... FM 2.1
Dub, Maksym ..... HL 52.2, HL 52.3
Dubacheva, Galina ..... CPP 26.5, •CPP 31.6
Dubail, Jérôme ..... TT 53.6
Dubey, Akhilesh ..... •HL 20.59
Dubey, Pralekh ..... •MA 49.9
Dubourdieu, Catherine ..... HL 25.3
Duboz, Jean-Yves ..... HL 26.2
Dubrovinskaia, Natalia ..... •TT 80.2
Dubrovinsky, Leonid ..... •FM 22.11, TT 80.2
Dubs, Carsten ..... MA 9.9, MA 9.12
Ducati, Caterina ..... FM 18.5
Ducci, Gianmarco . •DY 6.12, DY 14.5, O 23.5
Duchêne, Merle ..... •BP 7.32
Duchoslav, Jiri ..... MM 19.20
Dudy, L. ..... •O 85.2
Dudy, Lenart •O 8.5, TT 25.11, TT 29.3
Duelli, Marian ..... MA 33.1
Dufke, Paul ..... •BP 7.26
Dufouleur, Joseph FM 22.6, MM 40.4, TT 11.2
Dufresne, Eric ..... BP 20.6
Duft, Eva ..... MA 46.5
Duine, Rembert .... MA 51.5, TT 88.5
Duits, Michel ..... O 36.4
Duka, Tim C. ..... QI 14.10
Dulisch, Hubert ... HL 10.3, HL 20.26, TT 20.3
Dulle, Martin ..... MA 7.25
Dully, Timo ..... •MA 7.12
Duman, Emre ..... TT 15.11
Dumesnil, Karine .. MA 38.9, TT 14.12
Duncan, David A. ..... O 4.1, O 83.1
Duncker, Annalena ..... CPP 16.1
Dunin-Borkowski, R.E. ..... MA 3.8
Dunin-Borkowski, Rafal ... MA 38.10, MA 46.5
Dunin-Borkowski, Rafal E. .. MA 43.4
Dunsiger, Sarah R. ..... TT 52.5
Duong, Nhat Lam .. HL 20.14, O 10.6, TT 16.6
Dupont, Aurélie ..... •SYGF 1.6
Dupuy, Remi .... CPP 19.5, CPP 23.2, CPP 27.3, DY 20.5, DY 24.2, DY 26.3
Duque, Álvaro Díaz ..... O 87.7
Duran, Stefan ..... HL 52.5
Durand, Robin ..... •TT 83.2
Durate, Jazmin ..... FM 5.2
Durdiev, Dilshod ..... FM 15.3
Düren, Linda ..... •CPP 46.35
Düren, Oskar ..... O 58.3
Düreth, Johannes ..... HL 1.12
Durgun, Abdullatif MA 50.9, MA 52.31
Durgun, Engin ..... HL 10.6, MM 16.4, TT 20.6
Düring, Pia ..... FM 23.4
Düring, Pia Maria ..... O 93.2
Durmaz, Yasin C. ..... O 79.4
Dürr, Hermann ..... MA 24.4, TT 36.4
Dürr, Michael ... O 11.1, •O 11.4, O 31.2
Dürschmidt, Hannah Carolina •TT 61.11
Durst, Karsten ..... MA 50.5
Duru, Iremnur .... DS 20.14, MA 42.9, MM 12.9
Dusel, Felix ..... •DY 13.9, •TT 19.9
Dutke, Stephan ..... DD 12.1
Dutreix, Clement ..... O 62.2, TT 54.2
Dutta, Arka ..... •DY 14.12
Dutta, Arpita ..... •MA 45.2
Dutta, Ivan ..... •TT 86.5
Dutta, Sayan ..... •CPP 24.1
Dutta, Shovan .... DY 32.10, TT 45.10
Dutta, Soma ..... •MA 24.4, •TT 36.4
Dütz, Denny ..... QI 6.2, QI 14.23
Duvjir, Ganbat ..... •O 71.14, O 71.15, •TT 66.14, TT 66.15
Dyakonov, Vladimir ..... CPP 17.10, CPP 17.16, CPP 25.2, CPP 57.5, FM 11.20, HL 16.6, HL 20.61, HL 24.3, HL 26.29, HL 49.2, MA 13.8, •TT 24.2
Dye, Natalie A. ..... BP 3.4
Dyksik, M. ..... HL 54.10
Dylla, Carolin ..... SOE 12.2
Dzeik, Johann ... HL 20.49, •HL 20.51
Dzeroski, Saso ..... UP 5.5
Dzhagan, Volodymyr ..... HL 1.4
Dziadkowiec, Joanna ..... O 87.5
Dziegielewski, Przemyslaw •MM 19.3, MM 19.22
Dzinnik, Marvin J. ..... •HL 48.6
Dzubiella, Joachim ..... CPP 20.5, CPP 33.2, DY 23.5
E. Bürgler, Daniel ..... MA 42.4
E. Demidov, Vladislav ..... MA 52.5
E. Gruner, Markus ... MA 38.1, O 14.8
E. Mansour, Ahmed ..... AKjDPG 1.2
E.P. Umlandt, Marvin ..... AKBP 5.4
E. Shaw, Paul ..... CPP 48.5
E. Villegas, Javier ..... TT 69.5
Eaton, Alexander ..... TT 93.17
Ebad-Allah, Jihaan .. MA 11.2, TT 21.2
Ebbecke, Jens ..... DS 20.9, HL 24.3
Ebel, Frank T. ..... TT 13.1
Ebel, Lea Sophie ..... •UP 8.3
Ebeling, Daniel O 3.1, O 24.1, O 45.10, O 56.1, •O 58.1
Eberhard, Aurelia ..... HL 35.5
Ebert, Hubert ..... MA 14.3, MA 17.1, MA 35.7, •MA 35.8, TT 60.7, •TT 60.8
Ebert, Miriam R. ..... •TT 22.1
Eberts, Benedikt ..... •DS 20.17
Ebrahimi, Mahdieh ..... DY 44.3
Ebrahimi Viand, Roya ..... DY 43.4, DY 43.7, •MM 31.10
Echresh, Ahmad .. HL 17.9, HL 20.46, HL 20.56, HL 56.1
Echtenkamp, Will ..... O 60.6
Eck, Philipp ..... DS 20.43
Eckardt, André ..... •TT 18.3
Eckelt, Franz ..... •TT 93.14
Eckelt, Franz-Michel ..... TT 93.10
Eckerle, Simeon ..... MM 34.1
Eckert, Jürgen ... MM 18.2, MM 18.4, MM 35.1
Eckhardt, Janis K. ..... CPP 16.5, CPP 17.38, CPP 17.40, DS 8.2
Eckl, Emanuel ..... •HL 45.4
Eckrich, Jakob ..... •O 3.2
Eckseler, Jannis ... •DY 13.4, •TT 19.4
Eckstein, Jack ..... FM 12.10
Eckstein, Klaus H. ..... HL 45.6
Eckstein, Martin .. TT 4.12, TT 23.26, TT 23.27, TT 53.5
Eddhib, Ridha ..... •O 76.2
Edel, Eduard ..... CPP 19.3, DY 20.3
Edens, Leonard ..... •O 15.5, O 99.7, TT 73.5
Eder, Markus ..... CPP 20.2, DY 23.2
Eder, Moritz ..... O 94.3
Ederer, Claude ..... FM 7.7, MM 8.1
Edler, Karen ..... •CPP 30.1
Edmonds, Andrew ..... QI 13.5
Edossa, Nicole ..... O 84.6, TT 84.6
Edwards, Jordan ..... •O 96.10
Efferson, Charles ..... SYTP 1.1
Efremov, Dmitriy .. MA 7.37, MM 40.4
Egalla, Dinusha M. ..... •CPP 17.5
Ege, Lütfi Çağlar ..... •MM 19.33
Egenlauf, Patrick ..... •DY 6.2
Eger, Marc ..... •MA 52.21
Eggeler, Yolita M. ..... MM 3.6
Eggeling, Nico ..... •HL 38.10
Egger, David ..... MM 19.49
Egger, David A. .... FM 10.3, HL 23.7, HL 40.3, HL 42.1, MM 9.3, MM 9.5, MM 12.6, MM 22.8
Egger, Dominik ..... BP 15.10
Egger, Nadine ..... •O 93.10
Eggers, Vincent ..... O 38.6
Eggert, B. MA 23.5, MA 50.3, TT 35.5
Eggert, Benedikt .. MA 13.2, MA 36.1, MA 50.8, •MA 52.27
Eggert, Sebastian .. O 26.3, •TT 44.8, TT 78.4
Eglmeier, Geena ..... BP 14.4
Ehlert, Sascha ..... MA 7.25
Ehm, Alexander ..... •O 82.5
Ehresmann, Arno CPP 30.2, DY 41.13, MA 5.1, MA 7.23, MA 36.4, MA 36.5, MA 52.40, MA 57.6, TT 7.1
Ehret, Sonke ..... SYTP 1.1
Ehring, Felix ..... •HL 3.11, HL 20.19, HL 36.1
Ehrler, Bruno ..... HL 4.8
Ehrler, Rico ..... DS 18.1, DS 20.42, MA 57.6
Ehrlich, Jannis ..... MM 8.3, •QI 1.8
Eich, Sebastian .. CPP 15.5, MM 41.2
Eichel, Rüdiger-A. ..... FM 2.4
Eichhorn, Johanna CPP 44.3, DS 9.3, DS 12.3, HL 1.1, HL 12.6, HL 12.7, MM 4.2, MM 4.3, MM 4.5, •O 97.8
Eickhoff, Martin ..... HL 9.1, HL 12.3, HL 20.66, HL 24.1
Eikerling, Michael .. MM 25.5, O 39.4
Eilenberger, F. .... HL 54.10, HL 54.12
Einert, Marcus ..... O 54.5
Einfeldt, S. ..... HL 37.6
Eisebitt, Stefan ..... DS 6.1, MA 7.15, MA 7.19, MA 27.7, MA 27.11, MA 38.3
Eisele, Florian ..... •AKBP 8.10
Eisemann, Lukas ..... QI 14.1
Eisenbarth, Udo ..... AKBP 11.3
Eisenschmidt, Elias ..... •TT 22.35
Eisermann, Emilian ..... •HL 26.29
Eisert, Jens ..... QI 3.3
Eisfeld, Julian ..... QI 10.7
Eisner, Ludmila ..... •FM 11.30
Eixmann, Ronald ..... UP 3.4, •UP 3.5
Ejima, Satoshi ..... •QI 5.7
Ekitli, Burcak ..... •MA 50.4
Eklund, Tobias .... CPP 27.4, DY 26.4
El Alouani, Ahmed ... O 62.3, TT 54.3
El Azzouzi, Fatima ..... FM 14.4
El Dek, Samaa ..... MA 7.76
El Hamouz, Amer ..... O 65.2
El Haouari, Redouan ..... •CPP 9.4
El Kaderi, Yunos ..... •QI 16.6
El Kadri, Ahmad ... MA 9.13, MA 52.5
Elancheliyan, Rajam ..... CPP 35.2, DY 37.2
Elbakary, Nermeen Mohamed •BP 7.2
Elbakary, Omnia Ahmed Mohamed BP 7.2
El-Dabea, Tarek ..... •MM 19.27
Eldar, Avigdor ..... BP 14.15
Eleftheratos, Kostas ..... UP 3.3
Elgeti, Matthias ..... •BP 18.4
Elhanoty, M. ..... MA 7.14
El-Hussein Elnewishy, Ahmed •BP 26.2, •CPP 43.2
Eli, Zoghlin ..... TT 94.4
Eljaouhari, E.O. ..... TT 25.6
El-Kabil, Soufiane ..... HL 52.1
Elkaim, Erik ..... CPP 26.1
Eller, Fabian ..... CPP 44.6
Ellettari, Elisabetta ..... DY 7.2
Ellinger, Florian ..... O 93.8
Elliot, A. ..... MA 25.6
Elliott, Jenna ..... •BP 16.3, DY 47.1
Elm, Matthias T. ... DS 8.2, DS 20.20, HL 26.3, HL 42.2, HL 45.3
El-Mansi, Hogo ..... UP 6.2
El-Mansi, Hugo ..... UP 8.4
EL-Masry, Mai ..... •MM 19.28
Elmers, H.-J. . O 19.10, O 59.2, O 93.9, TT 48.2
Elmers, Hans-Joachim ..... MA 36.9, O 2.4, O 42.9, TT 14.4, QI 6.5
Elsaid, Abdelrahman ..... •MA 7.28
El-Said, Ayman .... DS 20.12, •FM 7.6
Elsaid, Mohammad ..... MA 7.42
Elsässer, Christian MM 8.3, MM 14.3, •MM 34.3, MM 39.8, QI 1.8
El-Sayed, Hesham ..... MA 7.24
Elsholz, Markus ..... DD 23.4
Elsner, Jan ..... •O 97.6
Elsonbaty, Sawsan Mohamed BP 7.2
Elstner, Marcus ..... CPP 14.2
Elu, Ugaitz ..... O 43.8
Elwakeel, Ahmed ..... •HL 20.46, HL 20.56
Elz, Jonas ..... •HL 26.19
Emami, Mohammadamin .. MM 18.6
Emami, Ronak Sarmasti ..... HL 48.5
Emde, Victor ..... BP 14.47
Emeis, Christoph ..... O 98.2
Emeis, Christopher . O 84.11, TT 84.11
Emmerling, Monika . HL 1.12, HL 15.2, HL 20.30
Emmrich, Lars ..... •TT 61.10
Emrick, Todd ..... CPP 17.42
Emtenani, Pouria ..... HL 40.6
Enderle, Mechthild ..... MA 3.6
Enderlein, Niklas .... O 71.12, O 71.13, O 84.3, TT 66.12, TT 66.13, TT 84.3
Enders, Axel ..... DD 36.2, DD 42.1
Enders, J. ..... AKBP 1.1
Enders, Joachim AKBP 2.3, AKBP 8.1
Endler, L. ..... •MA 7.14
Endres, Noah ..... O 42.7
Enenkel, Nicklas ..... MA 6.8
Ener, Semih ..... FM 9.4
Enezz, Mohammad ..... DY 25.5
Eng, L. M. ..... O 57.6
Eng, Lukas ..... FM 12.2, O 43.5
Eng, Lukas M. ..... •FM 12.6, FM 14.1, FM 14.2, FM 18.3, MA 6.6, O 52.3
Engart, Markus . AKBP 2.3, •AKBP 8.1
Engel, Andy ..... DS 21.9
Engel, Dieter ..... MA 27.1
Engel, Eric ..... •O 30.1, O 48.2
Engel, Lena ..... HL 34.2
Engel, Manuel ..... •HL 23.9
Engel, Nicole ..... HL 13.7, •HL 20.5, HL 20.6
Engelhardt, Felix ..... •MM 39.1
Engelhardt, Jonathan ..... O 58.3
Engel-Herbert, Roman ..... DS 20.26, HL 23.6, HL 40.1
Engelke, Fabian ..... •MA 10.2
Engelmann, Nora CPP 15.6, CPP 57.1
Engert, Florian ..... BP 14.38
Engin, Ibrahim ..... HL 20.41
Englhardt, Julian ..... •QI 2.7
Engstfeld, Albert ..... O 97.4
Engstfled, Albert K. ..... O 24.2
Engström, Lena ..... •DS 12.4
Ennen, Inga ..... CPP 46.14

Enns, Manuel ... MM 14.3, •MM 39.5
Enns, Walter ..... O 38.5, O 66.5
Enss, C. ..... TT 22.31
Enss, Christian ... TT 22.18, TT 22.19, TT 22.20, TT 22.21, TT 22.22, TT 22.27, TT 22.28, TT 22.29, TT 22.30, TT 28.2, TT 82.2
Enzner, Stefan ... DS 20.43, MA 24.1, O 74.4, TT 36.1, TT 68.4
Eobaldt, Edwin .. HL 20.21, HL 26.47, HL 35.5
Er, Chen-Chen ..... •MM 11.6
Erarslan, Zekiye ..... •CPP 7.3
Eratam, Fulden ..... O 83.1
Erb, Andreas ..... TT 22.25
Erb, Denise J. ..... •O 68.4
Erb, Roger ... DD 5.3, DD 6.1, DD 15.1, DD 28.3
Erbaş, Aykut ..... CPP 39.2
Erbe, Artur FM 11.36, HL 17.9, HL 18.4, HL 18.7, HL 20.46, HL 20.56, HL 47.3, HL 56.1, TT 32.4, TT 32.7
Erben, Daniel ..... •HL 54.11
Ercelik, Merve .O 15.11, O 17.4, O 77.6, O 99.11
Erdmann, Sebastian ..... •TT 72.7
Erdmenger, Johanna ..... •SYBS 1.4, TT 86.1
Eremenko, Zoya ..... •FM 11.11
Eremin, A. ..... MA 36.3
Eremin, Ilya MA 8.12, TT 5.6, TT 56.5, TT 69.9
Eremin, Ilya M. .... TT 43.10, TT 69.7
Erhardt, Jonas .... DS 14.3, DS 20.43, •O 63.5, O 63.8, O 74.4, •TT 55.5, TT 55.8, TT 68.4
Erhardt, Nina Girotto . O 71.8, TT 66.8
Erichson, Felix ..... BP 14.54, BP 18.2
Eriksson, O. ..... MA 7.14
Eriksson, Olle .... MA 34.1, MA 34.11, MA 50.7, MA 58.9, MM 37.5
Eriksson, Susanna ..... DS 3.3
Erlenbach, Alena ..... TT 24.3
Erni, Rolf ..... MA 3.11
Ernst, A. ..... MA 27.8
Ernst, Arthur ..... DS 11.8, O 2.1
Ernst, Frederik ..... UP 3.5
Ernst, Karl-Heinz ..... O 9.11, O 69.10
Ernst, Marcel ..... BP 14.95
Ernst, Matthias ..... DY 46.9, TT 75.9
Ernstofer, Ralph ... O 40.10, TT 37.10
Ernstorfer, Ralph .. MA 7.18, MA 27.2, MA 33.12, O 22.5, O 38.4, O 38.7, O 40.11, O 71.10, O 71.11, O 98.7, TT 37.11, TT 66.10, TT 66.11
Eroms, Jonathan . •HL 30.2, •TT 59.2
Errea, Ion ..... FM 6.6
Ersfeld, Klaus ..... BP 14.4
Ersoy, Ibrahim Talha ..... DY 58.10, SOE 17.10, •AKPIK 2.5, AKPIK 5.9
Erten, Onur ..... TT 86.5
Ertl, Berhard ..... DD 27.6
Ertural, Christina ..... MM 22.3
Erzberger, Anna .... BP 3.5, BP 12.10, BP 16.3, DY 47.1
Esat, Taner ..... O 9.5, O 17.1, O 83.7
Esattore, Mauro ..... •TT 28.3
Esch, Friedrich ..... O 23.9, •O 52.1
Eschenlohr, A. ..... MA 7.14
Eschrig, Matthias .. TT 73.8, TT 97.3, TT 98.6
Escobar-Galindo, Ramon ... FM 11.24
Escolano, Joan-Carles ..... BP 14.43
Escoto, Esmerando ..... AKBP 13.1
Esenkova, Nadezhda ..... •BP 8.5
Eserin, Samuel C. ..... HL 11.6
Eshaghi, Ghazaleh ..... •BP 26.11, •CPP 43.11, DS 14.9
Eskandari, Mohammad Amin BP 7.30
Esmann, M. ..... HL 54.10, •HL 54.12
Esmann, Martin .... HL 54.8, HL 54.9
Esparza, Rolando. .... O 67.3, O 67.11
Espinosa, Maria ..... HL 23.6
Espinosa Rodriguez, Edgar .. DY 62.5
Esposito, Marina .... TT 4.11, TT 49.2
Esposito, Massimiliano ..... DY 9.1, DY 27.5
Esposito, V. ..... MA 25.6
Esquembre-Kucukalic1, Ali .... O 7.2, TT 9.2
Essa, Ali ..... O 88.5
Esser, Norbert ..... O 13.11, O 58.3, •O 86.6, O 86.8
Esser, Sebastian ..... MA 52.37
Esses, Branden ..... HL 46.1
Essich, Leonard ..... •TT 93.1
Estabrook, Ian D. .. •BP 3.5, BP 37.12
Estandia Rodriguez, Saul .... TT 81.1
Esteban, Ruben ..... O 43.13
Esteve-Paredes, Juan Jose . •HL 36.3
Estevez Moya, Daniel ..... DY 6.7
Estevez Rams, Ernesto ..... DY 6.7
Estevo Silva Frehse, Vinicius •MA 11.3, •TT 21.3
Estillac Leal Silva, C. ..... •MA 52.24
Etehadi Abari, Najmeh ..... •QI 11.2
Etesse, Jean ..... QI 18.1
Etzkorn, Markus .. DS 20.21, FM 5.11, O 19.9, O 35.7, O 43.14, TT 81.5
Euchler, Eric .... •CPP 54.2, CPP 59.1
Eugenio, Carlos F. ..... MA 3.3
Eul, Tobias ... MA 54.8, O 8.1, O 14.2, •O 14.4, O 27.5, O 40.16, O 42.2, O 57.4, TT 37.16
Evangelou, Evangelos ..... DS 20.5
Evans, Martin R. ..... DY 7.7
Evans, Richard ... MA 7.39, •MA 14.5
Everett, Christopher ..... CPP 44.3
Everett, Christopher R. ..... CPP 53.2
Evers, Ferdinand ... DY 13.3, DY 42.9, MA 12.2, TT 19.3, TT 63.9, TT 92.10, TT 93.13
Everschor-Sitte, Karin •PLV II, DY 6.6, DY 61.4, FM 12.4, MA 7.38, MA 7.43, MA 7.71, MA 7.72, MA 37.3, MA 58.7, O 26.4, O 96.2, TT 6.6, AKPIK 5.2, AKPIK 5.4
Everts, Jeffrey .. CPP 10.10, DY 16.10, •DY 34.4, DY 34.5
Ewald, Björn ..... HL 15.2, O 96.1
Ewen, Yvonne ..... •JOB 2.3
Ewert, Moritz ..... O 84.6, TT 84.6
Expósito, Diego ..... O 15.1
Eyre, Lissa ..... MM 4.2
F. A. van der Vegt, Nico .. CPP 46.56, DY 43.8
F. Annett, James ..... MA 33.6
F. Dillenburg, Rodrigo ..... •BP 4.5
F.G.A Janssen, Johan .....CPP 58.2
F. Keller, Thomas ..... CPP 46.17
F.P. Seifert, Urban ..... TT 4.7
Faaber, Florian ..... O 43.6, O 80.4
Fabelo Rosa, Oscar Ramon MA 47.10
Faber, Christian ..... •BP 14.71
Fabian, Jaroslav ... DS 12.2, MA 7.45, MA 35.9, MA 58.10, TT 60.9, TT 73.9, TT 97.2
Fabian, Rachow ..... •O 88.9
Fabrizio, Michele .... TT 13.8, TT 14.6
Fabry, Ben ..... BP 14.64
Fachechi, Alberto •DY 45.3, •SOE 14.3
Facio, Jorge I. ..... MA 24.3, TT 11.4, TT 36.3
Facio, Jorge Ismael ..... O 2.5
Fackelman, Eric ..... O 45.9
Facsko, Stefan ..... DS 20.12, O 68.4
Fadler, Paul . O 14.9, O 38.8, •TT 4.12, TT 51.5, TT 91.3
Fadon, Andres Perez ..... TT 61.12
Faedi, Filippo ..... •DY 34.8
Fagan, William ..... BP 32.9, DY 52.9
Fähler, Sebastian .•MA 13.3, MM 21.8
Fahler-Muenzer, Philipp .... •FM 12.3, MM 4.4
Fahrensohn, Maike ..... •MA 40.5
Fairclough, Simon M. ..... FM 18.5
Fairman, Sam ..... O 96.5
FAIRmat team, The ..... AKjDPG 1.1
Faitsch, Marcin ..... TT 29.10
Faivre, Damien BP 1.1, CPP 1.1, DY 4.1
Fakhera, Fahmida ..... •FM 23.2
Fakhri, Nikta ..... SYBS 1.5
Falconer, Kathleen . •DD 38.1, DD 41.2
Falk, Stefanie . PSV I, •UP 6.2, UP 8.4
Falk, Sven ..... BP 14.64
Falke, Yannic ..... O 54.4
Falling, Lorenz ..... O 23.10
Falorsi, Francesca ..... DS 20.50
Falsina, Francesco ..... •CPP 17.37
Falta, Jens . HL 20.66, O 10.3, O 84.6, TT 16.3, TT 84.6
Falter, Christine ..... •QI 6.2, QI 14.26
Faltinath, Jonas ..... MA 49.4
Fan, Benshu ..... •O 49.4, O 79.3
Fan, Chongxiao ..... •O 79.1, O 79.3
Fan, Yinan ..... CPP 46.23
Fan, Yuzhe ..... BP 30.5, CPP 47.5
Fanciulli, Mauro ..... •O 14.1, O 93.6
Fandré, Jean Pascal ..... MA 36.1
Fändrich, Marcus ..... BP 20.3
Fandrich, Tom ... DS 20.21, HL 20.45, HL 20.51, •HL 55.10
Fang, Chi ..... •MA 35.4, •TT 60.4
Fang, Lei .... MA 43.5, O 15.6, O 15.9, O 56.3
Fang, Wei ..... AKPIK 5.10
Fang, Xufei ..... MM 23.1, MM 23.2, MM 23.3, MM 23.5, MM 27.3, MM 34.2
Fang, Yindong ..... MM 19.31
Fang, Yue-Wen ..... •FM 6.6
Fangohr, Hans .... MA 34.4, MA 50.2, •MA 58.1
Fantauzzi, Marzia .. MA 29.3, TT 46.3
Fantin, Andrea ..... MM 11.1
Faouri, Sinan S. ..... •MM 13.8
Farace, Bonaventura ..... AKBP 13.1
Farago, Jean ..... CPP 46.22
Farajian, Mahboubeh ..... BP 7.43
Faramarzi, Farzad ..... QI 11.8
Faramawy, Ahmed ..... •MA 7.24
Faravelli, Tiziano ..... DY 28.3
Farenbruch, Andreas ..... HL 49.3
Farhan, Ahlam ..... •FM 11.38
Farhood, Amir . •AKBP 9.3, AKBP 9.4
Faria Junior, Paulo E. ..... DS 12.2
Farinacci, Laëtitia ..... •O 9.9, O 15.7, O 89.1, O 89.5
Farkas, Lorant ..... QI 21.9
Farle, Michael ..... MA 50.1, MA 50.8
Farrel, Aloysius ... •HL 18.8, •TT 32.8
Farrell, Patricio ..... HL 4.8, HL 38.9
Farutin, Alexander ..... BP 27.5
Fasano, Yanina ..... TT 11.3, TT 11.4
Fasel, Roman ..... MA 5.9, TT 7.9
Fassbender, Jürgen ..... MA 12.4, MA 30.8, MA 35.6, MA 49.1, MA 57.2, TT 60.6
Fassl, Paul ..... HL 4.5
Fatayer, Shadi ..... O 58.5, O 99.11
Fatemi, Valla ..... TT 43.8
Fatihi, Mohamed Yassine .... O 86.6, •O 86.8
Faugéras, Clément ..... DS 12.8
Faugier-Tovar, Jonathan ..... QI 18.1
Faupel, Franz ... CPP 15.3, CPP 17.48
Fauseweh, Benedikt .. TT 29.4, QI 1.4, •QI 1.6, QI 3.2, QI 5.7
Faust, Rüdiger ..... TT 92.9
Fawaz, C. ..... O 19.10
Fawaz, Chafic ..... •TT 14.4
Fayaz, Muhammad •O 70.6, •TT 65.6
Fayet, Olivier ..... •TT 61.1
Fazlizhanova, Dina I. ..... TT 5.6
Fecher, Gerhard . MA 39.9, MA 52.28, MA 52.29
Fechner, M. ..... •MA 4.4
Fechner, Michael ..... MA 4.3
Fedchenko, O. O 19.10, O 59.2, O 93.9, TT 48.2
Fedchenko, Olena ..... O 2.4, TT 14.4
Federl, Maria ..... O 40.7, TT 37.7
Federl, Maria-Elisabeth ..... •O 66.2
Federolf, Mathias ..... HL 20.30
Fedorov, Alexander ... MA 8.5, TT 5.7
Fedorov, Arkady ..... O 48.6
Fedorov, Kirill ..... QI 2.4
Fedorov, Kirill G. ..... TT 28.7, QI 14.7, QI 14.8, QI 18.2, QI 18.3
Feenstra, Louw ..... TT 41.6
Feggeler, T. ..... MA 50.3
Fehér, Titusz ..... MA 16.8
Fehlinger, Paula ..... DD 27.6
Fehrenbach, Miriam ..... HL 12.5
Fehrenbach, Miriam J. ..... •HL 9.4
Feigl, Julius ... QI 8.3, •QI 11.6, QI 11.9
Feis, Joshua ..... DY 48.6
Feist, Armin O 49.3, •QI 2.6, AKBP 9.6
Feitosa, Victor ..... O 9.8
Fejes, Ignác ..... •MA 16.8
Felber, Korbinian .. •HL 16.6, HL 20.61
Felderer, Michael ..... QI 5.5
Feldkamp, Finn ..... •MA 7.72
Feldmann, Claus ..... BP 9.5
Felekary, Arash ..... •BP 40.4
Felgner, Judith ..... TT 28.6, TT 28.9
Felixberger, Fabian ..... •DS 21.8
Feller, Déborah CPP 17.44, •CPP 42.2
Fellows, Alex ..... O 61.3
Fellows, Alexander P. . O 87.7, O 95.5, TT 96.5
Felsen, Frederic ..... O 23.4
Felser, Claudia ..... DS 4.1, DS 20.51, FM 22.1, FM 22.2, HL 8.11, MA 7.36, MA 24.2, MA 33.5, MA 40.8, MA 52.28, MA 52.29, MM 30.6, MM 40.1, MM 40.3, O 43.5, O 63.4, TT 3.1, TT 4.10, TT 36.2, TT 44.2, TT 49.2, TT 49.5, TT 55.4, TT 57.7, TT 93.15
Felton, Solveig ..... MA 42.7
Fendler, Cornelius ..... MA 39.7
Feneberg, Martin ... HL 57.1, HL 57.2, HL 57.3
Feng, Kai ..... CPP 28.1, DY 29.1
Feng, Liwen ..... •TT 14.8
Feng, Shi . •DY 13.2, •TT 19.2, TT 72.9
Feng, Wuhu ..... UP 6.6
Feng, Xiaolong ... MA 54.3, MM 40.1, MM 40.3, •TT 3.1
Feng, Xinliang ..... O 6.2
Feng, Xu Yang ..... TT 69.1
Feng, Yuzhen ..... •BP 7.17
Feng, Zili ..... TT 41.4
Feoktystov, Artem ..... MA 7.25
Feraco, Giovanna .... O 76.4, TT 27.4
Ferch, Marc ..... CPP 17.36
Ferenz, Hannah ..... •BP 41.2
Fergusson, Joannah ..... BP 14.42
Feringa, Ben L. ..... O 69.11
Feringa, Stijn ..... FM 12.10
Fernandes Eleno, Luiz Tadeu TT 80.9
fernandes, rafael .. MA 20.4, TT 57.11
Fernandes, Rafael M. ..... MA 8.8, MA 47.6
Fernandes, Thales ..... BP 41.1
Fernández, Cynthia C. ..... O 4.2
Fernandez, Javier ..... QI 15.5
Fernández Scarioni, Alexander MA 7.77
Fernandez-Diaz, Maria Teresa MA 19.6, TT 31.6
Fernández-Fernández, David •HL 38.4
Fernández-íiaz, María Teresa .MA 7.2
Fernández-Pacheco, Amalio .MA 6.5, MA 55.6, MA 59.6
Fernández-Rossier, Joaquín .. DS 1.3, MA 5.9, O 15.1, TT 7.9
Fernando Cardozo Licha, Andrés AKPIK 2.5
Fernengel, Bernd Michael .. •DY 51.3, •SOE 15.3
Ferosh, Fathima .. BP 31.2, CPP 50.2
Ferran pousa, Ángel ..... AKBP 12.3
Ferrari, Franco . •CPP 24.4, CPP 29.5
Ferrarini, Alberta ..... CPP 9.5
Ferree, Maria ..... •HL 15.1
Ferreira, Matheus ..... HL 4.1
Ferreira, Pedro ..... O 35.2
Ferrer, Jaime .... MA 42.2, MA 58.10
Ferretti, Alessandro ..... MA 30.9
Ferretti, Andrea ..... O 84.7, TT 84.7
Ferro, Giuseppe Maria ..... SOE 9.5
Fery, Andreas ..... BP 7.8, CPP 41.7
Feser, Daniel ..... •MA 52.40
Feser, Markus S. ..... DD 39.3
Fessler, Florent ..... BP 16.10
Festring, Lars ..... •AKBP 3.2
Feuerle, Marius ..... UP 7.3
Feyer, Vitaliy .... O 9.1, O 61.1, O 69.2, O 69.6, O 83.4, O 83.6
Feyerherm, Ralf .... •MA 7.1, TT 23.1, TT 26.7, TT 26.8, TT 26.10, TT 57.2
Feyrer, Simon ..... TT 22.24, TT 73.7
Fialkowski, Jan ..... •SOE 9.4
Fichte, Lydia ..... •O 18.5
Fiebig, Manfred .... FM 4.7, FM 23.5, MA 7.32, MA 24.2, MA 27.9, O 98.2, TT 25.1, TT 25.3, TT 33.3, TT 36.2
Fiedler, Jill ..... DD 8.3
Fiedler, N. ..... •TT 22.31
Field, Mitchell ..... QI 11.4, QI 11.5
Fiete, Gregory A. ..... HL 8.11
Figge, Stephan ..... HL 12.3
Figueiredo, Johannes ..... HL 13.2, •HL 13.5
Fikáček, Jan ..... TT 52.5
Fikar, Jan ..... MA 34.5
Filip, Radim ..... QI 9.2, QI 14.2
Filipiak, Zuzanna Helena . •MM 19.43
Filipp, Stefan .. TT 28.7, QI 2.1, QI 2.7, QI 8.3, QI 11.6, QI 11.9
Filippozzi, Davide ..... •AKPIK 5.10
FILIZ, Volkan ..... MM 16.4
Filk, Thomas ..... DD 6.2, DD 17.1, •DD 19.2
Filsinger, Luis ..... TT 14.4
Filzmoser, Johannes ..... •O 94.3
Finco, Aurore ..... MA 59.7, •TT 24.5
Findeisen, Stefan .... HL 56.2, QI 2.9
Fingerhut, Benjamin Philipp CPP 23.5, DY 24.5
Fingerhut, Jan ..... •O 34.7

Fingolo, Ana C. ..... DS 21.2
Finizio, Simone ..... DS 6.1, MA 7.81, MA 8.13, •MA 46.4
Fink, Jörg ..... •TT 14.3
Fink, Nico ..... •DY 41.6
Fink, Tim ..... DS 20.49
Fink-Bauer, Christa ..... •FM 11.27
Finke, Birk .... O 10.10, O 72.1, O 85.5, O 98.4, TT 16.10, TT 67.1
Finkelstein, Ran ..... QI 2.3
Finkler, Jonas A. ..... MM 19.1
Finley, Jonathan J. ..... O 38.4
Finn, R. ..... MA 25.6
Finnseth, Øyvind .. •MA 3.4, MA 24.3, O 2.5, TT 36.3
Finocchio, Giovanni ..... MA 55.2
Fiolka, Reto ..... BP 14.38
Fiore Mosca, Dario •MA 19.2, •TT 31.2
Fiorenza, Shane ..... •BP 2.3
Fiorenza, Shane A. BP 32.11, DY 52.11
Firschke, Caroline ... •O 43.6, O 43.9, O 80.4
Fischbach, Sarah ..... •PSV II
Fischer, Ammon ... •TT 12.4, TT 44.4
Fischer, Benedikt ..... BP 12.2
Fischer, Carolin ..... CPP 54.4
Fischer, Charlotte ..... •DD 16.2
Fischer, Elias ..... •BP 1.3, •CPP 1.3, •DY 4.3
Fischer, Franz ..... HL 3.4, •HL 13.6
Fischer Friedrich, Elisabeth . BP 27.11
Fischer, Inga A. ..... O 96.6
Fischer, Jannis ..... •BP 7.30
Fischer, Jeison .. •O 7.1, O 7.6, O 10.1, O 10.5, O 10.8, O 15.4, O 17.7, O 17.12, O 59.1, O 62.8, O 64.3, O 89.8, O 99.10, •TT 9.1, TT 9.6, TT 16.1, TT 16.5, TT 16.8, TT 48.1, TT 54.8
Fischer, Kira ..... •CPP 3.5
Fischer, Kirsten .... DY 58.7, DY 58.8, SOE 17.7, SOE 17.8
Fischer, Lukas .. CPP 42.6, •MA 35.3, •TT 60.3
Fischer, Marisa .. •DY 51.2, •SOE 15.2, SOE 16.1
Fischer, Mark ..... TT 57.7
Fischer, Max ..... •TT 62.8
Fischer, Mirko ..... •CPP 46.53
Fischer, Peer ..... BP 7.55, BP 7.56, BP 30.2, CPP 47.2
Fischer, Peter ..... MA 44.6, TT 76.6
Fischer, Roland A. ..... CPP 16.2
Fischer, Saskia F. ... •HL 23.6, TT 5.5
Fischer, Tobias .. BP 26.11, CPP 43.11
Fischer, Tristan ..... MA 36.9
Fisher, Ian R. ..... O 84.8, TT 84.8
Fistul, Mikhail V. ..... TT 43.10
Fittipaldi, Rosalba .... O 80.3, TT 81.3
Fittipaldi, Rosalba Tatiana ... HL 23.1
Fitzek, Frank ..... HL 56.4
Fitzek, Frank H. P. .. HL 55.7, HL 56.5
Fitzgerald, J. M. ..... HL 54.10
Fitzgerald, Jamie ..... HL 54.9
Fitzpatrick, Erin G. ..... AKBP 5.2, AKBP 8.5
Fitzpatrick, Erin Grace ..... AKBP 5.1
Fix, Andreas ..... UP 7.4
Fix, Mario ..... MA 38.4
Fjellvåg, Ø. S. ..... TT 25.9
Fjellvag, Oystein ..... MA 17.2
Flacke, Luis ..... MA 51.8, TT 88.8
Flasby, Alexander ..... SYBT 1.2
Flashar, Katarina S. . HL 9.4, •HL 12.5, HL 12.7, HL 42.3
Flasse, Lydie ..... BP 14.49
Flathmann, Christoph ..... TT 5.6
Flatté, Michael ..... MA 48.10
Fleck, Julian ..... SOE 16.1
Fleck, Julian Luca •DY 51.4, •SOE 15.4
Flege, Jan I. ..... O 96.6
Flege, Jan Ingo .... CPP 16.4, DS 9.4, DS 9.5, DS 11.5, MA 7.76, O 10.3, O 23.3, O 84.6, O 88.7, O 88.9, O 88.10, TT 16.3, TT 84.6
Flegr, Salome ..... DD 27.2, DD 30.4
Fleig, Jürgen ..... O 52.4
Fleischmann, A. ..... TT 22.31
Fleischmann, Andreas ..... TT 22.18, TT 22.19, TT 22.20, TT 22.21, TT 22.22, TT 22.27, TT 22.28, TT 22.29, TT 22.30, TT 28.2, TT 82.2
Fleischmann, Thomas ..... HL 15.2
Flemming, Moritz ..... CPP 17.24, •CPP 38.5
Flenner, Silja ..... BP 14.44
Flommersfeld, Constantin .... O 71.4, O 99.5, TT 66.4
Florea, Ileana ..... HL 20.34, HL 57.5, O 62.3, TT 54.3
Flores- Calderón, Rafael ..... TT 44.5
Flores Calderon, Rafael Alvaro •TT 86.2
Flores, Marcos ..... O 67.3
Florez-Ablan, Diego ..... •TT 13.2
Florian Deißenbeck, Florian ... O 13.3
Florian, Schneider ..... O 5.2
Flory, Mario ..... QI 21.2
Flöter, Eberhard Lukas ..... •MM 31.1
Flötotto, Aaron ... CPP 9.6, •MM 26.2
Flurin, Emmanuel ..... TT 50.6
Fodor, Etienne ..... •DY 49.3, DY 49.4
Foerst, M. ..... MA 4.4
Foerster, Johannes M. ..... BP 2.11
Foerster, Moritz ..... AKBP 8.7
Foffi, Giuseppe ..... DY 62.7
Foggetti, Francesco ..... •MA 12.6
Föhlisch, Alexander ..... TT 14.5
Foini, Laura ..... DY 59.11, TT 99.11
Fokdal, Christian V-B. ..... O 95.11, TT 96.11
Folkers, Bart ..... •DD 36.3
Folland, T. G. ..... O 57.6
Fölsch, Stefan ..... HL 48.1
Fomin, Mykola ..... BP 20.9
Fomin, Vladimir M DS 20.29, FM 11.11
Font-Martín, Daniel ..... BP 3.3
Foppa, Lucas ..... MM 5.3, •MM 5.6, MM 13.6
Forbert, Harald ..... TT 91.4
Forero-Martinez, Nancy C. ... DY 54.5
Förg, Michael ..... DS 21.8
Forker, Roman O 6.8, O 30.2, •O 45.3, O 45.8, O 45.11, O 83.2
Fornoville, Max ..... •TT 2.7
Forozi Sowmeeh, Paria ..... •HL 4.7
Forrer, Luca ..... QI 14.25
Forschner, Lukas ..... O 24.2
Först, Michael ..... MA 4.3, •MA 25.1
Förster, Mona ..... BP 11.11
Förster, Moritz ..... •DD 3.1, DD 30.2
Forster, Robin P. ..... •O 2.2
Förster, S. ..... HL 45.1
Förster, Stefan O 28.5, O 40.9, O 55.1, TT 37.9
Förster, Stephan ..... •CPP 36.1
Forsthuber, Hannah ..... •AKBP 10.4, AKBP 11.1
Forti, Mariano ... •MM 11.4, MM 19.17
Fortmann, Jill ..... FM 6.8
Fortmann, Jonas D. ..... •O 85.5
Fortunato, Isabela Corina ... BP 27.2
Fösel, Angela ..... DD 42.2
Fossati, Félix ..... •TT 13.3
Foster, Adam ..... O 44.4, AKPIK 5.11
Foster, Adam S. ..... O 5.5, O 12.2
Foster, Brian ..... AKBP 12.4
Fountoulakis, Ilias .... UP 3.3, UP 5.2
Fowley, Ciaran ..... HL 18.4, TT 32.4
Fraboni, Beatrice ..... •HL 2.4
Fraboulet, Kilian ..... TT 2.7, TT 13.4, •TT 13.10
Fraenkel, Shachar ..... •QI 2.3
Fragkopoulos, Alexandros A. BP 1.10, CPP 1.10, DY 4.10
Fragkos, Konstantinos ..... UP 3.3
Fraile-Carmena, Álvaro ..... O 47.4
França, Hugo ..... •DY 34.3
Franceschi, Giada ..... •O 80.1
Franchetti, Giuliano ..... AKBP 7.4
Franchini, Cesare .... MA 3.2, O 93.8
Francini, Niccolò ..... •TT 26.5
Franco-Oñate, Maria-Jose .. •BP 3.11
Frank, Bettina . O 26.4, O 57.3, O 79.5, O 85.7
Frank, Felix ..... MM 40.7
Frank, Jonathan ... DS 20.31, DS 21.1
Franke, Katharina ..... O 9.9
Franke, Katharina J. .. O 43.6, O 43.9, O 46.1, O 71.4, O 80.4, O 99.5, TT 50.8, TT 66.4, TT 73.3
Franke, Lars ..... MA 9.1, •TT 10.5
Franke, Oliver ..... MA 27.1
Franke, Tristan ..... •BP 7.36
Frankenfeld, Katrin ..... BP 26.11, CPP 43.11
Fransson, Jonas ..... MA 58.12
Frantz, Alexander ..... TT 81.5
Frantz, David ..... SOE 6.3
Franz, Christoph ..... TT 23.3
Franz, Marcel ..... O 84.9, TT 84.9
Franz, Martin ..... O 58.2, •O 58.3
Franze, Kristian ..... BP 3.6, BP 7.45, BP 7.46, BP 7.50, BP 7.53
Franzka, Steffen ..... O 72.1, TT 67.1
Franzke, Katharina Lorena . HL 20.60
Frasca, Chiara ..... HL 4.7
Fraser, Marie-Louise ..... O 58.2
Frasetto, Fabio .... O 40.19, TT 37.19
Frassetto, Fabio ..... O 14.10
Fratino, Lorenzo ..... •DS 7.1
Fratus, Keith R. ..... •MA 6.8
Fraxanet, Joana ..... QI 3.1
Frédéric, Piéchon ..... TT 61.1
Frederik, Bub ..... •DD 15.3
Frederiksen, Thomas . O 3.4, TT 26.6, TT 42.2
Frederking, Felix ..... •TT 44.11
Fredersdorff, Philipp ..... O 88.6
Fredersdorff, Philipp Alexander •O 81.1
Freeman, Mark ..... TT 2.5
Fregin, Bob ..... BP 7.34, •BP 7.35, BP 7.36, BP 7.38, BP 37.3
Frehse, Vinicius ..... TT 81.6
Freibert, Antonia ..... BP 9.6
Freitag, Lasse ..... •CPP 17.8
Frenzel, Jan ..... MM 19.42
Frenzel, Maximilian . MA 25.3, O 49.2
Frerichs, Hajo ..... O 44.11
Freudenberger, J. ..... MA 52.22
Freudenstein, Josef ..... MA 12.2
Freudig, Manuel ..... •QI 3.5
Freund, Daniel ..... HL 22.4
Freund, Robert ..... QI 16.1
Freville, Robin ..... MM 7.10
Frey, Erwin .. BP 1.9, BP 10.9, BP 12.5, BP 12.8, BP 14.48, BP 14.51, CPP 1.9, CPP 18.9, DY 4.9, DY 18.9, DY 22.4, DY 41.8
Frey, Felix ..... •BP 16.6
Frey, Martha ..... •O 72.4, •TT 67.4
Freysoldt, Christoph MM 26.3, O 13.3, O 13.6, •O 48.1
Friák, Martin .... MA 34.5, •MM 8.10, MM 19.26, O 50.4, QI 14.16
Fricke, Kristina ..... DD 38.3
Fricke, Mathis ..... DY 28.3
Friedel, Anna Maria ..... MA 45.5, •MA 48.1
Friedemann, Sven ..... •TT 80.3
Friederich, Pascal ..... •SYAI 1.4
Friedrich, Alexandra ..... CPP 22.2
Friedrich, Benjamin M. ..... BP 14.49, BP 14.62, BP 36.2, •BP 37.12, DY 57.2
Friedrich, Christoph ..... •O 37.6
Friedrich, Florentine ..... •HL 54.2, HL 54.3
Friedrich, Lena . BP 14.24, •MM 19.30, MM 19.48
Friedrich, Niklas ..... •O 12.8
Friedrich Peter Seifert, Urban TT 33.6, TT 86.7
Friedrich, Rico ..... •FM 6.2, FM 6.3, MM 11.6, MM 19.2, O 18.6, O 71.6, O 95.4, TT 66.6, TT 96.4
Friedrichsen, Jan •MA 7.50, MA 47.11
Friege, Gunnar ..... DD 16.2, DD 26.1, DD 27.2
Fries, M. ..... MA 18.1, TT 30.1
Friese, Jan ..... •O 43.15
Friha, Feriel ..... HL 48.6
Friis, Nicolai ..... QI 7.2, QI 16.10
Frijters, Jasmine .... QI 14.7, •QI 14.8
Frion, Anthony ..... UP 5.4
Frisch, Alexander ..... •MM 27.3
Frischknecht, Friedrich ..... BP 1.4, CPP 1.4, DY 4.4
Fritsch, Daniel .... HL 38.9, •HL 40.11
Fritsch, V. ..... TT 25.9
Fritsche, Sarah ..... •BP 7.50
Fritschle, Felix ..... DD 30.7, DD 30.8
Fritz, Jonas H. ..... •DY 7.4
Fritz, Torsten ... O 6.8, O 10.7, O 28.3, O 30.2, O 44.14, O 45.3, O 45.8, O 45.11, O 83.2, TT 16.7
Fritze, Holger ..... FM 11.30, FM 14.4
Fritzsch, Felix ..... DY 32.4, •DY 32.5, TT 45.4, •TT 45.5, QI 7.1
Fritzsche, Marco ..... BP 14.42
Fritzsche, Stephan ..... O 66.5
Fröba, Michael ..... CPP 46.5
Froehlich, Paul ..... O 81.1
Froelich, Benjamin ..... TT 22.3
Froh, Jan ..... UP 3.5
Fröhlich, Kristina ..... FM 2.4
Fröhlich, Markus ..... CPP 26.2
Fröhlich, Paul ..... O 88.6
Fröhlich, Simon ..... MA 55.8
Fröhlich, Simon M. ..... •MA 21.1
Frohme, M. ..... BP 27.8, BP 37.2
Frohn, Marius ..... •TT 43.2
Frölich, Benjamin ..... •O 44.7
Frömter, Robert .. MA 55.2, MA 55.3, MA 55.5, MA 55.9
Frontzek, Matthias •TUT 5.2, •MA 1.2, MA 13.1, •MA 31.11, •TT 47.11
Fruhling, Kyle ..... MA 59.1
Frühwald, Daniel ..... •DY 22.6
Frunzio, Luigi ..... QI 6.10
Fu, Linhui ..... CPP 28.1, DY 29.1
Fu, Meirui ..... •CPP 17.43
Fu, Mengqi ..... HL 18.2, TT 32.2
Fu, Ming ..... O 96.10
Fu, Mingxuan ..... TT 41.4
Fu, Zouchen ..... HL 52.1
Fuchs, Alexander ..... •AKjDPG 1.3, AKPIK 6.3
Fuchs, Andreas ..... DD 6.2, DD 17.1
Fuchs, Florian ..... HL 48.8
Fuchs, Jean-Noël ..... TT 61.1
Fuchs, Josefin ..... MA 7.67
Fuchs, Laura ..... •CPP 53.4
Fuchs, Matthias ..... AKBP 8.3
Fuchs, Maximilian ..... CPP 6.4
Fuchs, Till ..... •FM 5.4
Fuente Santiago, Carmen .... DS 12.6
Fuerst, Mia ..... O 4.6
Fuhrberg, Andreas .. •QI 6.5, QI 14.23
Führer, Julian ..... HL 13.7, HL 20.6
Fuhrmann, Benjamin ..... O 58.3
Fuhrmann, Falko ..... HL 15.7
Fuhrmann, Felix ..... MA 2.8
Fuhrmann, Jana F. ..... BP 3.4
Fuhrmann, Martin ..... HL 15.7
Fujan, E. ..... BP 27.8
Fujii, Minoru ..... BP 9.4
Fujii, Syuji ..... CPP 33.4
Fujimoto, Naoki ..... HL 57.1
Fujta, C. ..... MA 18.1, TT 30.1
Fujta, Christopher . CPP 28.1, DY 29.1
Fukaya, Yuri ..... TT 98.5
Fulga, Cosma ..... AKPIK 5.12
Fulga, Ion Cosma . MM 19.24, O 63.6, TT 41.8, TT 55.6
Fullerton, Eric ..... MA 14.4
Füllgraf, Merlin ... DY 59.10, •TT 53.8, TT 99.10
Fumega, Adolfo O. ... O 59.7, TT 48.7
Fünfhaus, Axel ..... •TT 83.1
Funk, Johannes .... DD 30.7, DD 30.8
Fürch, Elise ..... O 83.2
Furlanetto, Federica ..... BP 14.64
Furo, Mizuki ..... O 84.5, TT 84.5
Fürst, Maximilian ..... •TT 61.8
Fürthauer, Sebastian ..... BP 29.3, BP 36.3, CPP 45.3, DY 57.3
Furusaki, Akira ..... TT 6.5
Furuta, Kanji ..... •HL 20.40
Fußangel, Jonas ..... •O 89.9
Fusek, Lukáš ..... O 13.12
Fyta, Maria ... BP 2.7, BP 2.8, BP 2.9, CPP 46.42
Fytas, Nikolaos G. ..... DY 15.5
G. G. de V. D. Da Silva, Luis . TT 69.10
G Gopakumar, Thiruvancheril O 46.10
G. Henriques, João C. ..... DS 1.3
G. L. Brito, Thiago ..... O 9.8, •O 12.6, O 95.6, TT 96.6
G. Vergniory, Maia MA 47.4, TT 14.10
Gaafer, Haitham ..... •MM 22.4
Gaal, Peter ..... MM 21.8
Gabathuler, Jérôme ..... UP 6.1
Gaber Abdelmagid, Ahmed .. HL 15.3
Gabriel, Philipp ..... MA 50.5
Gachon, Emilie BP 1.1, CPP 1.1, DY 4.1
Gacka, Ewelina ... •HL 18.3, •TT 32.3, QI 2.9
Gadge, Karun ..... O 86.7, •TT 44.9, TT 70.3
Gadjisade, Natawan ..... •BP 11.10
Gadzekpo, Aaron ..... •BP 15.4
Gaebel, Simon ..... MA 7.67
Gaël, Reecht ..... O 83.3
Gaerner, Maik ..... MA 5.1, MA 7.62, MA 7.63, MA 39.6, MA 39.13, •MA 47.8, MA 54.11, TT 7.1
Gahl, Cornelius ..... O 42.4
Gaikwad, Vikram ..... BP 20.5
Gaimann, Mario U. ..... DY 6.3
Gaisina, Elvina ..... •MM 34.1
Gajda, R. ..... CPP 32.3, DY 35.3
Gajdics, Marcell ..... •DS 6.4
Gajendra Babu, Keshav ..... BP 27.10
Gajendragad, Vaishnavi ..... DY 49.1

Galanis, Thanos ..... TT 81.1
Galazka, Zbigniew ... DS 9.5, HL 35.1, HL 40.2, HL 40.6
Galdino, Carlos William ..... MA 30.4
Galesic, Mirta ..... SOE 2.8
Gali, Adam ..... •HL 11.5
Gali, Virginia ..... TT 40.4, TT 41.10
Galiana, Beatriz ..... HL 20.34
Galicia, Asier ..... QI 8.5
Galindez Ruales, Edgar .... MA 29.10, TT 46.10
Galíndez-Ruales, Edgar ..... MA 2.8, MA 29.9, MA 47.9, TT 46.9
Galinski, Henning ... DS 16.1, O 96.12
Galinski, Maximilian ..... O 88.6
Galla, Tobias ..... •DY 8.8, DY 33.10, DY 48.3, SOE 10.2
Gallardo, Rodolfo ..... MA 57.2
Gallardo-Navarro, Oscar ..... BP 1.9, CPP 1.9, DY 4.9
Gallego, Fernando ... MA 3.1, TT 81.1
Gallego Lacey, Oliver ..... O 54.4
Gallegos, Alejandro ..... CPP 21.3
Gallegos, Miguel ..... BP 15.6
Galleogos Gonzalez, Miguel CPP 29.2
Galler, Anna ..... •TT 12.2
Gallet, J.-J. ..... O 85.2
Galliano, Leonardo ..... DY 62.7
Gallo, Alejandro ..... TT 51.3
Gallo, Marta ..... •BP 16.11
Galm, Anja ..... DD 30.7, DD 30.8
Gambardella, P. ..... MA 48.11
Gambardella, Pietro MA 29.3, TT 46.3
Gammon-Smith, Adam TT 70.5, QI 1.9
Gampl, Niklas ..... •BP 3.6
Gan, Ziyang ..... HL 30.2, TT 59.2
Gandhi, Hensi ..... •BP 7.13
Gandhi, Yashas Tejaskumar •CPP 49.3
Gandorfer, Simon .... QI 14.7, QI 14.8, QI 18.2, •QI 18.3
Ganduglia-Pirovano, Verónica O 23.3
Ganesan Sekar, Bharathi Ganesh •MM 34.4, MM 39.9
Ganesh, Sandhra ..... •AKPIK 5.7
Ganeva, Marina ..... DS 21.4
Gangadharaiah, Suhas ..... •HL 17.10
Gangloff, Dorian ..... •PLV IV
Ganguli, Ashok Kumar ..... MA 7.26, TT 41.7
Gansäuer, Arvid ..... •AKPIK 5.8
Ganschow, Steffen ..... FM 11.30, FM 14.3, FM 14.4
Ganser, Niels O 33.6, •O 72.1, •TT 67.1
Ganser, Romana ..... •O 42.6, O 80.5
Ganshow, Steffen ..... FM 11.3
Ganss, F. ..... TT 74.5
Ganss, Fabian .... FM 11.24, HL 23.1, MA 45.4, MA 51.1, MA 57.2, MM 21.8, TT 88.1
Ganswindt, Patrick ..... HL 48.4
Ganzer, Fabian ..... •QI 14.3
Gao, Lei ..... MA 39.1
Gao, Qingwei ..... O 87.4
Gao, Y ..... MA 19.7, TT 31.7
Gao, Yongxiang ..... DY 34.1
Gao, Yuan ..... •QI 8.5
Gao, Yueze ..... O 3.2, O 9.12
Garate, Ion ..... TT 83.2
Garbarino, Gaston ... TT 4.8, TT 49.1
Garbellini, Matteo ..... •QI 7.3, QI 9.5
Garcia de Andoin, Mikel ..... QI 3.6
Garcia de Figueiredo, Benjamin BP 32.9, DY 52.9
García de Viedma Guerra, Dolores •CPP 46.46
Garcia Fuente, Amador .... MA 58.10
García Iglesias, Miguel ..... CPP 17.7
Garcia Jr., Ailton José ..... HL 20.38
García Lastra, Juan Maria ... MM 8.4
García, Rodrigo ..... DY 62.8
Garcia Saez, Ana J. ..... •BP 16.1
Garcia, Vincent ..... •FM 18.1
Garcia-Belles, Raquel ..... QI 3.4
García-Blázquez, Manuel A. ... O 15.1
García-Cristóbal, Alberto ..... HL 8.3, O 59.3, O 71.2, TT 48.3, TT 66.2
García-Fuente, Amador ..... MA 42.2
Garcia-Gassull, Laura ..... •MA 33.10
Garcia-Goiricelaya, Peio O 7.4, TT 9.4
Garcia-Herrero, Victor ..... •HL 8.9
García-Iglesias, Miguel .... CPP 22.6
García-Mochales, Paula ..... O 33.5
Garcia-Page, Ana ..... •TT 2.8
Garcia-Ripoll, Juan Jose ..... TT 43.6
García-Tabarés, Elisa ..... HL 20.34
Gardelis, Spiros ..... DS 16.2
Gardiner, Jeff ..... O 44.11
Gareev, Timur ..... MA 30.3
Garg, Bharti ..... •O 27.3, O 27.4
Garg, Nikhil ..... SYBT 1.2
Garg, Shreya ..... •O 35.2
Garg, Sonali ..... •CPP 14.2
Gargiani, Pierluigi ..... O 10.2, O 84.9, TT 16.2, TT 84.9
Gargiulo, Roberto ..... •QI 15.1
Garima, Garima ..... •MA 33.8
Gärner, Maik ..... MA 7.54
Garny, Hella ..... UP 8.6
Garrahan, Juan P. ..... DY 7.3
Garratt, Samuel ..... TT 53.6
Garreis, Julian ..... AKBP 6.1
Garside, Antje ..... BP 27.10
Garst, Markus ..... MA 9.1, MA 9.11, TT 10.5, TT 23.4, TT 81.7
Garthe, Jonathan Linus Samuel •CPP 30.5
Gartmann, Robert ..... TT 22.12
Gärtner, Michael ..... O 46.11
Gärttner, Martin ..... QI 5.9, QI 21.7
Gary, Dominik ... BP 26.11, CPP 43.11
Gaß, Sebastian ..... TT 11.1
Gaspard, Pierre ..... BP 36.6, DY 57.6
Gasser, Marcel .... MA 29.9, TT 46.9
Gastaldo, L. ..... TT 22.31
Gastaldo, Loredana ..... TT 22.21, TT 22.22, TT 22.27, TT 22.28, TT 22.30, TT 82.2
Gastalo, Loredana ..... TT 22.29
Gastiasoro, Maria N. ..... HL 36.3
Gather, Malte ..... BP 14.39
Gather, Malte C. ..... HL 15.3, HL 15.7
Gati, Elena . MA 6.12, MA 8.5, MA 8.8, MA 42.11, TT 25.7, TT 41.5, TT 57.12
Gatti, Gianmarco ..... •O 66.8, O 76.5
Gatti, Matteo . O 38.2, O 59.6, TT 48.6
Gatto, Salvatore ..... •TT 53.4
Gatzmaga, Stefan ..... AKBP 2.2
Gatzsche, Ben Simon ..... AKBP 2.4
Gauch, Kaya ..... •MA 52.11
Gauges, Maira ..... DY 28.3
Gault, Baptiste ..... FM 5.2, MA 50.4, MM 39.6, O 48.1
Gaur, Kartik ..... HL 54.6, HL 55.1
Gaurdascione, Marcello ..... QI 6.9
Gaus, Anna-Laurine ..... O 54.7
Gaus, Katharina ..... •CPP 46.21
Gautam, Aarti ..... MA 7.26, •TT 41.7
Gautam, Randeer Pratap ... BP 14.44
Gautam, Sunny M P ..... •O 46.10
Gauthier, Georges ..... DY 25.1
Gauthier, Maxence ..... AKBP 6.1
Gautier, Brice ..... FM 4.1
Gautier, Pierre ..... •MA 7.15
Gautier, Ronan ..... QI 17.7
Gavara, Miguel ..... O 69.10
Gavrishev, Alexander ..... •TT 61.12
Gawalleck, Luca ... •DY 42.1, •TT 63.1
Gaydamachenko, Victor .... TT 28.6, TT 28.8, TT 43.5
Gazibegovic, Sasa ..... HL 20.40
Gázquez, Jaume ..... TT 81.1
Ge, Jian-Feng ..... TT 4.10, TT 73.1, •TT 78.5, TT 93.15
Ge, Jin ..... MA 49.1
Ge, Wenbo ..... MA 17.6
Ge, Wuzheng ..... •HL 18.4, •TT 32.4
Ge, Yuru ..... MM 21.8
Gebauer, Andreas .... O 14.11, O 38.5, O 41.3, •O 66.5, TT 38.3
Gebauer, Philipp ..... FM 4.2
Gebbett, Suzannah ..... SOE 2.5
Gebel, Jan ..... TT 62.11
Gebel, Steven ..... MA 16.1, TT 4.8
Gebhart, Philipp ..... CPP 24.2
Gebski, Marcin ..... AKPIK 3.4
Geck, Jochen ..... MA 33.8, TT 4.8, TT 5.7, TT 61.5, TT 62.6
Geckle, Stephan ..... CPP 41.7
Geelhaar, Lutz ..... DS 4.5, DS 11.3, HL 23.10, HL 33.4, HL 57.5
Geers, Patrick ..... •O 60.5
Geerts, Yves ..... O 61.8
Geese, Anne ..... DD 8.1
Gefen, Yuval ..... QI 17.5
Gegenwart, Philipp . MA 8.5, MA 18.7, MA 23.2, MA 37.9, MA 52.37, TT 22.34, TT 30.7, TT 35.2, TT 52.6, •TT 57.4, TT 57.5, TT 72.4, TT 72.6, TT 72.7, TT 79.4, TT 89.2, TT 98.2
Gehrig, Lukas ..... DS 14.3, DS 20.43, •O 74.4, TT 5.6, •TT 68.4
Gehrke, Kai ..... DS 20.4
Geibel, Christoph ... TT 25.7, TT 29.5
Geier, Levi ..... •MA 45.5
Geilen, Leonard ..... HL 3.9, HL 18.8, TT 32.8
Geilhufe, Matthias . DY 61.1, MA 40.5, MA 40.7
Geilhufe, R. Matthias DY 9.9, •DY 9.10
Geilhufe, Richard Matthias .. DY 60.5
Geirhos, Korbinian ..... MA 17.6
Geirsson, Torsten ..... •MA 7.31
Geisert, Simon ..... TT 14.2, TT 43.6, QI 8.1, QI 11.4, QI 11.5
Geisler, B. ..... TT 69.3
Gekle, Stephan ..... BP 2.2, BP 7.33, •BP 40.5
Gelczuk, Łukasz ..... HL 20.7
Geldiev, Begmuhammet ..... O 42.7
Geldiyev, Begmuhammet ..... O 76.1, O 80.5
Gelen, Ismet ..... •DS 4.2
Geller, M. HL 17.7, HL 20.27, HL 20.39
Geller, Martin ..... HL 17.3, HL 17.8, HL 20.12, HL 47.1, HL 55.5, HL 55.6
Gelzinyte, E. ..... O 57.6
Gelzinyte, Elena ..... O 96.8
Gemen, Julius ..... CPP 46.32
Gemmer, Jochen . DY 46.4, DY 59.10, TT 53.8, TT 75.4, TT 99.10
Gemming, Sibylle ... DS 18.4, DS 18.5, DS 18.6, •DS 18.7, DS 20.46, DS 20.47, HL 48.8, MM 3.9, MM 19.33, MM 19.34, O 62.5, O 74.2, O 74.3, TT 54.5, TT 68.2, TT 68.3
Géneaux, Romain ..... O 14.1
Geng, Daiyu . O 42.1, •O 70.7, •TT 65.7
Gengo, Takumi ..... •MA 3.10
Genix, Anne-Caroline ..... CPP 42.1
Geoffroy, Mario ..... •TT 23.34
George, Antony .... HL 30.2, TT 59.2
George, Janine ..... •FM 6.1
George, Mike ..... BP 14.24
Georges, Antoine .. DY 58.1, SOE 17.1
Georgiadis, Dimitrios . QI 8.2, •QI 13.7
Georgiev, Asen ..... TT 22.12
Georgiev, Asen L ..... TT 28.6
georgiev, asen Lyubenov .... TT 43.5
Georgiev, Petar A. ..... MA 7.22
Georgiev, Yordan ..... HL 20.46
Georgiev, Yordan M. ..... HL 17.9
Georgieva, Borislava ..... •MA 7.27
Georgieva, Milena T. ..... MA 7.22
Georgiou, Theoni K. ..... CPP 46.12
Georgopoulos, Nicolas ..... O 10.8, TT 16.8
Geprägs, Stephan MA 7.48, MA 30.5, MA 33.11, MA 59.5
Gerace, Federica .. DY 45.5, SOE 14.5
Gerasimenko, Yaroslav ..... O 12.8
Gerasimenko, Yaroslav A. ..... O 12.5
Gerber, Eli ..... TT 10.7
Gerber, Iann ..... HL 20.13
Gerber, Simon ..... TT 62.6
Gerdau, Rolf-Werner ..... TT 28.9
Gerhard, Lukas ..... •O 12.1
Gerhard, Marina .. HL 20.20, HL 45.8
Geringswald, Arik ..... O 25.1
Gerjets, Peter ..... DD 13.2, DD 27.7
Gerken, Martina ..... HL 26.17
Gerlach, Sonja . AKBP 8.7, AKBP 10.4, AKBP 11.1
Gerland, Ulrich .... BP 14.53, BP 15.8
Germann, Natalie ..... CPP 15.2
Gerntke, Tom ..... TT 25.10
Gerstenberg, Antonia ..... •O 18.1
Gerstenberger, Konstantin •CPP 60.2, DD 42.3
Gerster, Thomas ..... HL 25.1
Gerstmann, Uwe . HL 20.60, HL 49.3, O 16.1
Geske, Michael ..... O 81.7
Gessert, Denis ..... •DY 60.2
Gessler, Philipp ..... O 96.2, •TT 6.6
Gessler, Phillip ..... O 26.4
Gessner, Manuel ..... QI 14.11
Geuder, Colin ..... •O 43.11
Geulig, Laura D. •AKBP 5.1, AKBP 5.2, AKBP 8.5
Gevers, Lennart . •BP 30.6, •CPP 47.6
Gewinner, Sandy ..... O 85.4
Geyer, Daniel ..... •HL 52.1
Geyer, Philipp ... MA 48.10, MA 52.21
Geyer, Veikko F. .... BP 36.2, DY 57.2
Ghadiyali, Mohammed ..... MA 13.9
Ghaebi, Omid .... HL 20.21, HL 20.31, HL 26.47, HL 35.6
Ghafoor, Atif ..... •TT 42.8
Ghaith, Amin ..... AKBP 13.3
Ghaith, Jamal ..... •O 68.5
Ghalami, Farhad ..... CPP 14.2
Ghalgaoui, Ahmed .. MA 12.4, O 94.9
Ghan, Simiam ..... •O 50.3
Ghanbari, Azadeh ..... DD 30.10
Ghannadan, Azadeh ..... MA 36.2
Ghara, Arindam ..... •TT 25.7
Ghara, Somnath ..... •MA 17.6
Gharu, Amit ..... MA 7.74
Ghasemian, Saber Izak ..... BP 30.5, CPP 47.5
Ghassemizadeh, Reyhaneh .. MM 3.7
Ghazinezhad, Zahra ..... TT 23.13
Ghazinezhad, Zahrasadat .... MA 3.7
Ghebretinsae, Bereket ..... MA 7.70
Ghelev, Chavdar ..... MA 7.27
Ghihor, Anamaria ... TT 5.8, •TT 17.2, •QI 4.2
Ghimire, Nirmal ..... MA 8.3
Ghimire, Nirmal J. MA 33.11, MA 54.8
Ghiotto, Augusto ..... •FM 10.5
Ghiringhelli, Giacomo ..... •O 67.10
Ghodrati Saeini, Hadis ..... •DS 18.4, DS 20.46, DS 20.47
Gholami, Shirin . CPP 19.5, •CPP 27.3, DY 20.5, •DY 26.3
Ghorbani-Asl, Mahdi DS 12.5, •FM 2.2, O 7.7, O 84.10, TT 9.7, TT 84.10
Ghorbanietemad, Armin .... QI 14.27, •QI 21.3
Ghosal, Chitran ..... O 33.4
Ghosez, Philippe ..... FM 18.2
Ghosh, Bristi ..... •TT 92.11
Ghosh, Kanka ..... •MM 3.3
Ghosh Roy, Anindya ..... BP 15.9
Ghosh, Santanu .. HL 26.14, MM 30.5
Ghosh, Sayantan . •HL 17.9, HL 20.46, HL 20.56
Ghosh, Shreenanda ..... •TT 41.4
Ghosh, Subhadip ..... •MA 12.3
Ghosh, Sudeep Kumar ..... MA 2.2, TT 97.4
Ghosh, Sumit ..... •MA 42.4
Ghoshal, Arkajyoti . BP 1.11, CPP 1.11, DY 4.11
Giacobino, Elisabeth ..... •PSV VII
Giaconi, Niccolò ..... O 42.4
Giannini, Samuele ..... CPP 25.1
Giantomassi, Matteo ..... AKPIK 6.7
Gibbins, Molly ..... TT 70.5
Gibelli, Lucia ..... •TT 56.13
Gibertini, Marco ..... HL 35.9, MA 2.1
Gibson, Graham W. ..... MM 19.39
Giedke, Géza ..... TT 26.6, TT 42.2
Gierß, Peter ..... HL 34.5
Gierz, Isabella O 40.7, O 66.2, O 98.9, TT 37.7
Giesbrecht, Patrick ..... •O 65.5
Gieseler, Niels .. •BP 30.3, •CPP 47.3
Gieselmann, Luis Rolf ..... •MA 52.1
Gießelmann, Niels C. ..... CPP 46.5, •CPP 58.1
Giesen, Jan Mathis . O 26.3, •TT 78.4
Gießibl, Franz ..... O 40.8, TT 37.8
Giesinger, Nora-Elen ..... •CPP 17.1
Giessen, Harald ..... HL 55.7, O 26.4, O 57.3, O 79.5, O 85.7
Giessibl, Franz O 3.6, O 56.2, TT 74.12
Giessibl, Franz J. . O 3.4, O 3.5, O 4.6, O 12.5, O 41.2, O 99.11, TT 38.2
Giessibl, Franz Josef ..... O 63.10, TT 55.10
Giessibl, Valentin ..... O 12.5
Gievers, Marcel ..... TT 13.10
Giez, Tobias ..... CPP 17.48
Gil, Bernard ..... O 95.6, TT 96.6
Gilbert, Audrey ..... DS 11.3, DS 20.18
Gilbert, Mathew ..... DS 11.8
Gill, Deepika ..... •MA 38.14
Gilliot, Rémi ..... HL 8.12
Gillioz, Valentine ..... •FM 4.7
Gillmeister, Konrad .. O 40.9, TT 37.9
Gindorf, Mick ..... •CPP 46.27
Ginga, Victoria ..... MA 2.6, •TT 57.5, TT 94.6
Gingras, Michel J. P. MA 31.1, TT 47.1
Ginossar, Eran ..... QI 11.7
Ginot, Felix ..... •DY 21.10, DY 21.11
Ginzburg, Samuell ..... CPP 26.2
Giordano, Livia ..... MM 8.1
Gioria, Esteban ..... O 23.4
Girard, Martin ..... BP 4.4, BP 4.5
Giraud, Manuela ..... •BP 21.2

Giri, Bharat ..... O 60.6
Giri, Debasmita ... •DY 32.3, •TT 45.3
Girot, Antoine ..... BP 7.29
Girschik, Justin ..... O 88.6
Giselbrecht, Felix ..... O 9.10
Gispert, Peter ..... BP 29.4, CPP 45.4
Gisti, Martina ..... •TT 17.3, •QI 4.3
Gittinger, M. ..... HL 54.10
Gity, Farzan ..... HL 24.11
Giuntoli, Andrea ..... DS 16.4
Gkikas, Antonis ..... UP 5.2
Gladich, Ivan ..... CPP 19.5, DY 20.5, UP 6.1
Gladitz, Franziska ..... •O 73.2
Glamsch, Stephan .. MA 9.4, MA 12.1, MA 52.33, TT 79.4
Glaser, Niklas ..... QI 2.7
Glaser, Timo ..... O 11.4
Glatz, Fabian ..... •HL 20.18
Glatz, Lion Cornelius ..... •DD 6.1
Glaum, Julia ..... FM 18.8
Glazman, Leonid I. . DY 32.2, TT 45.2
Glazov, Michail ..... HL 10.5, TT 20.5
Glazov, Mikhail .... HL 20.13, HL 35.3
Glazov, Mikhail M. ..... HL 39.5
Gleichmann, Jonas ..... DD 25.2
Gleixner, Andreas ..... •JOB 2.1
Glezakou, Vassiliki-Alexandra O 65.10
Glier, Tomke ..... MA 39.18
Glitsch, Felix ..... DY 14.1
Glock, Marvin ..... CPP 39.5
Głodzik, Szczepan DY 32.12, TT 45.12
Gloistein, Felix ..... QI 20.6
Gloppe, Arnaud ..... O 12.9
Glorius, Frank ..... CPP 46.32, O 58.3
Glosemeyer, Matthias ..... MM 32.3
Gloskovskii, A. ..... DS 3.4, O 59.2, TT 48.2
Gloskovskii, Andrei DS 20.41, FM 4.2, FM 23.4, •MA 39.9, O 19.2, O 93.2, TT 25.11
Gloskovskii, Andrej ..... QI 14.23
Gloter, Alexandre ... FM 18.6, TT 69.4
Glotter, A. ..... TT 69.3
Gluch, Jakub ..... •HL 26.45
Gluth, Nils ..... DY 59.1, TT 99.1
Gmitra, Martin ..... DS 12.7, DS 14.2, MA 35.5, TT 60.5
Gnandt, Christian ..... QI 11.6, QI 11.9
Gnecco, Enrico ..... O 87.4
Gnezdilov, Vladimir ..... MA 40.8
Go, Ara ..... MA 3.10
Go, Dongwook ... MA 20.5, MA 29.4, MA 29.9, MA 51.4, MA 51.7, TT 46.4, TT 46.9, TT 88.4, TT 88.7
Göbel, Börge ..... MA 29.5, MA 38.11, MA 38.12, MA 55.1, TT 46.5
Göbel, Ida ..... MM 40.7
Göbel, Sophie ..... O 11.1, •O 31.2
Gödde, Lene A. ..... O 9.12
Göde, Sebastian ..... AKBP 6.1
Godec, Aljaž . DY 7.5, DY 9.5, DY 21.4, DY 41.10, DY 54.1, DY 61.2, DY 63.3, SOE 9.3
Gödecke, Gilles ..... •TT 81.5
Godfrin, Clement ..... QI 14.24
Godinho, Joao ..... O 96.5
Godinho, Maria Clara ..... HL 47.2
Goedecker, Stefan ..... CPP 46.54
Goennenwein, S. T. B. ..... MA 52.8, MA 59.8
Goennenwein, Sebastian ... MA 7.52
Goennenwein, Sebastian T. B. MA 29.8, MA 38.8, MA 39.24, MA 45.1, MA 51.8, MA 59.5, TT 46.8, TT 88.8
Goerbig, Mark Oliver ..... TT 83.13
Goerlich, Rémi ..... DY 21.9
Goerzen, Moritz ..... MA 21.5
Goerzen, Moritz A. ..... •MA 16.7
Goffman, Marcelo ..... TT 50.6
Göggelmann, Alexander ..... TT 82.3
Goh, Segun ..... SYGF 1.5
Göhler, Clemens CPP 37.4, CPP 37.6, CPP 40.5
Göhler, Fabian ... DS 20.42, MA 24.3, O 2.1, O 2.5, •O 76.6, TT 36.3
Gohlke, Matthias ..... •MA 19.10, •TT 31.10
Goian, Veronica ..... •MA 17.3
Gökce, Bilal ..... MA 13.7, MA 50.1
Göken, Mathias ..... •MM 32.6
Göken, Matthias ..... MM 32.3
Gokita, Takeaki ..... MA 59.6
Golam, Haider ..... TT 4.11
Golami, Shirin .... CPP 23.2, DY 24.2
Golan, Noam ..... BP 14.15
Goldberg, Phil ..... HL 26.23
Golden, Artemiy ..... BP 37.5
Golden, Mariia ..... BP 37.5
Goldhahn, Rüdiger . HL 57.1, HL 57.2, HL 57.3
Goldman, Nathan ..... TT 83.10
Goldmann, Mirko ..... AKPIK 3.4
Goldschmidt, Jan Christoph .. UP 8.5
Goldstein, Moshe ..... QI 2.3
Goldt, Sebastian ... DY 58.7, SOE 17.7
Golebiewski, Mateusz ..... MA 44.8, TT 76.8
Golestanian, Ramin ..... BP 7.48, BP 10.10, BP 37.9, CPP 18.10, CPP 28.4, DY 18.10, DY 27.6, DY 29.4, DY 33.2
Golež, Denis ..... TT 51.12
Golibrzuch, Kai ..... O 34.7
Golombiewski, Maik ..... TT 81.8
Goloviznina, Kateryna ..... •CPP 21.1
Golub, Leonid ..... TT 97.2
Golze, Dorothea ..... O 37.5
Gölzhäuser, Armin CPP 3.4, CPP 39.4
Gomes, Sofia ..... BP 11.6
Gómez, Alejandro S. •DY 8.7, TT 15.8
Gómez Flores, Claudia Leticia . O 9.8
Gomez Melo, Santiago .... •CPP 49.4
Gómez Ruiz, Mikel ..... •HL 23.10
Gomez, Samuel S. .. BP 5.6, •BP 16.2
Gomez-Leon, Alvaro ..... TT 15.7
Gómez-Rodrigo, Lucía ..... O 9.10
Gomonay, Olena . MA 29.10, MA 37.2, MA 51.7, TT 46.10, TT 88.7
Gompf, Bruno ..... O 96.1, TT 12.6
Gompper, Gerhard ..... •SYGF 1.5
Gonçalves de Sá, Joana ... •SYTP 1.4
Goncalves Faria, Marcos Vinicius •TT 57.6
Gong, Jiacheng ..... •HL 15.4
Gong, Junlu ..... AKPIK 6.4
Gong, Yilun ..... •MM 11.1
Goniakowski, Jacek .. O 52.2, O 52.5, O 55.2, •O 55.3
Gönnenwein, Jakob ..... •BP 14.3
Gönnheimer, Nils .. •MM 22.9, O 34.3
González Caminal, Pau ... AKBP 12.4
González Lastre, Manuel .... •O 35.6
Gonzalez, M. ..... TT 69.6
Gonzalez, Marta ..... •PLV X
Gonzalez Oliva, Ignacio ..... O 66.9
Gonzalez, Sara ..... FM 4.1
Gonzalez-Arciniegas, Carlos .. QI 18.1
Gonzalez-Diaz, Juan B. ... AKBP 11.2
González-Lastre, Manuel ..... O 33.2
Gonzalez-Navarrete, Barbara . O 54.5
González-Rodríguez, David CPP 17.7, CPP 22.6
Gonzalez-Ruano, Cesar ..... TT 73.9
Good, J. ..... BP 27.8, BP 37.2
Goodenough, Kenneth ..... QI 15.9
Goodge, B. H. ..... TT 69.6
Goodge, Berit ..... TT 40.1, TT 57.10
Goodge, Berit H. ..... •TT 39.4
Goodwin, Melissa ..... TT 28.5
Goodwin, Zachary A. H. ..... O 95.10, TT 96.10
Goossens, Annouk ..... FM 18.6
Gopakumar, Thiruvancheril ... •O 9.6
Gopakumar, Thiruvancheril g. CPP 17.47, O 10.4, O 48.4, TT 16.4
Gopalakrishnan, Sarang ..... QI 3.11
Gope, Monikana ..... •TT 22.4
Göpfrich, Kerstin ..... BP 7.37
Gopi, Ajesh K ..... TT 22.2
Gördes, Jendrik ... MA 7.47, MA 38.4, •MA 38.6
Gordeyeva, K. ..... MA 7.21
Gorfer, Alexander ..... •MM 37.2
Gorfman, Semën ..... FM 23.6
Gorini, Cosimo ..... HL 29.2, TT 58.2, •TT 74.7, TT 74.11
Gorkan, Taylan ... •FM 22.4, MM 16.4
Görling, Andreas ..... MA 5.4, TT 7.4
Görlitz, Sarah L. ..... •TT 71.6
Gorni, Tommaso ..... TT 95.8
Gornyi, Igor ..... •SYBS 1.2, QI 21.6
Gorobtsov, Oleg ..... •HL 8.6
Goroncy, Luca ..... •DD 42.2
Görsch, Julia ..... •DY 48.6
Gosálvez-Martínez, Daniel .. HL 30.7, TT 59.7
Gößler, Markus .. •MA 57.6, MM 39.1
Gosling, Nicolas .... TT 22.12, QI 11.5
Gossel, Lisanne ..... •DY 28.3
Gossen, Kai ..... •BP 7.8
Gossing, Florian ..... MA 21.3
Gossling, Nicolas ..... QI 11.4
Goswami, Ankur ..... HL 40.4
Goswami, Neerdhi ..... •O 22.6
Göth, Nils ..... •CPP 33.2
Gotszalk, Teodor ... HL 18.3, TT 32.3
Gottfried, J. Michael ... O 8.7, O 31.5, O 35.4, O 35.5, O 61.4, O 68.1, O 69.5, O 69.7, O 77.3
Göttlich, Richard ..... CPP 17.8
Gottschall, T. ..... •MA 18.1, MA 18.4, MA 18.5, MA 52.22, MA 52.24, •TT 30.1, TT 30.4, TT 30.5
Gottschall, Tino .... MA 18.2, TT 30.2
Gottwald, Georg ..... DY 8.5
Götz, Anika ..... TT 26.4
Götz, Klaus ..... BP 16.11
Gouder, Thomas ..... O 88.7
Goutier, Ann Chantal ..... •O 20.1
Goy, Claudia ..... CPP 27.5, DY 26.5
Goychuk, Andriy .. •BP 32.3, •DY 52.3
Graalmann, Jan-Hauke ..... •HL 3.2
Grabarczyk, Jakub ..... •DY 47.9
Grabarics, Marko ..... O 69.13
Grabowski, Blazej MM 11.5, MM 19.4, MM 35.6
Gradauskaite, Elzbieta ..... FM 18.6
Gradl, Johannes ..... O 66.2, •O 98.9
Gradwohl, Kevin-P. ..... QI 6.5
Graf, F. ..... MA 25.6
Graf, Isabella ..... BP 32.8, DY 52.8
Graf, Jonas ..... •O 96.1
Grafe, Hans-Joachim ..... TT 57.1
Gräfe, Markus ..... DD 30.5
Gräfe, Stefanie ..... CPP 21.5, HL 1.11
Grafenhorst, Judith ..... TT 79.3
Gräff, Kevin ..... CPP 26.4, CPP 49.5
Graffe, Timo ..... DD 14.2, •DD 23.2
Grafke, Tobias ..... DY 15.8
Graham, Jennifer ..... MA 8.3
Graichen, Lea ..... BP 7.40
Grambow, Eberhard ..... HL 22.4
Graml, Maximilian . BP 14.73, HL 54.1
Grammer, Benedikt ..... SOE 6.3
Grammer, Matthias HL 18.1, MA 7.48, MA 51.8, MA 52.18, •MA 59.5, TT 32.1, TT 88.8
Grams, Christoph ..... FM 18.8
Granas, O. ..... MA 7.14
Grånäs, Oscar ..... MA 24.4, TT 36.4
Granatelli, Gaetano ..... •BP 5.6
Granero, Alessandro ..... •MA 17.9
Granovski, Sergej .. MA 19.8, TT 31.8
Granovsky, Sergey . MA 7.2, MA 19.6, MA 31.9, TT 31.6, TT 47.9
Grant, Perry C. ..... DS 21.3
Granwehr, Josef ..... FM 5.5
Grap, Thomas .... HL 26.8, HL 26.33
Grapin-Botton, Anne ..... BP 14.49
Graß, Tobias ..... TT 26.6
Gräßel, Katharina ..... •JOB 2.2
Gräßer, Timo ..... •DY 46.9, •TT 75.9
Graßme, Florian ..... O 70.5, TT 65.5
Grässer, Timo ..... MA 58.8
Grasset, R. ..... TT 69.6
Grasset, Romain ..... MM 40.2
Grasset, Romian ..... TT 29.11
Grassi, Matías P. ..... MA 39.8
Grauer, Rainer ..... DY 15.8
Graus, Sven ..... MM 19.42, •TT 81.7, TT 81.8
Graw, Frederik .... BP 10.5, CPP 18.5, DY 18.5
Gray, Gabriel ..... •MA 57.2
Grebener, Lars ..... HL 20.12
Grebinyk, A. ..... BP 27.8, BP 37.2
Greco, Andres ..... TT 39.7
Green, Andrew ..... MA 23.3, TT 35.3
Greenberg, David S. ..... UP 5.4
Gregg, John F. ..... MA 9.5
Gregg, Marty ..... FM 12.5, FM 12.6
Gregor, Benz ..... •DD 12.2
Greichgauer, Adrian ..... TT 85.7
Greiner, Andreas ..... CPP 41.7
Greiner, Christian ..... MM 7.10
Gremmelspacher, Clara .... •BP 7.33
Grenz, Pascal J. ..... O 67.8
Grenzer, Patrick . HL 26.27, HL 26.55, •HL 45.6
Gresch, Alexander ..... QI 1.10
Gretarsson, Hlynur .. TT 3.2, TT 23.18
Greten, David .... MM 13.7, •MM 19.8
Greten, Lara ..... HL 30.4, TT 59.4
Grether, Luisa R. •DY 46.12, •TT 75.12
Greto, Eric ..... BP 14.50, BP 14.85
Greule, Paul .... O 15.4, O 17.7, O 17.9, •O 89.12, O 99.10
Greve, Daniel ..... DY 22.2
Greving, Imke ..... BP 14.44
Grewe, R. ..... AKBP 1.1
Grewe, Ruben .. AKBP 4.4, AKBP 14.1
Grieb, Tim ..... HL 12.3
Griedel, Markus ..... TT 22.11
Griesbeck, Michael ..... •DD 26.4
Grifoni, Milena ..... TT 56.13
Grigoletto, Massimo ..... HL 37.4
Grigorev, Vitalii ..... BP 14.51
Grill, Leonhard O 43.3, O 43.7, O 46.7, O 69.11, O 69.12, O 73.6
Grill, Stephan ..... BP 27.11
Grill, Stephan W. .... BP 3.9, BP 32.6, DY 52.6
Grilli, Lorenzo .... •MA 7.47, MA 38.6
Grimes, M. ..... MA 25.6
Grimm, Alexander ..... QI 3.4
Grimm, Benjamin Rasmus ... •O 88.8
Grimm, Philip ..... MM 3.9, MM 7.1
Grin, Yu. ..... TT 5.9
Grin, Yuri ..... TT 42.12
Grinenko, Vadim ..... TT 93.14
Grinko, Dmitry ..... QI 15.8
Grisan Qiu, Yan Yan ... O 69.2, O 69.6
Grisenti, Robert E. CPP 27.5, DY 26.5
Grisk, Holger ..... MA 54.11
Gröbmeyer, Franz ..... DS 12.3
Grockowiak, Audrey ..... TT 80.7
Groenhagen, Mathis ..... •DY 15.3
Groh, Henrik ..... •BP 14.1
Groh, Jordan D. ..... •DY 43.18
Groh, Jordan Dieter ..... BP 7.32
Groiss, Heiko ..... MM 19.20
Groll, Daniel ..... HL 3.6
Groll, Florian ..... •MM 41.2
Groll, Maja ..... HL 49.3
Grom, Daniel ..... •DY 59.4, •TT 99.4
Gröning, Oliver ..... MA 5.9, TT 7.9
Gröninger, Rebecca ..... HL 15.1
Gronwald, Imke ..... HL 39.8
Groot, Tijmen ..... MA 39.19
Groß, Axel . FM 5.6, FM 22.10, O 13.4, •O 39.6
Groß, Benjamin ..... DD 19.1
Gros, Claudius .... DY 45.6, SOE 14.6
Grosch, Lennart ..... HL 38.1
Grosche, F. Malte ..... TT 23.15
Grosche, Malte .... TT 29.11, TT 62.7, TT 93.17, TT 95.7
Grosfeld, Eytan ..... QI 11.7
Großmann, Fabian ..... HL 33.2
Großmann, Frank . DY 42.10, TT 63.10
Großmann, Max ..... HL 1.2, HL 26.4, •MM 17.2, MM 17.6
Großmann, Robert . BP 11.8, DY 33.5, •DY 55.2
Gross, Axel ..... MM 8.8, AKPIK 6.2
Gross, Boris ..... MA 49.2
Gross, Leo ..... O 3.2, •O 9.12, O 83.5
Gross, M. ..... BP 27.8, BP 37.2
Gross, Miela ..... MA 37.8
Gross, Miela J. ..... MA 37.2
Gross, Rudolf ..... MA 30.5, MA 51.8, TT 88.8, QI 2.4, QI 18.2, QI 18.3
Grossart, Hans-Peter ..... BP 1.11, CPP 1.11, DY 4.11
Grosser, Steffen ..... •BP 27.2
Grossi, Juri ..... MM 41.4
Grossmann, Max ..... •TUT 3.2, •AKPIK 1.2
Grothaus, Jonathan ..... •DD 14.3, DD 23.4
Grothues, Hans-Georg ..... PSV VI, •AIW 1.1
Grötzner, Gabriel .... HL 1.1, •HL 33.5, HL 42.3, HL 42.5
Grover, Catherine .... O 95.3, TT 96.3
Gruber, Christian ..... •O 19.5
Gruber, Manuel .... •MA 42.3, O 17.8, O 44.1, O 59.5, O 71.1, O 71.18, O 83.3, O 83.6, O 89.9, TT 48.5, TT 66.1, TT 66.18
Gruber, Maximilian A. ..... •HL 8.7, HL 57.4
Gruber, Patric ..... MM 7.10
Gruber, Philipp ..... O 58.2
Gruber, Raphael . MA 21.6, AKPIK 5.6
Grubisic-cabo, Antonija ..... O 76.4, TT 27.4
Grueneis, Andreas ..... TT 51.3
Gruenewald, Marco ..... HL 35.6
Gruhl, Robert ..... MA 52.37
Grumbach, Justus ..... •MA 55.11, MA 55.12

Grümbel, Jona ..... HL 57.2
Grumelli, Doris ..... O 8.7
Grumet, Manuel ..... MM 9.5
Grumm, Jonas ..... O 27.7
Grumser, Melvin ..... •O 46.1
Grun, Naemi ..... •TT 22.21
Grundler, Dirk ..... MA 44.8, TT 76.8
Grundmann, Marius .. HL 1.7, HL 9.3, HL 9.6, HL 26.19, HL 26.20, HL 26.21, HL 26.22, HL 26.32, HL 26.40, HL 26.42, HL 26.44, HL 40.7, HL 40.9
Grune, Elisabeth ..... •HL 20.25
Grünebohm, Anna ... FM 4.3, FM 4.8, FM 6.8, FM 11.6, FM 11.8, FM 11.19, FM 12.7
Grüneis, Alexander ... O 10.11, O 54.4, TT 16.11
Grüneis, Andreas ..... MA 39.25
Gruner, Markus E. MA 13.2, •MA 13.5, MA 18.3, MM 21.8, TT 30.3
Grunert, Malte .... •TUT 3.2, DY 43.2, •HL 1.2, HL 26.4, MM 17.2, MM 17.6, •AKPIK 1.2
Grünhaupt, Lukas . TT 22.8, TT 22.12, TT 28.6, TT 28.8, TT 43.5, •QI 11.1
Grüninger, Helen ..... CPP 17.14
Grüninger, Markus ..... TT 23.18
Grunwald, Joscha ..... TT 23.10
Grunwald, Lukas ..... O 79.1
Grunwitz, Tamina ..... AKBP 7.3
Grusche, Sascha ..... •DD 4.1
Gruschwitz, Markus .. O 33.4, •O 73.1
Grutter, Peter ..... O 33.2
Grützmacher, Detlev TT 73.6, TT 74.3, QI 6.9, QI 14.26
Gryko, Daniel T. ..... CPP 17.9
Grytsiuk, Sergii .... •MA 34.9, O 76.4, TT 27.4, TT 92.18
Grzeszczyk, Magdalena .... •HL 16.5
Grzyb, Andrzej ..... CPP 39.2
Gu, Genda ..... O 63.1, TT 55.1
Gu, Mong-Wen O 9.5, O 61.10, •O 69.8
Gu, Xinlei ..... MM 7.5
Gu, Yanwei ..... MA 5.9, TT 7.9
Guandalini, Alberto .. O 84.7, TT 84.7
Guardi, Giorgia ..... MM 3.6
Guarino, Anita ..... HL 23.1
Guatto, Manuel ..... •QI 16.5
Guazzelli, Elisabeth .DY 19.2, DY 19.5, DY 19.6
Gubler, Moritz ... CPP 46.54, MM 19.1
Guck, Jochen ..... BP 7.44
Gückelhorn, Janine MA 51.8, •TT 81.1, TT 88.8
Güdde, Jens ..... O 14.6
Gude, Maik ..... FM 19.4, MM 3.9
Guder, Adrian ..... MA 13.4
Gudim, I. A. ..... MA 17.7
Gudovannyy, Alexey ..... •CPP 25.3
Gueckstock, Oliver ..... MA 27.1
Guéneau, Mathis ..... •DY 49.7
Guenkel, Robin ..... •O 10.9, •TT 16.9
Guenther, Florian ..... DS 18.5
Guerci, Daniele ..... TT 6.4
Gueron, Sophie ..... •TT 50.4
Guerrero, Jorginho Villar .... MA 18.7, TT 30.7
Guerrini, Michele ... CPP 22.4, HL 1.6
Guevara, Jose M. ..... O 61.10
Guguchia, Zurab ..... MA 8.3
Guguschev, Christo ..... TT 79.4
Guha Ray, Chandraniva ..... •BP 3.9, DY 33.9
Gühne, Otfried ..... QI 12.7, QI 14.28, QI 15.9, QI 21.4
Guhr, Thomas ..... DY 15.10, DY 59.1, TT 99.1
Guillet, Alexandre ..... •DY 40.5
Guimarães, Jéferson ..... QI 8.5
Guinea, Francisco ..... TT 4.4
Gujare, Aditi .. CPP 31.2, •CPP 46.33, CPP 46.38
Gul, Iram .•CPP 2.3, •SOE 3.3, •UP 1.3
Gulácsi, Balázs ..... •QI 8.4
Gulans, Andris O 18.4, O 47.3, •O 84.1, •TT 84.1
Güleryüz, Oktay O 10.1, O 10.8, O 59.1, TT 16.1, TT 16.8, TT 48.1
Gülkaya, Aybüke ..... DS 18.1
Gülpen, Kamiel ..... •SOE 16.3
Gümbel, Lukas .... HL 23.8, HL 26.28
Gumbsch, Leah ..... BP 27.6
Gumeniuk, Roman ... FM 9.3, MA 7.2, MA 19.6, MA 31.9, MM 19.46, •TT 5.11, TT 25.8, TT 31.6, TT 42.12, TT 47.9
Gumm, Jens ..... AKBP 7.3
Gundermann, Laura ..... DS 20.40
Gundermann, Richard ..... DY 43.3
Gunkel, F. ..... MA 3.8
Gunkel, Felix ..... •DS 6.6, O 79.4
Günkel, Robin ..... O 70.1, O 95.12, TT 65.1, TT 96.12
Gunnink, Pieter ..... •MA 2.3
Gunny, Masoodah ..... •CPP 20.9, •DY 23.9
Günther, Clara Marie ..... TT 22.28, TT 22.29
Günther, Florian .. DS 18.4, •DS 20.47, O 62.5, TT 54.5
Günther, Gebhard ..... UP 5.3
Günther, Jarmo ..... •DD 23.3
Günzing, D. ..... MA 50.3
Günzler, Simon ..... QI 11.4, •QI 11.5
Guo, Chunyu ..... •TT 57.7
Guo, Emily ..... QI 2.1
Guo, Guangyi ..... MM 15.4
Guo, Haojie . O 86.4, TT 14.10, TT 74.1
Guo, Hua ..... O 34.7
Guo, Huixin ..... MA 44.8, TT 76.8
Guo, Jinhui ..... •O 43.1
Guo, Kaiwen ..... HL 15.4, •HL 15.6
Guo, Lin . FM 6.11, MA 49.5, •MA 49.6
Guo, Runjia ..... AKBP 5.2
Guo, Shanshan ..... •DS 20.51
Guo, Yingjian ..... •CPP 46.17
Gupta, Ajay ..... CPP 41.4
Gupta, Amitesh ..... •TT 22.10
Gupta, Ankita ..... •DY 63.3
Gupta, Arpan ..... MM 26.4
Gupta, Deeksha ... MA 27.2, MA 38.6
Gupta, Deepak ..... •DY 40.4
Gupta, Harsh DS 1.2, DS 16.6, QI 11.10
Gupta, Krishna ..... CPP 54.4
Gupta, Mitanshi ..... MM 21.7
Gupta, Rahul ..... MA 12.6, MA 39.1
Gurarie, Victor ..... TT 83.5
Gurevich, Svetlana V. DY 6.5, DY 22.2, •DY 22.9, DY 22.10, DY 41.9, DY 48.4, DY 48.5
Gurin, Péter ..... DY 47.4
Gurlek, Burak ..... DY 14.9
Gürlü, Oguzhan ..... O 69.9
Guskova, Olga .. CPP 14.6, •CPP 31.3
Gustavo, Frederic ..... TT 82.1
Guterding, Daniel . •MA 11.1, MA 11.2, •TT 21.1, TT 21.2, TT 69.11
Gutfleisch, O. ..... MA 18.1, MA 18.5, MA 50.3, MA 52.22, TT 30.1, TT 30.5
Gutfleisch, Oliver ... DS 7.5, MA 13.2, MA 13.4, MA 13.7, MA 18.2, MA 50.4, MA 50.5, MA 50.6, MA 50.7, MA 50.8, MA 50.9, MA 52.23, MA 52.27, MA 52.31, MA 52.32, TT 30.2
Gutfreund, Philipp ..... AKPIK 6.6
Gutierrez, Ignacio ..... MA 49.2
Gutierrez Ortigoza, Cristina Abril •CPP 46.7
Gutiérrez, Rafael ..... O 94.6
Gutierrez-Amigo, Martin ..... HL 8.11
Gutiérrez-Llorente, Araceli ... TT 69.5
Gutmann, Nicola ..... •HL 40.8
Gutt, Christian .... BP 14.44, BP 14.72
Güttinger, Johannes ..... MA 55.9
Guttmann, Dominic . DS 9.4, •DS 11.5, O 23.3
Guttmann, Martin ..... HL 37.3
Guzmán, Francisco ..... MM 40.8
Guzman, Horacio V. ..... BP 2.4
Guzman, Roger ..... TT 81.1
Gzyl, Tomasz ..... •HL 20.34
H. Beton, Peter ..... O 95.6, TT 96.6
H. Christensen, Morten .... •MA 33.3
H. F. Bunz, Uwe ..... O 46.2
H. Heenen, Hendrik ..... DS 14.1
H. Johansen, Christian ..... TT 56.1
H.M. van Loosdrecht, Paul . MA 27.10
H. Mir, Showkat ..... O 9.6
H. P. Pernice, Wolfram ..... MA 52.5
H. Patel, Jhanvi ..... BP 14.9
Ha Nguyen, Thi Ngoc ..... DS 20.48
Haag, Luca ..... MA 47.3, MA 54.8
Haag, Luca Felipe ..... •MA 8.6
Haag, Ruben ..... BP 7.14, BP 7.18, •BP 40.1
Haak, Inka ..... DD 39.1, •DD 39.3
Haake, Fabian ..... •O 54.6
Haar, Eduard ..... BP 20.9
Haas, Benedikt ..... TUT 1.1, FM 1.1, FM 15.1
Haas, Guillermo ..... O 3.7
Haas, Heinrich .... BP 31.3, CPP 50.3
Haas, Kaspar ..... •CPP 17.7
Haas, Lukas V. ..... BP 33.10
Haas, Michael .... TT 22.9, •TT 28.10
Haas, Pierre A. ..... BP 3.9, BP 14.94, BP 27.3, CPP 20.6, •DY 22.7, DY 23.6
Haase, Katherina ..... •DS 13.1
Haataja, Mikko ..... DY 41.11
Habenicht, Carsten ..... HL 22.2
Habenschaden, Christopher •MA 7.78
Haber, Simi ..... DY 47.2
Haberfehlner, Georg ..... O 96.12
Haberkamm, Hannes ..... O 48.5
Haberkern, Sebastian ..... HL 26.46
Haberl, Helmut ..... SOE 6.3
Haberland, Christian •O 28.3, O 44.14
Häberle, Patricio .... •O 67.3, O 67.11
Haberstroh, Florian ..... AKBP 8.7
Habibi, Mohammad ..... MM 31.2
habibipour, reza ..... •O 44.8
Hache, Toni ..... MA 39.7
Hackl, Lucas ..... TT 17.8, QI 4.8
Hackl, Rudi ..... MA 33.8
Haddad, Yorgo ..... TT 93.6, QI 8.5
Haddadi, Fatemeh ..... MA 2.1
Haddadi, Saeed ..... MA 36.2
Hadenfeldt, Hendrik ..... TT 22.27, •TT 82.2
Hadfield, Stuart ..... QI 1.7
hadipour, hanif ..... TT 56.7
Hadjadj, Sebastien MA 11.10, TT 21.10
Hadjadj, Sebastien E. ..... MA 38.4, •O 10.2, •TT 16.2
Hadjimichael, Marios ..... FM 12.3, FM 12.11
Hadjimichale, Yiannis ..... HL 38.9
Hadjivasiliou, Zena ..... BP 3.8
Hadlich, Christoph ..... FM 11.36
Hädrich, Julia ..... •DD 13.3
Hadzic, Elias ..... TT 29.8
Haeberle, Jan ..... CPP 15.2
Haessler, Max ..... •DY 43.22
Hafermann, Martin ..... DS 13.2
Häfner, Gregor ..... •CPP 3.2
Hagedorn, S. ..... HL 37.6
Hägele, Daniel ..... QI 14.27, QI 21.3
Hagenow, Alexander ..... MA 36.9
Hager, Martin ..... CPP 57.5
Haghighi, Nasibeh ..... AKPIK 3.4
Haghighirad, A. ..... O 59.2, TT 48.2
Haghighirad, Amir ..... TT 95.2
Haghighirad, Amir.A TT 23.31, TT 71.1
Haghighirad, Amir-Abbas . MA 39.18, O 22.3, TT 49.1
Hagiwara, Manabu ..... FM 22.8
Hagmann, Kevin .. HL 20.13, HL 39.7
Hähl, Hendrik ..... BP 14.17, O 54.1
Hahn, Alexander . HL 20.43, •TT 17.8, •QI 4.8
Hahn, Christian ..... PSV IV
Hahn, Dominik .... •DY 46.7, •TT 75.7
Hahn, Jan ..... BP 26.8, CPP 43.8
Hahn, Larissa ..... •DD 10.1, DD 26.3
Hahn, Nils-Torben ..... TT 93.10
Hahn, Robert ..... CPP 17.36
Hahn, Walter ..... •QI 13.3
Hähnlein, Bernd ..... HL 31.3
Haider, Golam ..... TT 49.2, TT 73.11
Haider, Michael ..... TT 28.7
Haindl, Rudolf ..... •O 49.3, QI 2.6, AKBP 4.3
Haink, David ..... •TT 29.4
HAJ TAIEB, Amine ..... •AKPIK 5.13
Hajdu, Janos ..... DY 53.1, TT 87.1
Hajiahmadi, Zahra ..... •FM 11.37
Hajizadeh, Nima ..... •HL 55.11
Hak, Victoria ..... O 78.1
Hakim, Bishoy ..... BP 16.11
Hakonen, Pertti ..... TT 97.1
Halas, Naomi ..... O 96.10
Halbauer, Max ..... •O 45.1
Halbritter, András ..... MA 17.6
Halbritter, Thomas ..... O 9.6
Haldar, Asmi ..... DY 46.6, TT 75.6
Haldar, Astik ..... •DY 44.10
Haldar, Soumyajyoti ..... MA 21.5
Haldar, Subhomoy ..... TT 78.1
Halder, Sandip ... •MA 11.11, •TT 21.11
Halder, Saronath ..... QI 12.3
Halder, Tanaya ..... TT 25.1
Hall, Darian ..... FM 10.5
Hallenbach, Elias ..... •CPP 39.5
Haller, Andreas ..... MA 7.4, MA 37.1, MA 52.15, TT 64.5, TT 83.12
Halliday, Daniel ..... TT 5.10
Hallilingaiah, Gowrishankar AKBP 2.2
Hallmann, Jörg .... O 40.15, TT 37.15
Hallsteinsen, Ingrid ..... MA 3.4
Hallwig, Olav ..... DS 18.3
Hals, Kjetil Magne Dørheim MA 30.11
Halun, Joanna ..... CPP 56.2
Haluszczynski, Alexander .... DY 6.8
Hamad, Hesham ..... •O 23.6
Hamada, Ikutaro ..•MM 39.4, O 12.10
Hamadeh, Abbass .MA 9.10, MA 9.12
Hamadeh, Alexandre Abbass MA 9.3
Hamann, Danielle ..... TT 5.5
Hamasaki, Kansuke ..... HL 57.1
Hambardzumyan, Karapet .. TT 22.16
Hambeck, Florin Leo ..... MA 57.4
Hambsch, Mike ..... DS 13.1
Hameed, Fareeha ..... FM 19.3
Hameed, Sadeed . MA 39.2, MA 43.4
Hamid, Sundas ..... •HL 26.3
Hamidreza, Esmaielpour .... FM 19.5
Hammad, Mohaned ..... HL 20.12
Hammer, Martin ..BP 14.29, BP 14.58
Hammer, René ..... FM 19.1
Hammer, Sebastian ..... CPP 22.2, HL 26.15, HL 26.54, O 96.1
Hammerschmidt, Thomas .. MM 7.2, MM 9.7, MM 11.4, MM 19.17
Hammoud, Julie ..... •MM 7.3
Hammouda, Sabreen ..... MA 47.10
Hammud, Adnan ..... O 43.2
Hampe, Jochen ..... HL 22.4
Hampel, Silke ..... O 70.2, TT 65.2
Hamrle, Jaroslav MA 39.6, MA 39.13, MM 19.7
Han, Dong ..... •O 69.5
Han, Jian ..... MM 30.1
Han, Kyunghoon ..... •CPP 29.2
Han, Xiufeng ..... AKPIK 6.4
Han, Yixuan ..... O 95.10, TT 96.10
han, zhangang ... BP 14.88, CPP 11.7, DY 17.7
hanaguri, tetsuo ..... O 95.9, TT 96.9
Handel, Mayra ..... •MA 7.56
Handschuh, Maria-Teresa .... QI 14.7, QI 14.8, QI 18.2, QI 18.3
Hanel, Joscha ..... HL 31.4
Hanemann, Paul ..... DD 16.2
Haniš, Jozef ..... •DS 12.7
Hänisch, Klara ..... HL 22.3
Hänisch, Philipp AKBP 2.4, AKBP 14.2
Hanke, Kai Daniel ..... •HL 26.13
Hanke, Michael ..... DS 4.5, HL 24.6
Hankiewicz, Ewelina M. ..... O 63.8, TT 55.8, TT 83.3
Hanna, Abanoub ..... •TT 26.8
Hanna, Michael ..... CPP 7.5
Hanna, Roudy ..... QI 6.9
Hannappel, Thomas ..... CPP 46.43, HL 12.4, HL 26.5, HL 26.11, HL 26.13, HL 26.41, HL 48.3, O 54.2
Hannebauer, Adrian ..... HL 48.6
Hannen, Volker ..... AKBP 7.3
Hannes, Weisbrich ..... TT 50.7
Hannezo, Edouard ..... BP 3.10
Hanrath, Friedrich ..... •O 37.3
Hans, Marcus ..... DS 7.5
Hans, Philipp ..... FM 19.3
Hänsch, Theodor ..... DS 21.8
Hansen, Andreas ..... O 77.4
Hansen, Ingvild ..... FM 12.4
Hansen, Luka ..... O 7.5, TT 9.5
Hansen, Mads ... •TT 29.11, TT 93.17
Hansen, Mads Fonager ..... TT 23.15
Hänseroth, Jonas ..... CPP 9.6
Hansmann, Philipp .. O 71.12, O 71.13, O 84.3, TT 3.5, TT 51.5, TT 66.12, TT 66.13, TT 84.3
Hantke, Nick ..... MM 19.48
Hantzko, Lukas ..... •QI 1.5
Hao, Maosheng ..... O 93.1
Hao, Y ..... MA 19.7, TT 31.7
Haque, Masudul .. DY 32.10, TT 45.10
Harasawa, Ayumi ..... O 60.7
Hardeweg, Lovis ..... •O 3.3, O 15.4, O 17.7, O 99.10
Hardt, Michael . CPP 41.6, CPP 46.36
Harfouche, Messaoud ..... DS 20.2, MA 7.76, MM 12.9, MM 19.28
Harfouche, Messoud ..... TT 93.4
Hargreaves, Cameron ..... AKPIK 6.7
Harich, Jessica ..... BP 9.6
Haridas, Hitha ..... •HL 48.3
Haridas, Shyamkumar Vadakket HL 53.4
Hariki, Atsushi ..... MA 8.13, O 84.5, TT 3.3, TT 84.5
Harling, Benno ..... O 73.3, O 73.4,

•O 74.9, •TT 68.9
Harmat, Adam L. . BP 26.5, CPP 43.5
Harmon, Tyler ..... BP 29.5, •BP 31.2, BP 39.2, CPP 45.5, •CPP 50.2, CPP 55.2
Harms, Christina ..... •HL 57.2
Harmsen, Frithjof .... •O 27.2, O 46.9
Harnack, Nele ..... •MA 6.9
Harnagea, Luminita ... O 2.3, TT 11.1, TT 11.3, TT 92.3, TT 93.5
Haronin, Vadzim ..... FM 4.4
Harre, Kathrin ..... CPP 41.7
Harris-Lee, Eddie ..... •MA 35.10, •TT 60.10
Härtel, Andreas ..... •CPP 20.12, •DY 23.12, •DD 6.2
Hartelt, Moritz ..... CPP 59.4
Harth, Kirsten ... •CPP 10.2, •DY 16.2, DY 25.3, DY 25.4, DY 25.5
Harting, Jens ..... CPP 33.3, DY 61.6, DY 62.8
Hartke, Bernd ..... O 88.6
Härtl, Patrick .... •MA 5.5, MA 39.20, O 44.2, O 60.4, O 63.2, •TT 7.5, TT 55.2
Hartl, Tobias ..... O 72.1, TT 67.1
Hartman, Felix ..... MA 7.39
Hartmann, Alexander K. ..... DY 7.9, DY 15.3, DY 15.4, •DY 60.3
Hartmann, Andreas ..... BP 14.79
Hartmann, Dirk ..... O 78.1
Hartmann, Fabian •HL 29.5, •TT 58.5
Hartmann, Felix ... •DY 61.1, MA 14.4
Hartmann, Jörg ..... UP 6.3
Hartmann, Roman ..... •TT 81.3
Hartsch, Muriel ..... •BP 18.3
Härtter, Daniel ..... BP 7.43
Hasan, M. Nur ... •MA 50.2, MA 58.1, MM 41.3
Hasan, Mahmudul ..... MA 52.32
Hasegawa, Yukio ..... O 42.5
Hashagen, Tim Julius ..... •HL 4.2
Hashimoto, Takahiro ..... O 2.6
Hasil, Serap ..... TT 23.23
Häsler, Benjamin ..... DY 21.6
Hassan, Anees Ul ..... DS 20.23
Hassan, Mariam ..... •DS 18.3
Hassan, Md. Farhatul ..... CPP 17.22
Hassanien, Ahmed MA 39.22, O 70.4, O 70.5, TT 65.4, TT 65.5
Hassanzadeh Sarhangi, Pouya MM 32.3
Hasse, Christian ..... DY 28.3
Hasse, Vicky ..... FM 11.2
Hassinger, Elena ... TT 29.5, TT 52.2, TT 62.6, TT 79.3, TT 94.5
Hassler, Fabian ..... HL 10.3, TT 2.10, TT 20.3, TT 42.7
Hastenteufel, Luca ..... •BP 7.21
Hatton, Peter ..... MA 16.6
Hauer, Jürgen ..... CPP 44.3
Hauet, Thomas ..... TT 14.12
Hauf, Julian ..... AKBP 4.4
Hauff, Dieter ..... TT 22.32
Haug, Rolf ..... DS 14.6
Haug, Rolf J. ..... HL 10.4, HL 17.6, HL 20.10, HL 24.5, HL 29.4, HL 30.5, HL 48.6, TT 20.4, TT 58.4, TT 59.5
Haugerud, Ivar ..... BP 14.86
Haugg, Stefanie ... DS 16.3, DS 20.10, FM 11.26, FM 11.29
Hauklien, Trond ..... MA 6.11
Hauner, Jonas ..... O 94.4
Häupl, Magdalena ..... •BP 14.86
Hauptmann, Nadine ..... O 99.3
Hauschild, Elisabeth ..... CPP 46.19
Hauschild, Johannes ..... •TT 51.7, TT 51.9
Hauser, Kevin ..... •FM 11.23, O 42.3, O 44.3, O 44.7, TT 22.3, TT 92.19
Häuser, Patrick ..... HL 26.5
häußler, ellen ..... TT 72.3
Häusler, Ines ..... HL 25.3
Häusler, Stefan ..... DS 21.4
Hausmann, Bruno ..... •HL 20.2
Hausmann, F. ..... BP 27.8, BP 37.2
Hausmann, Tim Bennet .... BP 14.70
Haverkamp, Nils ..... •DD 6.3
Haverkort, Maurits ..... TT 3.2
Haverkort, Maurits W. ..... MA 19.5, MA 52.6, TT 13.1, TT 23.32, TT 31.5, TT 51.4, TT 71.5, TT 71.6
Havlin, Shlomo ..... SOE 9.4
Hawashin, Bilal ..... O 62.8, TT 54.8
Hawkins, Rhoda ..... BP 40.2
Hayashida, Kenji ..... O 61.11
Hayen, Nicolas .. CPP 19.4, CPP 27.2, DY 20.4, DY 26.2
Haynes, Peter ..... O 50.7
Haze, Masahiro ..... O 42.5, O 64.2
Hazra, Sumeru ..... •QI 6.10
Hazra, Tamaghna .. •DY 13.1, •TT 19.1
He, Jiali .. FM 11.4, •FM 18.7, FM 18.8
He, Lianyi ..... TT 95.3
He, Ran ..... MM 19.44
He, Shikun ..... AKPIK 6.4
He, Yin-Chen ..... TT 2.11
He, Zhiyuan ..... •MA 7.60
He, Zhouyi ..... •BP 39.2, •CPP 55.2
Heber, Bernd ..... UP 7.5
heber, michael ..... TT 25.11
Heberling, Frank ..... O 36.5
Hébert-Dufresne, Laurent ... •SOE 7.2
Hebestreit, Lennart ..... CPP 58.3
Hecht, Bert ..... HL 15.2, O 96.1
Hecht, Daniel ..... •DD 27.8
Hecht, Lukas ..... DY 44.3
Hecht, Stefan ..... O 43.3, O 43.7
Heckel, Alexander ..... O 9.6
Heckens, Anton J ..... DY 15.10
Hecker, Katrin ..... HL 10.3, TT 20.3
Hecker, Tim K. ..... •MM 35.7
Heckmann, Olivier ..... O 93.6
Hedayati, Mehdi K. ..... •AKPIK 4.1
Hedevang, Martin ..... O 34.5
Hedwig, Sebastian ... O 14.2, O 40.16, TT 37.16
Heedt, Georg ..... •TT 15.9
Heenen, Hendrik ..... CPP 46.66
Heenen, Hendrik H. .. DY 14.5, O 13.1, O 34.1, O 81.3, O 86.10, O 97.11
Heering, Peter ..... •DD 38.2
Heger, Julian ..... CPP 15.1
Heger, Julian E. ..... CPP 53.2
Heggemann, Jonas ... •O 5.5, O 36.2, O 44.5
Hegner, Franziska S. ..... HL 40.3
Hehn, Anna-Sophia ..... HL 24.8
Hehn, Michel ..... O 40.15, TT 37.15
Heib, Tim ..... •QI 10.2
Heib, Tim Christoph ..... QI 10.1
Heid, Rolf ..... TT 49.1
Heide, Christian .... SYFC 1.5, O 74.1, TT 68.1
Heide, Gerhard ..... MM 19.46
Heidenreich, Sebastian ..... DY 44.6
Heidkamp, Jan-Niklas ..... •HL 24.9
Heidrich-Meisner, Fabian .. TT 23.29, TT 23.30, TT 44.3
Heidweiler, Leo .. •DY 51.6, •SOE 15.6
Heikkilä, Tero ..... TT 22.24
Heikkinen, Petri ..... TT 22.17
Heil, Christian ..... TT 22.34
Heil, Christoph .... •TT 80.5, TT 80.9
Heil, Jochen ..... CPP 46.61
Heiler, Jonah ..... HL 11.6
Heiliger, Christian ..... CPP 16.5, CPP 17.38, CPP 17.40, HL 37.1, HL 48.2, MA 10.2, MA 39.16
Heim, Kilian ..... •TT 22.32
Heimbold, Joram ..... CPP 46.60
Heimrich, Karl .. MA 48.10, •MA 52.17
Hein, Petra ..... O 84.11, TT 84.11
Heindel, Tobias ..... QI 18.7
Heindl, Moritz ..... HL 26.50
Heindl, Moritz B. ... HL 45.4, HL 45.5
Heine, Johanna .. HL 20.20, HL 23.8, HL 26.28
Heine, Thomas ... MA 36.6, MA 36.7
Heinemann, Thomas ..... BP 14.47
Heinen, Laura ..... •BP 8.3
Heinicke, Susanne . •TUT 2.1, •DD 1.1, DD 9.3
Heinisch, Nils ..... •HL 55.4
Heinke, Heidrun .... DD 8.2, DD 20.2, DD 23.1, DD 24.2, DD 25.1, DD 28.1, DD 30.6, DD 36.1
Heinrich, Andreas MA 43.5, MA 49.8, O 15.6, O 15.9, O 15.11, O 17.1, O 17.4, O 56.3, O 64.2, O 77.5, O 77.6, O 99.11
Heinrich, Benjamin ..... •TT 92.17
Heinrich, Lukas ..... BP 15.8
Heinrich, Matthias DY 48.6, HL 20.25, •MA 7.74
Heinrichs, Luzie Lina ..... •CPP 39.4
Heins, Christopher ..... •MA 10.4
Heinsdorf, Niclas .. •MA 10.5, O 84.9, TT 84.9
Heintz, Hannah .... BP 11.9, •BP 14.17
Heintzmann, Rainer ..... BP 14.33, BP 14.37, BP 14.45, BP 14.58
Heinz, Aaron ..... AKBP 7.4
Heinz, Björn ..... MA 9.3, MA 9.10, MA 9.12, MA 39.14, MA 48.1, MA 48.3, MA 48.4, MA 48.9, MA 52.19
Heinz, Cajetan ..... •TT 15.10
Heinz, Hendrik ..... CPP 39.1
Heinze, Leonie ..... MA 7.3
Heinze, Stefan ... MA 21.5, MA 39.21, TT 6.3
Heinzel, Thomas . BP 14.47, BP 14.56, HL 20.35, HL 20.36, HL 20.54
Heinzelmann, Sarah ..... TT 13.10
Heinzmann, Ulrich ..... O 66.5
Heise, Alexander ..... MA 12.1
Heise, Stephan ..... DS 20.4
Heißenbüttel, Marie-Christin . HL 25.2
Heisig, Marco ..... BP 33.4
Heisinger, Fabian ..... •O 23.9
Heitzig, Jobst ..... SOE 9.1
Heiz, Ueli ..... O 65.6, O 78.2, O 81.6, O 94.8, O 94.10
Hejtmánek, Jiří ..... MA 34.2
Held, Karsten ..... MA 11.6, TT 10.1, TT 13.1, TT 21.6, TT 23.23, •TT 39.3, TT 69.2
Held, Tobias .. O 40.1, O 40.2, O 40.3, O 40.4, O 40.6, O 98.6, TT 37.1, TT 37.2, TT 37.3, TT 37.4, TT 37.6
Helias, Moritz ..... DY 43.9, DY 58.5, DY 58.7, DY 58.8, SOE 4.8, SOE 17.5, SOE 17.7, SOE 17.8
Hellenes, Anna B. ..... MA 54.6
Hellenes, Anna Birk ..... •MA 10.6
Hellenkamp, Felix ..... MA 43.2
Heller, Lars ..... MA 7.81
Heller, Maximilian HL 20.49, HL 55.10
Heller, René ..... AKBP 3.6
Heller, Robert ..... •O 4.7
Hellman, Lukas ..... TT 13.1
Hellmann, Frank ... DY 51.6, SOE 15.6
Hellsvik, Johan ..... •MA 34.1
Hellweg, Thomas . CPP 7.4, CPP 31.2, CPP 46.33, CPP 46.38, CPP 58.5
Hellwig, Fabienne ..... MM 19.48
Hellwig, O. ..... TT 24.7
Hellwig, Olav ..... DS 18.1, DS 20.42, MA 57.6
Helm, Bernd ..... DS 21.4
Helm, Christiane A. ..... BP 5.4, CPP 46.28, CPP 46.29
Helm, Manfred ..... HL 17.5, TT 57.6, AKBP 2.1
Helm, T. ... MA 47.7, TT 29.1, TT 80.6
Helmbrecht, Katharina .... •FM 22.10
Helmer, Benjamin ..... TT 62.4
Helml, Jakob ..... O 38.6
Helten, Holger ..... CPP 22.2
Helversen, Martin von ..... QI 18.7
Hemberger, Joachim ..... FM 18.8, MA 23.6, MA 52.34, MA 52.36, TT 35.6
Hémery, Samuel ..... MM 36.5
Hemm, Ralf . •O 41.1, O 83.4, •TT 38.1
Hemmida, Mamoun ..... MA 31.2, MA 31.7, TT 47.2, TT 47.7
Hengstler, D. ..... TT 22.31
Hengstler, Daniel TT 22.20, TT 22.21, TT 22.22, TT 22.27, TT 22.28, TT 22.29, TT 22.30, TT 28.2, TT 82.2
Henk, Jürgen ... MA 38.11, MA 38.12, •O 60.1, O 64.8
Henke, Fritz ..... CPP 15.6
Henke, Jan-Wilke ..... QI 2.6
Henke, Marvin ..... •TT 92.14
Henke, Sebastian ..... O 69.6
Henkel, Carsten ..... MM 19.41
Henkel, Karsten .... CPP 16.4, DS 9.4
Henkel, Pascal ..... •HL 4.6, O 58.1
Henkelmann, Gideon ..... •MM 21.3
Henksmeier, Tobias ..... HL 48.7
Henn, Enno ..... CPP 59.1
Henn, Sebastian ..... HL 26.42
Henne, Julia ..... HL 22.4
Hennes, Marc ..... BP 11.5
Hennet, Louis ..... CPP 26.1
Hennig, Christoph ..... MM 19.46
Hennig, Fabian ..... •DD 25.2
Hennig, Joshua . •HL 52.5, AKPIK 5.3
Hennig, Richard ..... •MM 2.1
Henning, Pia ..... DS 16.10, MA 7.10
Henrichs, Luca .... HL 55.5, •HL 55.6
Henriksen, Annika ... O 84.6, TT 84.6
Henriques, Joao C. G. ..... O 15.1
Henríquez, Ricardo ..... O 67.3
Henschel, Cristiane ..... CPP 46.31
Henschel, Mara ..... •BP 14.79
Hensel, Daniel ..... MM 21.8
Hensen, Matthias .. HL 8.8, HL 26.55, HL 46.4
Henss, Anja ..... DS 9.1, DS 20.20
Henstridge, M. ..... MA 25.6
Hentrich, Richard ..... O 79.4
Hentschel, Mario . FM 11.34, MA 37.6
Hentschel, Martina ..... DY 42.12, DY 42.14, •DY 59.3, TT 63.12, TT 63.14, •TT 99.3
Henz, Jakob ..... •DS 21.5, HL 20.11, HL 25.2
Henze, Thomas ..... BP 14.43
Hepting, Matthias ... O 93.5, TT 39.6, •TT 39.7
Herb, Dennis ..... DY 40.3, •QI 20.2
Herb, Michael ..... O 40.7, TT 37.7
Herber, Andreas ..... UP 6.3
Herbert, Maximilian ..... •AKBP 2.3, AKBP 4.4, AKBP 8.1
Herbrych, Jacek ... DY 46.4, MA 47.1, TT 75.4
Herbst, F. S. ..... MA 52.8, •MA 59.8
Herbst, Franz Stefan ..... MA 38.8
Herbst, Lea ..... •DD 29.1
Herbst, Matthew ..... TT 22.22
Herbstritt, Lucas ..... TT 22.30
Herdman, Chris ..... TT 64.1
Herdt, Marija ..... DD 24.2
Heredia, Agustina ..... O 8.7
Herfort, Jens ..... HL 18.9, MA 37.5, TT 32.9
Hergenhahn, Uwe ..... CPP 23.4, CPP 27.3, DY 24.4, DY 26.3
Hergenhan, Felix ..... •CPP 22.3
Hergert, Hannes ..... •HL 42.2
Hering, Dag-Björn •TT 23.11, TT 23.12, TT 94.8
Hering, Matthias ..... •DY 48.5
Herink, Georg ... DY 22.10, HL 26.50, HL 26.51, HL 26.56, HL 45.4, HL 45.5
Herklotz, Andreas ..... MA 30.12
Herm, Michel ..... MM 36.4
Hermann, Johannes M. ..... •O 65.4
Hermann, Sophie ..... •DY 61.3
Hermanns, Maria ..... TT 23.18
Hermes, Ilka .... CPP 41.3, CPP 54.4, HL 3.5
Hermes, Sarah Tabea ..... BP 14.28, •BP 14.32, BP 14.36
Hernández Juárez, Beatriz CPP 46.46
Hernandez, R. G. ..... MA 47.7
Hernández-Mínguez, Alberto HL 11.7, HL 18.9, MA 37.5, TT 32.9
Hernangómez-Pérez, Daniel HL 24.8, •HL 39.10, O 7.4, TT 9.4
Herold, Anna ..... DD 14.3, •DD 23.4
Herper, Heike ..... MM 41.3
Herper, Heike C. . MA 50.2, •MA 50.7, MA 58.1, MM 37.5
Herranz, Gervasi ..... TT 81.1
Herranz, Jesús ..... HL 23.10
Herre, Philipp ..... TT 81.5
Herrera Rodriguez, Rosa ... CPP 17.4
Herrero, Aitziber ..... O 44.15
Herrero, Iker ..... HL 20.8
Herrero, Jorge Moreno ..... BP 31.3, CPP 50.3
Herrgen, Paul ..... MA 8.6, MA 38.7, •MA 47.3
Herringer, Paul ..... •TT 17.6, •QI 4.6
Herritsch, Jan ..... O 68.1
Herrlich, Tobias ..... MA 30.5
Herrmann, Carmen CPP 23.1, DY 24.1, TT 90.6
Herrmann, Cornelius ..... MA 47.11, MA 54.7
Herrmann, Franziska Marie AKBP 11.4, •AKBP 13.3
Herrmann, Paul ... HL 30.3, •HL 54.1, HL 54.2, HL 54.3, TT 59.3
Herrmann, Tabea . •DY 32.4, •TT 45.4
Herrmann, Xaver O. ..... •TT 89.1
Herrmannsdörfer, T. MA 23.5, TT 35.5
Herrmannsdörfer, Thomas MA 52.27
Herrschmann, Julian ..... MA 7.48
Hertel, Raphael ..... CPP 17.43
Hertel, Tobias ... HL 26.27, HL 26.55, HL 45.6
Herter-Lehmann, Tom ..... TT 5.5
Hertl, Nils ..... •O 80.2
Hertle, Lasse ..... UP 7.5
Hervé, Marie ..... TT 49.4
Hery, Benjamin ..... •DY 54.8
Herzen, Julia ..... CPP 46.4
Herzig, Eva M. . CPP 17.14, •CPP 22.1,

CPP 44.6, HL 53.5
Herzig Sheinfux, Hanan ..... HL 10.1, TT 20.1
Herzog, Marc ..... HL 26.52, O 40.15, TT 37.15
Herzog, Max ..... MA 7.17, •MA 27.4
Herzog, Vincent ..... O 46.1
Heß, Christian .... MM 19.44, TT 11.3
Heß, Justus ..... •O 43.8
Heß, Lars Nikolas ..... •MA 52.9
Heß, Regina ..... AKBP 7.4
Hess, Christian .... MM 40.4, O 63.2, TT 11.4, TT 55.2, TT 93.10, TT 93.14
Hess, Nathaniel ..... BP 20.6
Hesse, Vera Anna Nina Alina •CPP 46.11
Hesselmeier-Hüttman, Erik .. QI 20.6
Hetaba, Walid ..... CPP 4.3
Hetényi, Balázs ..... TT 17.7, QI 4.7
Hetzel, Mareike ..... QI 15.3
Heubach, Maren-Kathrin ..... •O 97.3
Heuer, Andreas .. BP 14.20, BP 14.59, CPP 14.4, CPP 17.34, CPP 17.35, CPP 35.4, CPP 46.53, DY 37.4
Heuplick, Lukas ..... O 68.1
Heurs, Michèle ..... •PSV VIII
Heusler, Stefan ..... DD 6.3, DD 23.3
Heuthe, Veit-Lorenz ..... •DY 6.1
Hevia, Samuel ..... O 67.3
Hexemer, Alexander ..... CPP 15.1
Heyde, Markus ..... O 65.5
Heyen, Hauke Lars •MA 21.3, MA 39.7
Heyl, Christoph ..... AKBP 13.1
Heyl, Markus ..... DY 13.5, DY 13.7, DY 14.12, TT 19.5, TT 19.7
Heymer, Oliver ..... •MM 19.5
Heyroth, Frank .. MA 48.10, MA 52.17
Hickel, Tilmann ..... TUT 6.1, FM 9.4, MM 1.1, •MM 5.5, MM 25.2, MM 25.3, MM 34.4, MM 34.7, MM 39.9
Hicken, Thomas ..... •MA 8.3
Hicken, Thomas J. .. MA 8.5, TT 57.2, TT 57.3
Hickey, Ciarán ..... TT 33.4
hidalgo, raúl c. ..... DY 19.3
Hidalgo, Raúl Cruz ..... DY 25.4
Hieckmann, Ellen ..... CPP 15.6
Higginbotham, Andrew P. ... TT 28.11
Higgins, Anthony ..... AKPIK 6.6
Higgins, Luke ..... MA 6.4
Highland, Wyatt ..... •O 35.1, O 35.3
Higueret, Stéphane ..... HL 26.2
Hilaire, Azeline ..... •CPP 46.22
Hilbert, Lennart ..... BP 15.4
Hilbig, Johan ..... HL 55.10
Hildebrand, Elias ..... •FM 11.7
Hildebrandt, Ron ..... HL 1.7
Hildebrnad, Elias ..... FM 11.2
Hilf, Lena ..... •CPP 46.20
Hilfert-Rüppell, Dagmar ..... DD 30.1
Hilgenkamp, Hans ..... TT 28.5
Hilgers, Yannis ..... •O 43.14
Hilken, Per-Ole ..... •CPP 46.29
Hille, Jacob ..... CPP 57.6
Hille, Paul ..... •MA 52.6
Hillebrands, Burkard ..... MA 48.7, MA 48.8, MA 52.7
Hillebrandt, Sabina . •HL 15.3, HL 15.7
Hillenbrand, Rainer . HL 20.8, HL 35.7
Hiller, Guido ..... •O 44.1
Hiller, Jonas ..... HL 4.1
Hillert, Wolfgang FM 11.29, AKBP 9.1, AKBP 9.2
Hillier, Adrian D. ..... TT 14.9
Hilmer, Hannah ..... O 28.6, •O 28.7
Hilscher, Sebastian ..... TT 22.28, •TT 22.29
Himanen, L. ..... AKPIK 6.5
Himanen, Lauri .... FM 6.5, MM 22.3, AKPIK 6.3
Himcinschi, Cameliu ..... FM 7.5, MM 13.3, MM 19.46
Himmelsbach, Jan •DY 32.7, •TT 45.7
Himmler, Wolfgang ..... TT 97.2
Hindenberg, Meike ..... AKPIK 6.4
Hinderhofer, Alexander .... CPP 12.3, CPP 12.5, CPP 48.1, DS 21.4, AKPIK 6.6
Hindriksen, Alina ..... DD 27.1
Hinduja, Chirag ..... CPP 8.5
Hinke, Tobias ..... O 78.2
Hinkelmann, Maria ..... •DD 8.2
Hinkov, Vladimir .. MA 24.1, TT 25.11, TT 36.1
Hinlopen, Roemer . TT 17.2, •TT 97.5, QI 4.2
Hinostroza Caldas, Alejandra •BP 14.63
Hinrichsen, Haye ..... MA 7.51
Hinsley, Gerard ..... HL 4.1
Hintze, Janos ..... •BP 14.70
Hinz, Brian ..... CPP 37.6
Hinz, Sebastian ..... HL 22.4
Hirel, Pierre ..... FM 11.6, •MM 27.1
Hirnet, Lena ..... •MA 47.5, O 48.5
Hirohata, Atsufumi ..... MA 52.28, MA 52.29
Hirsch, Florian ..... •HL 3.1
Hirsch Passicos, Arthur .. •AKBP 6.2
Hirschberger, Max MA 52.37, MA 54.1
Hirschberger, Maximilian .. MA 55.12
Hirschfeld, Lucas ..... O 46.5
Hirschmann, Eric .DS 20.22, MM 12.8
Hirschmann, Julian ..... HL 39.8
Hirschmann, Moritz M. ..... MA 8.1, MA 54.1
Hisatomi, Ryusuke ..... MA 52.13, •MA 59.4
Hitaishi, Prashant BP 14.24, CPP 19.4, •CPP 27.2, CPP 46.4, DY 20.4, •DY 26.2
Hlawacek, Gregor .. HL 18.3, HL 38.3, HL 38.11, •HL 40.5, HL 56.2, MM 11.2, TT 32.3, QI 2.9
Hlawatsch, Julius . DD 36.2, •DD 42.1
Hlawaty, Rebekka ..... MA 50.5
Ho, E. ..... MA 25.6
Ho, Hsin-Mei ..... •O 61.6
Ho Lee, Byung ..... BP 27.10
Ho, Sy Dat ..... •CPP 23.5, •DY 24.5
Hoang, T.P. ..... MA 7.30
Höcherl, Simon ..... TT 56.13
Hochhaus, Julian Andreas .... O 94.9
Höcker, Birte ..... PSV I, •SYSC 1.3
Hocker, Stephen ..... •O 29.1, O 29.3, O 94.11
Hodak, Richard ..... HL 4.1
Hodge, Themba ..... TT 15.1
Hodgson, Stephen ..... TT 95.7
Hodson, Wade ..... •DY 9.5
Hoecht, Jonas ..... TT 71.6
Hoehl, Arne ..... O 96.5
Hoepfner, Lara ..... BP 7.28
Hoeppe, Hannes P. CPP 27.4, DY 26.4
Hoesch, M. .. O 19.10, O 59.2, TT 48.2
Hoesch, Moritz .. MA 7.67, MA 39.18, O 42.9, O 63.4, TT 55.4
Hoesch, Mortiz ..... TT 14.4
Hofacker, Andreas .. •HL 2.7, HL 22.2
Hofemeier, Arne .... BP 7.43, BP 7.48
Höfer, Johannes ... •TT 78.1, TT 82.1
Hofer, Markus ..... •SOE 11.4
Höfer, Ulrich ..... SYFC 1.1, MA 12.2, O 14.6, O 38.6
Hofestädt, Jannik ..... •JOB 2.1
Hoff, Dominik ..... •TT 62.2
Hoff, Felix .DS 20.31, DS 21.1, FM 11.2
Hoffman, Bernd ..... BP 40.1
Hoffman, Jennifer E. ..... FM 11.23
Hoffman, Sebastian ..... MA 37.8
Hoffmann, Angélique ..... FM 11.30, FM 14.3
Hoffmann, Cedric ..... CPP 57.6
Hoffmann, Christoph G. .... •CPP 2.1, •SOE 3.1, •UP 1.1, UP 6.6
Hoffmann, Georg DS 20.26, •HL 40.1, HL 40.8
Hoffmann, Hendrik ..... O 46.2
Hoffmann, Kevin Marvin .. •CPP 60.1
Hoffmann, M. ..... MA 25.6
Hoffmann, Nico ..... DS 20.34
Hoffmann, Noah ..... •MM 9.6
Hoffmann, Raik ..... AKPIK 6.4
Hoffmann, Raja ..... •HL 20.31
Hoffmann, Rebecca ..... •HL 10.1, •TT 20.1
Hoffmann, Stefan . DD 38.1, •DD 41.2
Hoffmann, Sven ..... TT 11.3, TT 11.4
Hoffmann-Vogel, Regina .... O 44.12, TT 78.6, TT 90.1
Höffner, Josef ..... UP 3.5
Hofheinz, Max ..... TT 82.5
Höflich, Katja ..... FM 11.28
Höfling, Felix ..... DY 61.7
Höfling, Sven ..... HL 1.12, HL 20.30, HL 29.5, HL 34.2, TT 58.5, QI 18.7
Hofmann, Alexander ..... CPP 48.3
Hofmann, Andrea ..... QI 14.25
Hofmann, Anna-Lena ..... CPP 15.6, CPP 57.3
Hofmann, Caspar ..... QI 18.6
Hofmann, Jan Philipp ..... O 54.5
Hofmann, Johannes ..... MA 8.2
Hofmann, Johannes S. ..... •TT 4.5
Hofmann, Johannes Stephan TT 2.11
Hofmann, Jonas ..... DD 14.3
Hofmann, Jonathan K. ..... •O 41.4, O 54.3, •TT 38.4
Hofmann, Manuel ..... •CPP 46.3
Hofmann, Mario ..... HL 20.16
Hofmann, Niklas ..... O 98.9
Hofmann, Oliver ..... O 3.5
Hofmann, Oliver T. ..... O 6.8, O 8.4, O 30.2, O 30.4, O 58.7, O 69.6, O 93.10
Hofmann, Philip ..... O 66.8, O 76.4, O 76.5, O 85.3, TT 27.4
Hofmann, Stephan ..... O 98.10
Hofmeier, David ..... TT 2.3
Hofmeister, David Ari ..... •O 77.4
Hofmeister, Isabella Alexandra •O 40.7, •TT 37.7
Hogan, Conor ..... O 58.3
Höger, Sigurd ..... O 77.4
Hogg, Mark R. ..... HL 55.4
Hogger, Wolfgang .. DY 42.4, TT 63.4
Hoheneder, Alexander ..... O 80.1
Hohenwarter, Anton ..... MM 7.9
Hohls, Frank HL 17.2, HL 25.1, O 95.1, TT 96.1
Hohlstamm, Anselm ..... •BP 14.10
Hohmann, Judith ..... QI 11.4
Hohmann, Judith K. ..... QI 11.5
Höhn, Christian .... HL 12.4, HL 26.11
Höhndorf, Greta ..... •BP 7.14
Höhne, Jens ..... TT 89.1
Höhner, Lars ..... CPP 19.2, DY 20.2
Holder, Luise ..... MA 39.24
Holec, David ..... MM 7.5, MM 17.1, MM 21.5
Holeschovsky, Linus ..... TT 97.5
Holl, Klara ..... •CPP 46.2
Holl, Max Phillip ..... DY 41.11
Holland, Julian ..... •MM 22.1
Hollatz, Paul ..... •HL 20.19
Holldack, Karsten ..... MA 36.10
Holleitner, Alexander HL 3.9, HL 13.2, HL 13.5, HL 18.8, HL 20.9, HL 30.6, TT 32.8, TT 59.6
Holleitner, Alexander W. ..... HL 3.6, HL 8.4, HL 8.7, HL 57.4
Holler, Mirko ..... MA 7.81
Hölling, Michael ..... DY 8.4, DY 41.5
Höllmann, Davin ..... •HL 24.5
Hollo, Aron ..... •AKPIK 5.12
Hollstein, Helena ..... •HL 26.54
Hollweger, Simon B. ..... O 93.10
Holm, Christian . BP 7.13, CPP 46.25, CPP 49.1, CPP 49.3, DY 44.16
Holovatch, Taras ..... DY 54.2
Holovatch, Yurij ... •DY 54.2, SOE 5.2
Hölscher, Torsten ..... DS 4.3, DS 8.5
Holschuh, Lennard ..... •CPP 10.7, •DY 16.7
Holsgrove, Kristina .FM 12.5, FM 12.6
Holt, Samuel J. R. ..... MA 34.4
Holt, Samuel RJ ... MA 50.2, MA 58.1
Höltermann, Holger ..... •AIW 1.4, •AIW 1.5
Holters, Johannes ..... •HL 20.4
Holthaus, Martin ... DY 59.8, TT 99.8
Holtmann, Marcel ..... •O 67.8
Holzer, Christof ..... O 12.1
Hölzer, Jule S. ..... O 45.3
Hölzer, Laura ..... •CPP 46.50
Holzhacker, Daniel ..... •O 65.1
Holzhauser, Henrik ..... •DS 7.3
Holzmann, Christian ..... •MA 52.33
Holzmann, Thomas ..... O 56.2
Hömke, Franziska ..... •TT 22.37
Hommel, Caroline ..... O 8.6, •O 17.4, O 77.5, O 77.6, O 89.10
Hommelhoff, Peter •SYFC 1.5, O 74.1, TT 68.1
Honda, Yoshio ..... HL 57.1
Honecker, Andreas . TT 4.2, •TT 26.1, QI 16.6
Honerkamp, Carsten ..... DY 58.7, SOE 17.7, TT 29.7
Hong, Cheng-Lin ..... •QI 5.1
Hong, Chong-Wei ..... DY 19.2
Hong, Jinbao ..... AKBP 5.2
Hong, Jong-Am ..... O 82.2
Hong, Seong-Hyun ... O 17.4, •O 77.6
Hong, Xiaochen ..... TT 93.14
Hönicke, Philipp ..... MM 12.3
Honigmann, Alf .... BP 16.2, BP 27.10
Honma, Daichi ..... O 67.9
Honnigfort, Christian ..... CPP 5.3
Hooley, Chris .... •MA 23.3, •TT 35.3, TT 98.7
Hopf, Lennard ..... •HL 20.13
Hopfmann, Caspar HL 34.1, •HL 55.7, HL 56.4, HL 56.5
Höpfner, Jakob ..... HL 37.4
Hoppe, Harald CPP 17.22, CPP 17.25, CPP 17.41, CPP 48.4, •CPP 57.4, CPP 57.5
Hoppe, Josephine ..... BP 26.10, CPP 43.10
Hoppe, Wolfgang MA 7.13, MA 30.12, O 14.5
Höppel, Heinz Werner ..... MM 32.3
Horák, Aleš ..... MA 34.5
Horák, Michal ..... O 27.1, O 96.7
Horak, Sarah ..... O 94.5
Hörandl, Stefan ..... O 11.5
Horbach, Jürgen CPP 35.3, CPP 35.5, DY 37.3, DY 37.5
Horenburger, Tessa ..... •DD 8.1
Hörhold, Sebastian ..... •DY 42.13, DY 59.5, •TT 63.13, TT 99.5
Hörich, Florian ..... HL 33.2, HL 33.3
Horiike, Yoshiaki .. •DY 53.2, •TT 87.2
Hörmann, Lukas .. O 3.5, O 3.6, O 4.1, •O 33.7, O 62.4, TT 54.4
Hörmann, Max TT 2.6, TT 23.8, QI 5.4
Hörmann, Nicolas ..... O 65.3
Hörmann, Nicolas G. .•O 13.8, O 65.8, O 97.7, O 97.10, O 97.11
Horn, Alexander ..... DS 21.9
Horn, Sophia ..... SOE 10.3
Hornbostel, Jan-Lucas ..... •O 73.4
Horn-Cosfeld, Beate ..... HL 20.54
Horneber, Dominik ..... HL 1.12
Hornig, Dominik ..... DS 18.1
Horn-von Hoegen, Michael .. HL 52.4, O 10.10, O 26.4, O 33.6, O 72.1, O 85.5, O 86.9, O 96.2, O 98.4, TT 2.5, TT 16.10, TT 67.1
Horoz, Sabit ..... •DS 20.2
Horstink, Tim ..... TT 28.5
Horstmann, Jan Gerrit ..... MA 7.32, MA 27.9, O 86.7, •O 98.2
Horstmann, Lukas ..... •TT 51.10
Hortschitz, Wilfried MA 34.4, MA 58.1
Horvát, Szabolcs ..... BP 14.49
Horváth, Zsolt Endre ..... DS 6.4
Horz, Holger ..... DD 6.1
Hosaka, Yuto ..... SYBS 1.3
Hossack, Cedric ..... •UP 2.1
Hossain, Md. Tarik . HL 13.7, HL 20.6, HL 20.14, •O 10.6, •TT 16.6
Hosseinifar, Rahil ..... MA 38.4
Hötte, Nele ..... DD 30.6
Hötzel, Rudolfo ..... HL 12.3
Hötzinger, Andreas ..... DY 42.13, •DY 59.5, TT 63.13, •TT 99.5
Hou, Disha ..... •TT 26.4
Hou, Xiao ..... O 2.2
Houel, Arnaud ..... HL 38.11
Houmes, Maurits ... •O 71.3, •TT 66.3
Houzet, Manuel ..... TT 50.1
Hövel, Philipp ..... SOE 8.2, •SOE 8.4
Hövelmann, Svenja ..... BP 14.24
Hövelmann, Svenja C. ..... CPP 19.4, DY 20.4
Hoverath, Annika ..... DD 16.3
Howard, Ian ..... HL 45.8
Howard, Michael CPP 46.55, DY 41.16
Howson, Griffin C. .. MA 31.1, TT 47.1
Hoyer, Rhea ..... •MA 2.4
Hrabec, Ales ..... FM 23.5, MA 44.2, TT 76.2
Hrdlicka, Lutz ..... UP 7.2
Hricovini, Karol O 14.1, O 76.3, O 93.6
Hroncová, Beáta ..... •DS 21.7
Hrůza, Dominik .. •O 6.1, O 8.2, O 69.1
Hsieh, Ya-Ping ..... HL 20.16
Hsu, Chih-Yao ..... BP 14.38
Hsu, Hsiu-Chuan . MM 19.24, TT 41.8
Hsu, Jia-Xiang ... MA 31.10, TT 47.10
Hsu, Lan-Tien ..... •FM 12.7
Hsu, Tzu-Ching . •MM 19.24, •TT 41.8
Hu, Fangyi ..... •HL 20.65
Hu, Haiyang ... QI 8.3, QI 11.6, QI 11.9
Hu, Haoyu ..... TT 74.1
Hu, Kwangyul ..... MA 48.10
Hu, Mengli ..... •MA 47.4
Hu, Mengying ..... •QI 15.9
Hu, Pengyu ..... DS 11.1
Hu, Qi ..... •TT 83.5
Hu, Shiqi ..... •MA 38.5
Hu, Wenxiang ..... TT 62.6

Hu, Xiaopeng ..... TT 29.12
Hu, Yi ..... TT 29.12
Hu, Yu-Min ..... •QI 9.1
Hu, Zhiwei ..... •FM 11.17, MA 19.5, TT 31.5
Hua, Nelson ..... HL 8.6
Huang, Botsz ..... HL 29.1, TT 58.1
Huang, Chien-Lung MA 31.10, •TT 2.1, TT 47.10, TT 93.8
Huang, Dennis ..... •TT 49.3
Huang, Guanhao ..... QI 2.6
Huang, Jiayun ..... DY 41.1
Huang, Jie ..... O 5.5
Huang, Jingsong ..... O 54.4
Huang, Jun ..... MM 25.5, O 39.4
Huang, Junxiang ..... QI 12.7
huang, kai ..... DY 19.3, •DY 41.1
Huang, Lee-Kang ..... DS 6.6
Huang, Libai ..... TT 44.4
Huang, Lingen ..... AKBP 8.8
Huang, Meng-Jie ..... O 7.5, TT 9.5
Huang, Shirong ..... CPP 7.1
Huang, S-W ..... MA 25.6
Huang, Wantong ..... O 15.4, O 17.7, O 17.9, O 89.12, O 99.2, O 99.10, •TT 95.3
Huang, Xiaochun ... •O 63.2, TT 11.3, •TT 55.2
Huang, Xiaohan ..... •DY 61.6
Huang, Xuan-Fu ..... HL 20.55
Huang, Yao-Wei ..... BP 14.38
Huang, Yifan ..... •BP 31.1, •CPP 50.1
Huang, Yi-Ping .... •DY 2.4, DY 32.11, •TT 1.4, TT 45.11
Huang, Yu-Chi ..... •MA 25.4
Huang, Yunfei ..... •BP 7.24
Huang, Yushen ..... •MM 19.21
Huang, Zhen ..... TT 51.12
Huang, Zilong ..... •BP 14.37
Hub, Jochen S ..... •BP 20.4
Huber, David ..... •O 14.5, O 42.1
Huber, Dominik ..... •BP 33.2
Huber, Joel ..... •QI 12.4
Huber, Liam ..... MM 5.5
Huber, Marcus ..... QI 7.2, QI 16.10
Huber, Margaretha ..... •DS 9.3
Huber, Markus A. ..... O 12.5
Huber, Nico ..... TT 41.6
Huber, Patrick .... •CPP 6.1, CPP 6.5, CPP 46.9
Huber, Rupert ..... •SYFC 1.1, HL 8.1, HL 39.8, MA 12.2, O 12.5, O 12.8, O 38.6, O 40.8, TT 37.8
Huber, Tito ..... MM 19.15
Huber-Loyola, Tobias ..... HL 34.2
Hubert, Patrick ..... O 34.8, •O 88.6
Hübler, Alexandra ..... HL 3.1
Hübner, Jens ..... HL 38.10, •HL 55.8
Hübner, Julia-Maria ..... TT 5.8
Hübner, René ..... HL 17.5, HL 18.3, HL 40.5, MA 45.4, MA 51.1, MA 57.2, TT 32.3, TT 88.1
Hübner, Stefanie ..... BP 37.7
Hübner, Uwe ..... DS 14.9
Hübsch, Robert ..... •O 65.12
Hübschmann, Henry ..... HL 20.33, HL 49.3, •HL 54.4
Huc, Ivan ..... O 45.4
Hucht, Alfred ..... TT 2.5
Hucht, Fred ..... HL 20.43, MA 52.2, TT 42.3
Huck, Christian ..... DS 21.2, O 46.2, O 46.4
Huck, Maryam ..... AKBP 13.2
Hudson, Thomas ..... MM 27.5
Huebl, Hans ..... HL 18.1, MA 30.5, MA 37.7, MA 45.1, MA 51.8, MA 52.18, MA 59.5, TT 22.25, TT 22.26, TT 32.1, TT 43.9, TT 88.8, QI 2.4, QI 14.21
Huebsch, Marie-Therese ... MA 34.13
Huelga, Susana ..... •TT 18.2
Huepe, Cristián .... CPP 11.7, DY 17.7
Huettig, Annette O 9.4, O 45.4, O 78.3
Hufenbach, Julia ..... MM 3.9
Hufenbach, Julia Kristin ..... MM 7.1
Huffmann, Emilie ..... TT 2.11
Hüffmeier, Laurenz •DS 20.27, O 28.6
Hug, Florian ... •AKBP 4.1, AKBP 14.3
Hug, Hans ..... MA 44.2, TT 76.2
Hug, Hans J. ..... •O 64.1
Hug, Hans Josef ..... O 9.11
Hugenschmidt, Christoph ... MM 7.7
Hüger, Daniel ..... O 54.7
Hughes, Stephen ... HL 30.4, TT 59.4
Hugues, Maxime ..... HL 26.2
Hühn, Kai ..... HL 55.8
Huhnstock, Rico . CPP 30.2, DY 41.13, MA 7.23, MA 36.4, MA 36.5, MA 52.40, MA 57.6
Hui, Xingjian ..... •AKBP 12.3
Huijink, Roeland ..... TT 28.5
Huisinga, Margarete . •O 71.4, O 99.5, •TT 66.4
Hüllmandel, Laura ..... •HL 26.56
Hülsenbusch, Thomas .... AKBP 11.2
Hülser, Tobias ..... •DY 6.9
Hultzsch, Thomas ..... TT 78.6
Humbert, V. ..... TT 69.3
Humbert, Vincent ..... TT 69.5
Hummer, Fabian ..... AKBP 8.10
Hummer, Gerhard ..... BP 15.11
Hümmer, Thomas . DS 21.8, HL 26.26
Huňařová, Anna ..... MM 8.10
Hung, Tzu-Chao ..... O 9.10, O 12.8, •O 83.5
Hunger, David ..... BP 9.5, DS 21.8, HL 26.26
Hunger, Johannes ..... CPP 13.2
Hunger, Martin CPP 13.7, •CPP 46.28
Hungerland, Jonathan ..... BP 14.70
Hunkemöller, Marc ..... •SOE 4.6
Hunnestad, Kasper FM 18.8, MA 37.6
Hunter, Kye E ..... •BP 21.6
Hunter, Robert ..... CPP 26.1
Hunyady, Csongor ..... QI 6.3
Hupe, Lukas ..... BP 10.6, CPP 18.6, DY 18.6, DY 33.2, DY 44.12
Hüppe, Franziska ..... •CPP 4.4
Huq, Mashiat ..... CPP 46.65
Hurskyy, Stepan ..... FM 14.4
Hus, Saban ..... O 73.1
Huschle, Jonathan ..... •TT 22.11
Huse, Nils ..... BP 9.6
Hüser, Dorothee ..... FM 19.8
Huseynov, Elchin ..... •MM 36.3
Hussain, Muhammad ..... •HL 35.6
Hussain, Sajjad ..... •MA 42.10
Hussein, Tawfik ..... •DS 20.1
Hussey, Nigel ..... TT 97.5
Husstedt, F. ..... TT 25.6, •TT 29.1
Hutardo, Mar Alcazar ..... BP 2.4
Hütner-Reisch, Johanna I. .... O 55.4
Huttel, Erhard ..... AKBP 4.2
Hütten, Andreas CPP 3.4, CPP 46.14, DS 6.5, MA 7.62, MA 7.63
Hüttner, Celina ..... SYFC 1.5
Hüttner, Niklas ..... TT 97.2
Huxley, Andrew .... TT 29.2, TT 93.17
Huynh, Lilia ..... •FM 18.6
Hwang, H. Y. ..... TT 69.6
Hwang, Hyein ..... CPP 23.1, DY 24.1
Hwang, Sun-Yong ..... TT 42.11
Hwang, Younghun MA 33.12, O 71.14, TT 66.14
Hyder, Ali ..... •FM 2.6
Hyman, Anthony ..... •PLV XI
Hyman, Anthony A. . BP 32.6, DY 52.6
I S, Devamrutha ..... •MA 39.3
Iadecola, Thomas .. DY 46.2, TT 75.2
Iannetti, Mattia .... •O 63.8, •TT 55.8
Ibach, Harald ..... O 67.9
Ibanez-Aspiroz, Julen ..... HL 36.3
Ibañez-Azpiroz, Julen .. O 7.4, TT 9.4, TT 71.7
Ibrahim, Abdullahi ..... •SOE 4.5
Ibrahim, E. ..... FM 2.7
Ibrahim, Hamza ..... BP 15.6
Ickler, Maret ..... CPP 20.3, DY 23.3
Ide, K. ..... AKBP 1.1
Ide, Katharina E. AKBP 4.4, AKBP 14.1
Ide, Niklas ..... •O 69.4, O 83.8
ideta, satoshi ..... O 82.3
Idriss, Hicham ..... O 88.7
Iglesias, L. ..... TT 69.6
Iglesias, Lucia .... FM 18.6, •TT 69.4, TT 69.5
Iglev, Hristo ..... HL 46.1
Ihara, Yoshihiko .. •MA 19.4, •TT 31.4
Ihle, Thomas ..... DY 44.4, DY 44.8, DY 55.7
Ihssen, Sören ..... •TT 43.6, QI 8.1
Il'ichev, Evgeni ..... TT 93.6
Il'ichev, Evgenii ..... TT 5.1, TT 64.2
Iličin, Teodor ..... TT 22.6
Illing, Elias •BP 1.8, BP 14.3, •CPP 1.8, •DY 4.8
Illing, Rico ..... MA 49.1, MA 49.5
Ilyakov, Igor ..... MA 7.46, MA 12.4, MA 25.8, MA 35.6, O 41.3, TT 14.8, TT 38.3, TT 60.6
Ilyas, Ahmed ..... AKPIK 6.3
Ilyn, Maxim MA 11.10, O 10.2, TT 16.2, TT 21.10
Imada, Manami ..... •BP 14.77
Imam, Neama ... •CPP 16.4, MA 7.76, MM 19.28
Imamoglu, Atac ..... HL 13.4
Imamoglu, Mehmet Selim ... •O 69.9
Imamura, Masaki ..... O 42.5
Imbrasas, Paulius ..... HL 26.16
Imhof, Margarete ..... DD 23.2
Imperiale, Christian ..... O 56.6
in 't Veld, Yann ..... •TT 12.7
Inajetovic, Matteo ..... QI 3.7, •QI 5.3
Inami, Eiichi ..... O 64.7
Inayeh, Alex ..... O 56.6
Inckemann, Sebastian ..... FM 11.30, •FM 14.3
Ingebrandt, Sven ..... O 96.3
Ingo FLEGE, Jan ..... MM 19.28
Ingrosso, Alessandro ..... DY 45.5, SOE 14.5
Íñiguez-González, Jorge ..... FM 18.8
Inosov, Dmytro .... •TUT 5.1, •MA 1.1, MA 7.2, MA 19.3, MA 19.4, MA 19.6, TT 31.3, TT 31.4, TT 31.6
Inosov, Dmytro S. . MA 31.8, MA 31.9, TT 47.8, TT 47.9, TT 72.3, TT 93.15
Inoue, Ryota ..... O 64.5
Insuasti Pazmino, Bolivar Efrain •TT 72.9
Inzani, Giacomo ..... O 38.6
Inzenhofer, Tobias ..... HL 39.8
Iodchik, Andrey . CPP 17.24, HL 20.48
Ion, Lungu ..... •CPP 46.16
Ionov, Leonid ..... MA 49.1
Iori, Gianluca ..... FM 19.3
Ipek, Selman ..... •QI 12.5
Iraola, Mikel ..... MA 47.4
Irman, Arie ... AKBP 10.1, AKBP 10.2, AKBP 11.3, AKBP 11.4, AKBP 12.5, AKBP 13.3
Irmler, Andreas ..... •TT 51.3
Isacsson, Andreas . CPP 10.1, DY 16.1
Isaeva, Anna ..... FM 11.25, MA 3.3, MA 24.3, •MA 39.19, MA 52.35, O 2.5, TT 36.3
Isaia, Daniel ..... MM 27.3
Isbrandt, Gloria ..... •TT 72.1
Isele, Ricco ..... O 94.11
Isensee, Jonas .... BP 7.48, DY 44.12
Ishida, Hiroshi ..... MA 55.4
Ishikawa, Hikaru ..... O 64.5
Ishimori, Issei ..... O 67.9
Ishiwata, Shintaro ..... FM 9.2
ishizaka, kyoko ..... O 95.7, O 95.9, TT 96.7, TT 96.9
Işik, Berkay ..... DD 7.2
Islam, A.T. M. Nazmul ..... TT 26.8
Islam, ATM Nazmul ..... TT 26.10
Islam, Md. Moidul ..... CPP 17.22, CPP 57.4
Islam, Md Mursalin ..... •TT 44.5
Islam, Nazmul ..... TT 26.7
Islam, Rabiul ..... HL 2.5, HL 20.48, •HL 22.6, HL 26.18
Ismail, Hassan . •CPP 48.4, CPP 57.4
Isobe, Masahiko .... O 93.5, TT 39.6, TT 39.7, TT 49.3, •TT 49.8
Israel, Noel ..... MA 36.12
Issa, Sally ..... •HL 23.2
Issac, Abey ..... UP 8.1
Iten, Aaron ..... FM 12.7
Ito, Naoki ..... O 84.5, TT 84.5
Ito, Shunichiro ..... O 82.4
Ito, Suguru ..... O 14.6, O 38.6
Itto, Yuichi ..... •DY 27.1
Ivády, Viktor ..... QI 20.6
Ivakhno-Tsehelnyk, Oleksandra •HL 1.4
Ivanjek, Lana ..... DD 14.1
Ivanov, Alexandre ..... TT 95.7
Ivanov, Viktor CPP 46.59, •CPP 46.60
Ivanova, Vladislava ..... HL 20.64
Ivanovic, Filip ..... •CPP 25.1
Iwahara, Naoya ..... MA 3.10
Iyer, Priyanka ..... SYGF 1.5
Izadi, Zohreh ..... •O 31.4
Izquierdo, Manuel ..... O 98.7
J. Bukas, Vanessa ..... O 65.11
J. Mellor, Christopher O 95.6, TT 96.6
J. R. Costa, Fábio .. •O 95.6, •TT 96.6
J. Simpson, Grant ..... O 69.12
J. Willatt, Michael ..... DY 14.10
Jabbari-Farouji, Sara ..... DY 7.8
Jabeen, Ayesha . O 6.1, O 8.2, •O 69.1
Jablonka, Kevin Maik ..... •SYAI 1.5
Jablonowski, Krystian .... •MM 19.40
Jabr, Ahmad ..... •O 65.2
Jabri, Slaheddine ..... •FM 5.11
Jäck, Berthold ..... TT 82.4
Jäckel, Kevin ... MA 39.12, •MA 54.11
Jäckering, Lina ..... O 26.5, O 96.3, O 96.4, •O 96.11
Jackson, Jonathan ..... BP 3.9
Jacob, David MA 5.9, •O 15.10, O 17.6, TT 7.9
Jacob, Stefan ..... BP 14.74, HL 22.2
Jacob, Timo .. O 24.2, O 65.4, O 97.4
Jacobi, Hans-Werner . UP 6.2, UP 8.4
Jacobs, Karin ..... BP 7.41, •BP 11.7, BP 11.9, BP 14.17, O 54.1
Jacobs, Tom .... •DY 45.4, •SOE 14.4
Jacobsen, Gabriel ..... HL 47.2
Jacobsen, Karsten W. ..... MM 17.7
Jacobsen, Nils ..... •O 66.3
Jacobsen, Sol .... •MA 44.3, •TT 76.3
Jacobson, Peter ..... O 48.6, O 58.7
Jacques, Vincent ..... MA 59.7
Jadhav, Ashish .. TT 22.28, TT 22.29
Jadoenathmissier, Hiresh .. TT 22.12
Jaeck, Berthold ..... •MA 8.4
Jaeger, Arndt ..... •HL 26.46
Jaekel, Finn ..... HL 22.3, •HL 22.4
Jaeschke, Frederike ..... •HL 12.1
Jaeschke, Henrik ..... BP 37.5
Jaeschke Ubiergo, Rodrigo .. MA 2.7, MA 7.55, MA 20.6
Jaeschke-Ubiergo, Rodrigo .. MA 2.5, MA 7.53, MA 20.2
Jaeschke-Uiergo, Rodrigo .. •MA 47.6
Jafarizadeh, Arash ..... TT 70.5
Jaffres, H. ..... TT 69.3
Jäger, Lukas ..... HL 35.5
Jäger, Lukas Raam ..... •HL 35.4
Jah, Neha ..... MA 39.7
Jahn, Falko ..... •DS 4.6
Jahnel, Marcus ... BP 31.2, CPP 50.2
Jahnke, Frank ..... HL 13.3, HL 54.11
Jaime, Marcelo ..... O 95.1, TT 96.1
Jain, Arpit . DS 21.5, HL 20.11, O 33.3, O 66.4
Jain, Purnima ..... •DY 62.9
Jain, Sourabh ..... HL 35.3
Jaiswal, Ankita ..... O 46.10
Jakob, C. A. ..... TT 22.31
Jakob, Gerhard ..... DS 6.5, •MA 2.8, MA 21.4, MA 29.9, MA 39.1, MA 47.3, MA 47.9, MA 51.2, TT 46.9, TT 88.2
Jakob, Kai-Luis ..... •FM 19.5
Jakob, Konstantin ..... MM 19.8
Jakob, Konstantin S. ..... •MM 13.5, MM 13.7
Jakovljevic, Sara ..... HL 55.7
Jakowetz, Tom ..... DD 16.3
Jakowski, Jacek ..... O 54.4
Jaksch, Kevin ..... QI 14.1
Jakub, Zdeněk .. O 6.1, •O 8.2, O 69.1
Jalaal, Maziyar ..... DY 34.3
Jalas, Sören ..... AKBP 8.4
Jalil, Abdur R. ..... QI 6.9
Jalil, Abdur Rehman ..... TT 74.3
Jamalzadeh Kheirabadi, Sharieh •HL 24.11
Jamebozorgi, Vahid ..... •FM 11.9
James, Mathew .. MA 29.11, MA 37.7, •MA 51.6, TT 46.11, •TT 88.6
Jamet, Francois ..... TT 17.5, QI 4.5
Jamnik, Simon ..... •MM 19.36
Jamotte, Maxime .. TT 61.9, •TT 83.4
Jamshidi, Kambiz ..... HL 56.1
Jan, Asghar Ali ..... •HL 24.2
Jana, Bapan ..... MA 42.6
Jana, Debayan ..... •DY 43.13
Janas, David ..... •O 83.6
Janas, David Maximilian ... MA 30.9, O 84.4, TT 84.4
Janda, Tomas ..... O 96.5
Janek, Jürgen ..... CPP 4.4, O 24.1
Jang, Harim ..... •O 15.8, O 99.6
jang, iksu ..... •MA 20.4, TT 95.4
Jang, S. ..... O 85.2
Jang, Seunghyeok ..... •MA 49.8
Jang, Won-Jun .. •MA 43.5, MA 49.8, O 56.3
Jang, Wooik ..... CPP 15.6
Jangid, Darshit ..... O 44.11
Janićijević, Željko ..... FM 6.11
Janikwska, Oliwia ..... HL 54.9
Janiš, Václav ..... TT 62.11
Janisch, Rebecca ..... MM 15.5, MM 19.17, MM 19.25, MM 34.6
Janiszewska, Natalia ..... O 87.4

Janke, Una ..... BP 14.25
Janke, Wolfhard . CPP 38.6, •DY 15.1, DY 43.12, DY 60.2
Jankiewicz, Antoni ..... •TT 78.3
Jankovic, Denis .... MA 49.8, •O 89.2
Janmey, Paul ... •BP 35.5, •CPP 51.5
Jannasch, Anita ..... BP 9.4
Janod, Etienne ..... TT 49.4
Jánossy, András ..... MA 16.8
Jansen, Daniel . •O 7.6, O 15.4, O 17.7, O 62.8, O 99.10, •TT 9.6, TT 54.8
Jansen, G.S.Matthijs MA 7.10, O 14.3, •O 14.10, O 19.6, O 38.1, O 40.19, O 40.21, O 66.9, O 98.10, TT 37.19, TT 37.21
Janßen, Martin .... •DY 53.1, •TT 87.1
Jansen, Marvin Marco ..... •HL 17.1
Jansen, Thies ..... •HL 38.2
Janshoff, Andreas .. BP 7.14, BP 7.27
Janson, Kevin ..... BP 33.10
Janson, Oleg ..... TT 11.4, TT 98.4
Jansons, Ernests ..... O 84.1, TT 84.1
Janssen, Foelke ..... •DS 6.3
Janssen, Jan ..... •SYAI 1.3, MM 5.5, MM 13.4, MM 22.4, MM 32.2
Janssen, Lucas M. ..... QI 11.8
Janssen, Lucas Marten ..... TT 15.6, •TT 74.2
Janssen, Lukas ..... TT 26.5, TT 27.3
Janzen, Andreas ..... O 2.6
Janzen, Christian CPP 30.2, MA 36.5
Janzen, Daniel ..... •HL 26.7
Janzen, Philipp ..... •O 45.11
Jaouen, N. ..... MA 25.6
Jarecka, Anton .. •TT 22.18, TT 22.19
Jarecki, Jasmin ..... •MA 38.3
Jaroš, Petr ..... MM 16.6
Jarosik, A. ..... MA 36.3
Jarošová, Markéta ..... DS 7.5
Jarrahi Zadeh, Yasaman .. •HL 20.12
Jäschke, Frederike ..... O 65.12
Jasmeen, Jasmeen .. O 17.8, •O 83.3
Jasti, N. P. ..... HL 54.10, HL 54.12
Jatkar, Kasturie ..... MA 12.6
Jauernik, Stephan .. O 84.11, TT 84.11
Jauk, Thomas ..... MA 27.11
Jauma, Gabriel ..... TT 43.6
Jaurigue, Lina ..... DY 6.5, QI 10.4, AKPIK 4.3
Javaloyes, Julien .... DY 6.5, DY 22.2, DY 22.9, DY 22.10, DY 41.9, DY 48.4, DY 48.5
Javanmard, Younes .. TT 17.6, QI 4.6
Javed, Mohammad Atif ..... TT 53.7
Jaworski, Leonie ..... AKBP 11.2
Jay, Sarah ..... BP 3.10
Jayabalan, Jesumony O 59.5, •O 71.1, O 71.18, TT 48.5, •TT 66.1, TT 66.18
Jayakumar, Vaishnavi ..... •SOE 16.2
Jayalatharachchi, Vishakya ... O 77.1
Jayaram, Sreehari . TT 24.6, •TT 92.5
Jefferson, Ro .... •DY 58.2, •SOE 17.2
Jefremovas, Elizabeth ..... MA 21.6, MA 55.5
Jehl, Xavier ..... QI 2.10
Jehle, Tom ..... •O 44.6, O 79.2
Jehn, Lukas ..... O 22.3
Jeindl, Andreas ..... O 58.7
Jelínek, Pavel O 10.2, O 69.13, TT 16.2
Jeng, Hao ..... QI 2.6
Jenni, Kevin ..... MA 3.6
Jensen, Carl ..... •O 84.11, •TT 84.11
Jentsch, Patrick ..... •BP 12.10
Jentsch, Silas A. ... HL 26.3, HL 42.2, HL 45.3
Jeon, Hoyeon ..... O 73.1
Jeon, Jae-Chun ... MA 7.82, MA 30.2, MA 35.3, TT 22.2, TT 60.3
Jeong, Jong-Ryul ..... MA 52.12
Jeong, Seonghyeon ..... BP 9.6
Jerabek, Paul ..... MM 13.8
Jerger, Markus ..... QI 8.5
Jerkiewicz, Gregory ..... O 97.3
Jeromin, Arno .. CPP 15.1, CPP 46.17, O 28.7
Jeromin, Maren .. •MM 18.3, MM 18.5
Jesche, Anton ..... MA 8.5, •MA 18.7, •TT 30.7, TT 52.6, TT 89.2, TT 98.2
Jeschke, Harald O. MA 11.1, •MA 11.2, TT 21.1, •TT 21.2, TT 57.2
Jester, Stefan-Sven ..... O 77.4
Jestin, Jacques ..... •CPP 36.1
Jetter, Daniel ..... MA 49.2, •MA 49.3
Jetter, M. ..... HL 55.9
Jetter, Michael .. HL 20.37, HL 20.38, HL 20.42, HL 31.4, HL 34.2, HL 34.4, HL 34.5
Jha, Menaka ..... HL 26.14, MM 30.5
Jhankar, Soumyaranjan ..... O 44.16, O 44.17
Ji, Jing-Rong ..... O 84.9, TT 84.9
Ji, Lichen ..... •TT 29.12, TT 95.3
Ji, Shuai-Hua ..... TT 29.12, TT 95.3
Ji, Xinru ..... DS 16.8, DS 20.33
Jia, Guobin ..... O 73.2
Jia, Lei ..... O 4.4
Jia, Ran Sheng ..... TT 69.1
Jia, Xiaoqing ..... TT 71.2
Jiang, Bo ..... FM 10.2
Jiang, Hao ..... O 43.2
Jiang, Nan ..... O 55.4
Jiang, Shuhan ..... •BP 16.9
Jiang, Song ... O 12.4, O 12.7, O 43.16
Jiang, Xinyu ... •CPP 17.19, CPP 44.5, CPP 46.45
Jiang, Xiongzhuo CPP 44.5, CPP 48.2
Jiang, Yi ..... TT 74.1
Jiang, Zenghui . DS 20.21, •HL 20.52, HL 31.4
Jiang, Zhihao ..... O 66.8
Jiang, Zhongyi ..... •QI 8.1
Jiménéz-Calvo, Pablo ..... HL 23.4
Jin, Biaobing ..... TT 71.2
Jin, Hanshang ..... TT 2.1
jin, haolin .. TT 5.3, TT 17.2, TT 22.23, TT 40.1, TT 57.10, QI 4.2
Jin, Kang ..... MA 7.46, •MA 35.6, •TT 60.6
Jin, Keda ..... •MA 43.3
Jin, Limei ..... •DY 41.12
Jin, Yichen ..... •O 42.4
Jin, Zhaonan ... •CPP 44.5, CPP 53.6
Jing, Weiguo ..... AKPIK 6.7
Jirák, Zdeněk ..... MA 34.2
Jo, Wonhyuk ..... O 40.15, O 98.3, TT 37.15
Jobst, Bernhard ..... QI 15.6
Jobst, Johannes ..... QI 20.8
Joch, Alina ..... QI 1.6
Jocher, Roman ..... O 97.4
Jochum, Johanna .MA 7.33, MA 46.2
Jocic, Angelina ..... O 46.4
Joffre, Manuel ..... HL 8.12
Johánek, Viktor ..... O 13.12
Johannesmann, Florian ..... MA 7.9
Johannsen, Sven ..... O 89.9
Johannsmann, Diethelm ..... BP 11.1, CPP 60.1, CPP 60.3
Johannsmann, Felix ..... O 28.4
Johansson, Annika ..... MA 24.5, MA 29.6, MA 51.3, TT 36.5, TT 46.6, TT 88.3
Johansson, Fredrik O. L. ..... TT 14.5
John, Alen ..... •MA 21.4
John, Ben .... O 61.3, O 95.5, TT 96.5
John, Karin BP 11.6, BP 12.3, DS 20.6
John, Philipp ..... HL 24.6, •HL 57.5
John, Philipp M. ..... DS 4.5
John, Thomas ..... •BP 7.7, BP 7.20, BP 7.21, BP 14.28, BP 14.32, BP 14.35, BP 14.36, BP 36.7, DY 57.7
John, Ti ..... AKPIK 2.1
Johnson, Agaya .. BP 14.76, •BP 39.4, •CPP 55.4
Johnson, David C. ..... TT 5.5
Johnson, Jeremy ..... MA 25.6
Johnson, Philip ..... BP 9.6
Johnson, S. ..... MA 25.6
Jöhrens, Korinna ..... BP 14.34
Jolie, Wouter ... O 7.6, O 10.5, O 15.4, O 17.7, O 17.12, O 59.1, O 62.8, O 89.8, O 99.10, TT 9.6, TT 16.5, TT 48.1, TT 54.8
Joll, Kit ..... •O 97.2
Jolly, Spencer W. ..... AKBP 8.4
Jomard, François ..... FM 11.17
Jonay, Cheryne ..... •DY 2.5, •TT 1.5
Jonda, Lukas ..... •O 40.3, •TT 37.3
Jones, Alfred ..... O 66.8
Jones, Alfred J. H. . O 95.11, TT 96.11
Jones, David ..... CPP 48.5
Jones, Dylan ..... MM 41.8, TT 81.2
Jones, Harry .. AKBP 12.4, AKBP 13.2
Jones, T. ..... O 88.11
Jöns, Klaus ..... HL 20.33, HL 49.3, HL 54.4
Jöns, Klaus D. ..... HL 55.4
Jonsson, Hannes ..... •O 37.1
Joos, Raphael .... HL 20.42, HL 31.4, HL 34.1, HL 34.2, QI 18.6
Joost, Jan-Philip .. DY 42.3, MA 7.59, TT 63.3
Joppe, Philipp ..... UP 3.5
Jordan, Mareike ..... BP 27.11
Jordt, Philipp ..... CPP 19.4, DY 20.4
Jörg Neugebauer, Jörg Neugebauer O 13.3
Jorio, Ado ..... HL 47.2
Jose, Anagha ..... MA 19.5, TT 31.5
Jose, Juwana ..... •HL 34.3
Jose Palliyan, Annarose .... •TT 26.7
Jose, Stephy ..... DY 49.8
Josef Ribeiro Parteli, Eric ..... UP 3.2
Joseph, Darin ..... •O 93.8
Joseph, Jerelle ..... BP 20.6
Joseph, Ronald ..... AKBP 7.4
Josephy, S. ..... TT 24.7
Josephy, Simon ..... MA 6.9, DD 7.2
Joshi, Aprajita .... •MA 19.9, •TT 31.9
Joshi, Radhika Hemant ..... •QI 2.2
Joshi, Vidul R. ..... QI 6.10
Joshi, Yug ... FM 2.1, FM 5.2, FM 5.8, MM 16.2, MM 34.5, MM 35.4, MM 35.5, •MM 39.6
Josiek, Joris ..... O 62.1, TT 54.1
Josse, Pierre . •O 8.6, O 77.5, O 89.10
Jost, Daniel ..... MA 33.11
Josteinsson, Björn ... MA 6.9, DD 7.2
Josten, Nicolas ..... •MA 50.8
Jouaiti, Elise ..... O 12.9
Jouault, Benoit ..... HL 29.5, TT 58.5
Jouneau, Agathe ..... •BP 37.4
Jourdan, Martin ..... MA 38.6
Jourdan, Thomas ..... FM 11.17
Jousten, Karl ..... O 78.5
Jovanović, Mateja ..... •MM 32.5
Jovic, V. ..... O 85.2
Joy, Ajin ..... TT 22.2
Joy, Krishnanjana ..... MA 37.8
Jozwiak, Christopher . MA 5.8, TT 7.8
Juan, Fernando de ..... TT 74.1
Juarschek, Dominik ..... MA 40.9
Jugovac, Matteo ..... O 61.1
Juhin, Amélie ..... CPP 20.7, DY 23.7
Jülicher, Frank ..... BP 7.47, BP 10.3, BP 10.7, BP 10.11, BP 14.11, BP 14.92, BP 14.93, BP 27.11, BP 32.6, CPP 18.3, CPP 18.7, CPP 18.11, DY 18.3, DY 18.7, DY 18.11, DY 34.7, DY 52.6
Jünemann, Cedric ..... •CPP 60.3
Jung, Felix ..... SOE 6.5
Jung, Hyein ..... •MA 27.2, O 22.5, O 40.10, O 71.11, TT 37.10, TT 66.11
Jung, Hyunwook ..... •O 34.1, O 81.3
Jung, Jannis ..... O 3.1, O 58.1
Jung, Martina ..... •QI 5.9, QI 21.7
Jung, Niklas ..... •QI 17.1
Jung, Philipp ..... BP 7.41
Jungb, Hyun ..... O 65.2
Jungfleisch, M. Benjamin .... MA 6.1
Junghans, Kira ..... •O 15.3, O 89.4
Jungwirt, Tomáš ..... MA 47.6
Jungwirth, Pavel .. CPP 19.5, DY 20.5
Jungwirth, Tomas ..... MA 20.6
Junkar, Ita ..... BP 26.2, CPP 43.2
Junkes, Heinz ..... O 81.7
Junquera, Javier ..... HL 39.10
Juntilla, Markus ..... O 12.2
Jurado Jiménez, Alejandro . •BP 7.48
Juranyi, Zsofia ..... UP 6.3
Juraschek, Dominik ..... FM 23.3, MA 25.3, MA 25.4, •MA 25.9, MA 40.3, MA 40.4
Jurczyk, Jakub ..... MA 6.5
Jureczko, Paulina •MA 35.5, •TT 60.5
Jürgensen, L. ..... AKBP 1.1
Jürgensen, Lars AKBP 4.4, AKBP 14.1
Jussios, Louis ..... DY 42.2, TT 63.2
Just, Wolfram ..... O 44.13
Juzak, Robert ..... DS 21.4
Jyothi Bhasu, Anjali ..... •MA 58.5
Jyoti, Divya ..... O 15.5, •O 69.3
K. G. Johansson, Mats ..... CPP 58.2
K.Hurley, Paul ..... HL 24.11
K. Paul, Robin ..... •DS 7.5
K. Singh, Jayant ..... O 9.6
K. Vayali, sarathlal ..... CPP 46.17
Kaap, Fabian ..... TT 28.6, TT 28.8, TT 43.5
Kaatz, Martin ..... BP 14.34
Kabachnik, Nikolay M. ..... O 66.5
Kabanova, Victoria ..... BP 9.6
Kabát, Jiří ..... O 96.7
Kachel, Stefan R. ..... O 8.7, O 31.5, •O 35.4, O 35.5
Kachula, Oleh ..... •UP 5.3
Kaczmarek, Alix ..... O 69.7
Kaczorowski, Dariusz ..... TT 29.5
Kadashchuk, Andrey ..... CPP 57.2
Kaden, Cornelia ..... MM 11.2
Kaden, Felix ..... HL 26.16
Kadlec, Christelle . MA 7.30, MA 17.3, •MA 25.8, TT 93.12
Kadlec, Filip ..... •MA 7.30, MA 25.8
Kadri, Ahmad El ..... MA 52.14
Kadwe, Trideep ..... O 98.7
Kaemmerer, Jonas ..... TT 43.4
Kaestner, Lars ..... BP 36.7, DY 57.7
Käferstein, Leonard ..... •HL 26.40
Kaganer, Vladimir .. FM 7.8, HL 23.10
Kageyama, Hiroshi ..... FM 22.9
Kahana, Tom ..... •TT 23.27
Kahl, Jasmin ..... •DS 20.16
Kähler, Jana . •O 7.5, O 71.16, O 71.19, •TT 9.5, TT 66.16, TT 66.19
Kahng, Sejong ..... MA 49.8, O 77.6
Kahraman, Bilge ..... •HL 22.5
Kai, Masaya ..... O 67.9
Kaib, David A.S. ..... TT 33.2
Kaidisch, Siegfried ..... O 61.7
Kaifler, Natalie ..... UP 8.6
Kainka, Lucina ..... BP 12.6
Kaiser, David .... BP 26.11, CPP 43.11, DS 14.9
Kaiser, David L. .... •O 40.4, •TT 37.4
Kaiser, Florian ..... HL 11.6, HL 31.5, TT 22.21
Kaiser, Julian ..... MA 8.5, TT 52.6, •TT 98.2
Kaiser, Katharina ..... O 12.4, O 12.7, O 12.9
Kaiser, Marius ..... •CPP 17.14
Kaiser, Markus ... DS 20.32, HL 26.8, HL 26.33
Kaiser, Sebastian ..... •CPP 29.1
Kaiser, Stefan ..... MA 19.8, •O 41.3, TT 14.8, TT 31.8, •TT 38.3, TT 49.2, TT 49.5, TT 74.6
Kaiser, Ute ..... O 10.6, TT 16.6
Kaiser, Waldemar •FM 10.3, MM 12.6, MM 22.8
Kákay, A. ..... TT 24.7
Kakugo, Akira ..... •DY 62.1
Kakuschke, Hannes ..... •HL 30.5, •TT 59.5
Kalady, Mohammed Fayis .. •FM 19.9
Kalaidzidis, Yannis ..... BP 27.3
Kalavalapudi, Keerthika ..... O 26.1
Kälber, Julian ..... •TT 83.9
Kalcheim, Yoav ..... HL 8.6
Kalina, Karl A. ..... CPP 24.2
Kalinin, Mikhail ..... O 69.5
Kalkan, Kübra .... •MA 7.38, MA 58.7
Kalkan, Sirri Batuhan ..... TT 92.15
Kallam Valli, Anjima ..... •DS 13.3
Kalläne, Matthias ..... O 7.5, O 70.3, O 71.16, O 71.17, O 71.19, O 71.21, TT 9.5, TT 25.11, TT 65.3, TT 66.16, TT 66.17, TT 66.19, TT 66.21
Kallappara, Shashank ..... •DY 15.6
Kallikkunnath, Akshay ... •CPP 10.13, •DY 16.13
Kalsberger, Tim ..... •MA 7.59
Kaltenbrunner, Martin ..... MA 49.1
Kaltenecker, Korbinian ..... HL 35.7
Kalvoda, Lukas ..... •BP 14.89
Kalz, Erik ..... •DY 34.10
Kam, Chonfai ..... QI 1.11
kamal, Asif ..... •BP 14.13
Kamalakar, M. Venkata .... MA 24.4, TT 36.4
Kamalasanan, Anoop ..... MA 48.10
Kamali Ashtiani, Mohammad Javad •MA 9.3
Kaman, Ondřej ..... DS 7.5
Kamaric, Alisa ..... O 25.1
Kamat, Aneesh Anand ..... •QI 8.2
Kamath, Sandesh ..... UP 3.2
Kamba, Stanislav .. MA 17.3, MA 25.8
Kamber, Aurèle ..... QI 14.25
Kaminski, Adam ... O 63.11, TT 55.11
Kaminski, Jochen ..... DD 16.3
Kaminski Lenzi, Ervin ..... DY 42.15, TT 63.15
Kamm, Moritz ..... •MA 7.40
Kammerbauer, Fabian ..... DS 6.5, MA 7.66, MA 21.1, MA 29.2, MA 55.2, MA 55.8, MA 55.9, TT 46.2
Kämmerer, G. ..... MA 50.3
Kämmerer, Gérald ..... MA 42.3, •AKPIK 2.4
Kämmerer, Jonas N. ..... •TT 22.16
Kämmerer, L. ..... MA 7.14, •MA 50.3

Kämmerer, Lea . . . •MA 36.1, MA 42.3
Kamp, Martin . . . . . DS 20.43, HL 1.12, O 74.4, TT 68.4
Kampermann, Hermann . . . . QI 10.10, QI 14.9, QI 15.2, QI 18.4, QI 18.8
Kämpfe, Thomas . . . . . AKPIK 6.4
Kämpfer, David . . . . . O 54.3
Kampfrath, Tobias . MA 7.8, MA 27.1, O 80.4
Kamps, Oliver . . . . . DY 6.13
Kamra, Akashdeep HL 39.11, MA 9.5, MA 30.5, MA 51.8, TT 88.8
Kanatani, Sachie . . . . BP 1.4, CPP 1.4, DY 4.4
Kanazawa, Kiyoshi . . . . . SOE 9.2
Kanazawa, Naoya . . . . . MA 37.6
Kandappanthodi, Chithra . . •FM 11.18
Kandil, Eman Ibrahim . . . . . BP 7.2
Kanduč, Matej . . . •CPP 27.1, •DY 26.1
Kanekar, Advait . . . . . AKBP 12.4
Kaneko, Yuya . . . . . •O 61.11
kang, chang jong . . . . . TT 25.11
Kang, Chang Wan . . . . . O 33.2
Kang, Faming . O 61.4, O 69.5, •O 77.3
Kang, Jingxuan . . . . . HL 33.4
Kang, Kisung . . . . . HL 23.5, MM 31.5
Kang, Kyongok . . . BP 39.4, CPP 55.4
Kangen, Ashish Yashwanth •TT 23.22
Kanhaiya, Krishan . . . . . CPP 39.1
Kanistras, Nikos . . . . . •MA 7.8
Kanitz, Rouven . . . . . QI 5.10
Kankanamge, HIran . . . . . •FM 11.19
Kansari, Mayukh . . . . . BP 2.9
Kantelberg, Richard . . •HL 2.6, HL 2.7, HL 22.2, HL 22.4
Kantian, Adrian . . . . . TT 56.9
Kantorovich, Sofia •BP 14.76, BP 39.4, CPP 20.7, CPP 24.3, CPP 42.4, CPP 55.4, DY 19.9, DY 23.7, DY 25.2, DY 41.2, DY 44.11, DY 44.21, DY 44.22
Kantz, Holger . . . . . DY 6.4, •DY 6.7, DY 48.2, SOE 4.9
Kao, Ming-Chao . . . . . DS 9.5
Kapaklis, Vassilios . . . . . MA 39.8
Kapás, Kornél . . . . . QI 3.1
Kapil, Venkat . . . . . MM 22.9
Kapitein, Lukas . . . . . •BP 12.1
Kapon, Yael . . . . . MA 7.66, MA 29.2, TT 46.2
Kapoor, S. . . . . AKPIK 6.5
Kapoor, Sarthak . . . . . •AKPIK 6.3
Kapp, Alexander . . . . . •CPP 46.30
Kappes, Manfred . . . . . O 23.2
Kappl, Kim . •DD 7.1, DD 21.1, DD 30.7, DD 30.8
Kappl, Michael . . . . . CPP 33.4
Kaps, F. G. . . . . O 57.6
Kapuscik, Paulina . . . . . DS 11.5
Kar, Ritama . . . . . MM 19.6
Kar, Satyakam . . . . . MA 13.3
Karaca, Ezgi . . . . . •BP 18.1
Karadimov, Todor R. . . . . •MA 7.22
Karajic, Eric . . . . . •DS 1.1
Karaka, Abdallah . . . . . •O 10.5, O 10.8, O 62.8, •TT 16.5, TT 16.8, TT 54.8
Karakachian, Hrag . . . . . •O 2.6
Karakaya, Tarik . . . . CPP 5.1, CPP 8.3
Karaman, Tamer . . . . . •MA 37.8
Karan, Sujoy . . . . . O 17.8, O 83.3
KARATUTLU, Ali . CPP 17.30, DS 20.2, DS 20.14, FM 19.3, FM 19.6, HL 20.1, MA 42.9, •MM 12.9, MM 16.4
Karbowniczek, Paweł . . . . . CPP 56.2
Kärcher, Victor . . . . . •DS 20.7
Karczewski, Grzegorz . . . . . HL 26.45
Karetta, Bennet . . . . . MA 20.2
Karfusehr, Christoph . . . . . CPP 20.2, DY 23.2
Karg, Alexander . . . . HL 9.1, HL 20.66
Karg, Matthias •CPP 17.44, CPP 20.3, CPP 30.5, CPP 42.2, DY 23.3
Kargl, Florian . . . . MM 21.1, •MM 21.9
Karić, Ajla . . . O 44.7, O 44.9, •TT 22.3
Karimi, Ali . . . . . CPP 46.61
Karimi, Amin . . . . . O 31.3, O 61.10
Karimian, Maryam . . . . . •SOE 4.4
Karlinger, Daniel . . . . . •CPP 17.33
Karlova, Katarina •MA 31.6, MA 36.11, TT 26.1, •TT 47.6
Karmakar, Mintu . . . CPP 11.1, DY 17.1
Karmakar, Sreejani . . . . . •MM 13.6
Karn, Abhishek . . . . . O 62.3, TT 54.3
Karnatak, Paritosh . . . . . •MA 49.2
Karner, Carina . . . . . •DY 14.4
Karow, Marisa . . . . . BP 14.64
Karpitschka, Stefan . . . BP 1.3, BP 1.8, BP 7.4, BP 7.26, BP 14.2, BP 14.3, CPP 1.3, CPP 1.8, CPP 5.2, CPP 5.4, DY 4.3, DY 4.8
Karr, Leonie . . . . . •BP 7.52
Karrai, Khaled . . . . . MA 6.2
Karsch, Stefan . . . . . AKBP 8.7
Kartsovnik, Mark . . . . . TT 23.17
Karube, Shutaro . . . . . MA 59.4
Karunanathan, Kethusan . . . DS 20.24
Karyofylli, Violeta . . . . . DY 41.12
Kasaian, Kiarash . . . . . BP 33.4
Kasatkin, Alexander . . . . . TT 14.12
Käsehagen, Julia . . . . . •BP 7.19
kashimoto, yuki . . . . . •O 82.3
Kashirina, Olga . . . •O 71.12, •TT 66.12
Kashkanova, Anna . . . . . BP 16.9
Kasotakis, Emmanouil . . . . . •MA 50.1
Kassaiyan, Parsa . . . . . CPP 30.4
Kassem, Aahmed . . . . . O 94.11
Kassem Arrak, Ahmad . . . . . •O 29.3
Kassubek, Timo . . . . . MM 16.3
Kastell, Jannis . . . . . •TT 44.6
Kasten, Nils . . . . . •HL 26.28
Kastl, Christoph . . . HL 20.9, •HL 30.1, HL 30.6, •TT 59.1, TT 59.6, TT 74.4
Kästner, Bernd . . . . . O 96.5
Kastner, Carolin . . . . TT 23.1, TT 57.2, •TT 57.3
Kastner, Caroline . . . . . TT 57.1
Kästner, Markus . . . . . CPP 24.2
Kataev, Vladislav . . . . . TT 79.5
Katayama, Naoyuki . . . . . TT 49.8
Kathiresan, Muthukani . . . . . •HL 33.3
Katnagallu, Shyam . . . . . O 48.1
Kato, Moyu . . . . . MA 19.4, TT 31.4
Katoorani, Parya . . . . . TT 2.5
Katsnelson, Mikhail . . O 76.4, TT 27.4
Katsnelson, Mikhail I. . . . . MA 34.9, MA 58.9, TT 12.7
Katsumoto, Hiroshi . . . . . •MA 8.11, MA 55.4
Katter, Benjamin . . . MA 24.1, TT 36.1
Katzenbach, Dieter . . . . . DD 31.1
Kauch, Anna . . . . . TT 10.1, TT 23.23
Kaufer, Luca . . . . . •O 24.1
Kaufhold, Leonard . . . . . •HL 38.5
Kaufman, Seth . . . . . MA 39.10
Kaulich, Burkhard . . MA 6.4, MA 6.10
Kaupp, Jochen . . . . . QI 18.7
Kaur, Guratinder . . . . . •MA 3.5
Kaur, Harmanjot . . CPP 23.4, DY 24.4
Kaur, Sarabjeet . . . . . O 51.2
Kaus, Anton . . . . . DS 6.6
Kaushik, Ravi . . . . . •MA 27.6
Kautz, Christian . . . . . TUT 2.1, DD 1.1, DD 10.2
Kautzsch, Malte . . . . . CPP 46.60
Kauwtilyaa Krishnaswamy, Gunasheel MA 29.3, TT 46.3
Kawa, Karol . . . . . •QI 9.2
Kawaguchi, Kaishu . . . . . O 60.7
Kawaguchi, Yuki . . . . DY 53.2, TT 87.2
kawamura, keita . . . . . O 82.3
Kawamura, Mitsuaki . . . . . TT 91.1
Kawde, Trideep . . •HL 3.10, HL 26.53
Kayatz, Florian . . . . . •TT 56.4
Kaye, Jason . . . . . TT 51.12
Kaymazlar, Koray . . . . . •QI 18.7
Kaynar, Emine . . . . . •HL 33.2
Kayser, Yves . . . . . MM 12.3
Kazantzidis, Andreas . UP 3.3, UP 5.2
Kazarian, Karina . . . . . TT 62.6
Kazemian, Majid . . . . . MA 6.10
Kazimierczak, Honorata . . . . . BP 7.56
Kazimir, Aleksandr . . DS 18.1, DS 18.2
Kazmaier, Stefan . . . . . HL 34.1
Ke, Chung-Ting . . . . . TT 4.1
Kedia, Mayank . . . . . MM 16.2
Kehr, S. . . . . O 57.6
Kehr, Susanne C. . . . . FM 14.1, O 52.3
Keienburg, Jan . . . . . O 7.6, TT 9.6
Keil, Julia . . . . . •BP 4.3
Keim, Peter . . . . . •CPP 35.1, •DY 37.1
Keimer, Bernhard . . MA 48.5, TT 39.6, TT 39.7, TT 40.1
Kelai, Massine . . . . . O 8.6
Keles, Mervenur . . . . . •MA 7.37
Keller, Elisabeth . . . . . •MM 17.7
Keller, Lucas . . . . . TT 52.3
Keller, Nils . . . . . •MA 7.53
Keller, Philip . . . . . O 11.4
Keller, Thomas . . . . . CPP 15.1
Keller, Thomas F. . . . . O 34.6
Kellerer, Thomas . . BP 26.3, CPP 43.3
Kellerer, Wolfgang . . . . . BP 5.1
Kellers, Simon G. •CPP 35.4, •DY 37.4
Kelling, Jeffrey . . . . DS 18.4, DS 20.34, DS 20.46, DS 20.47, DS 21.4, AKBP 6.5, AKBP 8.8, AKBP 11.3, AKBP 13.3
Kellner, Matthias . . . . . •CPP 9.7
Kellner, Philipp . . . . DS 20.49, HL 31.3
Kellner, Phillip . . . . . FM 7.1
Kelly, Angela M. . . . . DD 40.1
Keloth, Anurag . . . . . CPP 17.42
Keloth, Anuragk . . . . . CPP 17.15
Kelvin von Grundherr, Christopher MA 6.2
Kemerink, Martijn . . . . . CPP 17.7, CPP 22.6, CPP 37.2, CPP 37.4, CPP 37.6, CPP 40.5, DS 7.3, FM 4.9, HL 53.2, HL 53.4
Kempa, H. . . . . HL 45.1
Kempa, Mariel . . . . DY 46.3, •DY 46.4, TT 75.3, •TT 75.4
Kempf, Merlin . . . . . MM 14.4
Kempf, Niklas . . . . . •DD 23.5
Kempf, Sebastian . . . . . TT 82.3
Kempter, Richard . . . . . DY 33.8
Kendir Tekgül, Esra . . . . . FM 19.3, MM 12.9, •MM 16.1
Kennes, Dante . . . •SYFC 1.4, DY 32.1, O 79.1, TT 45.1
Kennes, Dante M. . . . . TT 44.4
Kentsch, Ulrich . . . . . HL 47.3
Kepič, Peter . . . . . O 96.7
Kera, Alessia . . . . . •QI 10.9
Keren, Kinneret . . . . . BP 3.2
Keresteš, Jiří . . . . . O 13.12
Kermode, James . . . . . MM 9.4
Kern, Christian S. . . . . O 9.1
Kern, Christian Simon . . . . . O 61.1
Kern, Johannes . . HL 20.59, MA 9.13, MA 52.5, MA 52.14
Kern, K. . . . . TT 24.7
Kern, Klaus . . . O 9.8, O 35.7, O 44.16, O 95.6, TT 73.2, TT 92.2, TT 96.6
Kerner, Nadine . . . . . MM 35.4
Kerschenbauer, Thomas . . •MA 52.38
Kerstan, Marc P. . . . . •AKBP 3.4
Kersting, Elias . . . HL 20.44, HL 20.47, •HL 26.31
Kerth, Gerald . . . . . BP 7.35
Keßler, P. . . . . O 85.2
Keßler, Philipp . . . . . DS 20.43
Kesselheim, Stefan . . . . . BP 14.57
Kessler, Philipp . . . . . •HL 8.8
Kettler, John . . . . . •AIW 1.1, •AIW 1.5, •AIW 2.5
Ketzmerick, Roland . . . . . DY 42.11, DY 59.2, TT 63.11, TT 99.2
Keußen, Justus . . . . . •DY 22.2
Keyser, Ulrich . . . . . O 13.9
Kézsmárki, István . MA 7.35, MA 7.50, MA 8.9, MA 16.5, MA 16.8, MA 16.10, MA 17.6, MA 23.2, MA 23.4, MA 31.2, MA 37.9, MA 51.6, MA 54.2, O 42.2, TT 35.2, TT 35.4, TT 47.2, TT 57.6, TT 88.6
Khain, Tali . . . . . •SYBS 1.1
Khajavikhan, Mercedeh . . . . . DY 48.6
Khajenooriranjbar, Shakiba . •DY 41.9
Khajetoorians, Alexander . . . . . O 99.3
Khajetoorians, Alexander A. . . O 15.3, O 89.4, O 89.7, O 99.9
Khalaf, Eslam . . . . . TT 4.5
Khalakhan, Ivan . . . . . O 13.12
Khaliq, Ahmar . . . . . FM 19.2
Khaliullin, Giniyat . . . . . TT 39.7
Khammee, S. . . . . BP 27.8, BP 37.2
Khan, Amrita . . MA 52.31, •MA 52.32
Khan, Ayesha . . . . DS 21.8, •HL 26.26
Khan, Kacho Imtiyaz Ali . . . . . DS 12.9
Khan, Latif . . . . . TT 93.4
Khan, Latif Ullah . . BP 33.12, DS 20.2, MM 12.9
Khan, Mayana Yousuf Ali . . . MA 49.9
Khan, Ramsha Wasi . . . . . •CPP 46.45
Khan, Zahid Ullah . •BP 33.12, FM 2.6
Khandelwal, Shishir . . . . . QI 15.2
Khanenko, Pavlo . MA 23.4, •TT 29.5, TT 35.4
Khaoula, Djennane . . . . . HL 49.3
Kharbanda, Vansh . . . . . •DY 43.16, DY 43.17
Kharik, Dmytro . . . . . AKPIK 5.3
Kharsah, Osamah . . . . . O 34.4
Khatua, Subhankar •MA 31.1, •TT 47.1
Khelfallah, Malika . . . . . •CPP 20.7, •DY 23.7
Khemani, Anirudh . . . . . •BP 33.4
Khera, Natasha . O 6.2, •O 6.5, O 45.5, O 58.4
Khera, Nikhita . . . •MA 52.39, TT 24.3
Khidr, Esraa . . . . . AKBP 4.1
Khim, Seunghyun . MM 40.2, TT 29.5, •TT 52.1, TT 52.2, TT 62.6
Khizar, Asma . . . . . •O 73.6
Khodabakhshi, Alireza . . . . . DY 19.5, •DY 19.8
Khodachenko, Daniil . . . . . •MM 21.4
Khodakarami, Mohammad AKBP 9.3
Khodakovskiy, Nikita . . . . . AKBP 13.1
Khodam Hazrati, Mehrnoosh . BP 2.5, BP 15.3
Khokhlov, Nikolai . MA 27.6, MA 30.3
Khoromskaia, Diana •BP 3.8, BP 7.51
Khosroshahi, Negin . . . . . •CPP 46.40, CPP 46.41
Khudaiberdiev, Daniiar . . . . . •HL 10.5, •TT 20.5
Khudoyberdiev, Asliddin . . . . . •MA 7.9
Khujakulov, Anvar . . . . . •HL 1.8
Khurram, Muhammad . . . . •CPP 13.7, CPP 46.28
Kibler, Ludwig A. . . . . O 65.4
Kichanov, Sergei . . . . . MA 7.30
Kick, Matthias . . MM 19.14, MM 37.2, O 18.5
Kiefer, Lara . . . . . •MA 3.7
Kiehn, Alexander . . . . . •DS 20.39
Kielar, Charlotte . . . . . FM 11.36
Kieler, Maximilian . •DY 59.6, •TT 99.6
Kieler, Maximilian F.I. . . . . DY 32.7, TT 45.7
Kieler, Oliver . . . . . TT 22.7, TT 22.9, TT 28.3, TT 28.9, TT 28.10
Kielesiński, Łukasz . . . . . CPP 17.9
Kiemle, Christoph . . . . . UP 7.4
Kiemle, Jonas . . . . . HL 13.2
Kienle, Lorenz . . . HL 20.23, HL 20.24, HL 26.23
Kiens, Ellen . . . . . FM 12.10
Kierfeld, Jan . . . . . BP 14.22
Kiermaier, Eva . . . . . BP 27.4
Kiese, Dominik . . . . . TT 13.11
Kieser, Fabian . . . . . •DD 37.1
Kihou, Kunihiro . . . . . TT 93.14
Kikkawa, Akiko . . . . . MA 16.6
Kikkawa, Takashi MA 29.10, TT 46.10
Kikkinides, Eustathios . . . . . DS 6.2
Kikuchi, Hiroto . . . . . •FM 22.9
Kilicaslan, M. Fatih . . . . . MA 42.9
Kiln, Julius . . . . . •DY 34.6
Kim, Changho . . . . . •DY 6.10
Kim, Dong-Jik . . . . . HL 25.3
Kim, Dongwook . . . •MA 11.6, O 71.10, •TT 21.6, TT 66.10
Kim, Gideok . . . . . DS 11.3
Kim, Hobeom . . . . . CPP 17.10
kim, hyeong do . . . . . TT 25.11
Kim, Jinkyung . . . . . •O 99.6
Kim, Ji-Seon . . . . . CPP 57.3
Kim, Jungdae . . . . . O 71.14, O 71.15, TT 66.14, TT 66.15
Kim, Kab-Jin . . . . . MA 52.12, MA 59.9
Kim, Kyoohyun . . . . . BP 27.10
Kim, Min Gyu . . . . . TT 26.9
Kim, Mincheol . . . . . O 71.15, TT 66.15
Kim, Moonjoo . . . . . FM 6.10
Kim, Philip . . . . . TT 12.3
Kim, Rebekah Seonggyeong •HL 37.4
Kim, Sanghoon . . . . . MA 59.9
Kim, Se Kwon . . . . . MA 59.9
Kim, Se-Ho . . . . . O 48.1
Kim, Seo-Jin . . . . . MA 34.2, TT 94.3
Kim, Steven . . . . . TT 42.7
Kim, Tae Kyu . . . . . BP 9.6
Kim, Taewook . . . . . TT 42.6
Kim, Timur . . . . . O 74.4, TT 68.4
Kim, Yeon-Ji . . . . . O 56.3
Kim, Yewon . . . . . O 56.3
Kim, Yong-Baek . . . . . TT 57.11
Kim, Younghyuk . . . . . DS 11.8
Kimata, M. . . . . TT 29.1
Kimel, Aleksei . . . . . MA 27.6, MA 30.3
Kimoto, Yuta . . . . . •MA 30.1
Kimouche, Amina . . . . . MA 7.47
kimura, fumihiko . . . •O 95.9, •TT 96.9
Kimura, Shin-ichi . . . . . HL 42.4
Kimura, Shojiro . . . . . MA 17.8
Kinaret, Naomi . CPP 48.3, •CPP 57.2
Kincal, Cem . . . . . O 69.9
Kind, Yanick S. . . . . •QI 1.4
King, Phil . . . . . O 76.7
King, Phil D. C. . . . . TT 5.10
Kingston, Alex . . . . . BP 3.6
Kinikar, Amogh . . . . . •MA 5.9, •TT 7.9

Kintrup, Katharina .....•CPP 14.4
Kipke, Felix ..... MM 35.6
Kippenberg, Tobias DS 16.8, DS 20.33
Kippenberg, Tobias J. ..... QI 2.6
Kira, Mackillo ..... HL 8.1
Kirchberg, Henning ..... TT 53.2
Kirchen, Manuel ..... AKBP 8.4
Kirchlechner, Christoph ..... MM 7.8, MM 7.10, MM 34.2, MM 36.1, MM 36.4
Kirchmair, Bernhard .....•BP 26.3, •CPP 43.3
Kirchmann, Patrick S. O 84.8, TT 84.8
Kirchner, Alexander .....TT 22.24, •TT 73.7
Kirchner, Nico .....•TT 33.5, TT 51.7
Kirk, Isolde .....•BP 18.2
Kirsch, Andrea ..... MA 3.3
Kirschbaum, Jan ....BP 32.1, DY 52.1
Kirschke, Jule ..... MA 33.4, TT 5.6, •TT 23.10
Kirschner, Stefanie CPP 5.1, •CPP 8.3
Kiselev, Alexei .....UP 8.3
Kiselev, Mikhail ..... TT 42.4
Kiselev, Nikolai ..... MA 46.5
Kiselev, Nikolai S. .•MA 16.9, MA 37.1
Kiseleva, Iuliia .....•FM 12.2
Kishonti, Adrian .....CPP 57.1
Kislitsyn, Matvei ..... O 10.9, •O 70.1, O 95.12, TT 16.9, •TT 65.1, TT 96.12
Kissling, Christoph TT 28.6, •TT 28.8, TT 43.5
Kitamura, Sota .....•TT 44.1
Kitatani, Motoharu ..MA 11.6, TT 21.6
Kitou, Shunsuke ..... FM 9.2, FM 9.5, O 95.9, TT 96.9
Kitsopoulos, Theofanis ..... O 34.7
Kivala, Milan .. O 35.1, O 46.3, O 46.4
Klammes, Sebastian .....AKBP 7.3
Klamser, Pascal .... BP 8.1, •SOE 2.3
Klapp, Sabine H.L. . DY 27.2, •DY 34.9
Klar, Lena ..... HL 55.8
Klar, Peter J. .. DS 8.2, DS 9.1, HL 9.2, HL 42.2, MM 35.7
Klare, Johann .....MA 7.73
Klaß, Yannick .....HL 18.6, TT 32.6
Klaßen, P. ..... MA 50.3
Klassen, Matthias .....•DD 27.2
Klatt, Michael .....O 54.1
Klatt, Michael A. ..... BP 11.9
Kläui, Mathias ..... DS 6.5, MA 2.8, MA 7.66, MA 21.1, MA 21.4, MA 21.6, MA 29.2, MA 29.9, MA 29.10, MA 39.1, MA 39.2, MA 43.4, MA 47.3, MA 47.9, MA 51.2, MA 51.7, MA 55.2, MA 55.3, MA 55.5, MA 55.8, MA 55.9, TT 46.2, TT 46.9, TT 46.10, TT 88.2, TT 88.7, AKPIK 5.6
Klauß, Hans-Henning ..... MA 54.7
Klaus, Matthias .....•SOE 4.8
klauss, hans henning .....TT 72.3
Klauss, Hans-Henning ..... MA 7.50, MA 47.11
Klavins, Peter .....TT 2.1
Klawohn, Sascha ..... MM 22.3
Klebl, Lennart .....TT 51.1
Kleemann, Hans ..BP 41.2, CPP 38.5, •HL 2.2, HL 2.6, HL 2.7, HL 22.1, HL 22.2, HL 22.3, HL 22.4, HL 22.5
Klees, Raffael L. ... TT 78.2, •TT 78.7
Kleeschulte, Julian .. O 62.8, TT 54.8
Kleibert, Armin .....MA 7.81
Klein, Edina ..... BP 7.9, BP 11.2
Klein, Idan .....•MM 21.2
Klein, Julian .....HL 13.5, HL 20.13, •TT 12.5
Klein, Marten ..... DY 28.4
Klein, Matthias ... HL 20.9, •HL 30.6, •TT 59.6
Klein, Pascal .....DD 10.1, DD 25.3, DD 26.3
Klein, Sebastian .....•CPP 37.4
Klein, Tobias .....FM 19.8
Kleine, Hannah ..... AKjDPG 1.4
Kleinherbers, E. .....HL 17.7
Klein-Hitpass, Annika ..... HL 35.7
Kleinke, Tobias .....MA 39.7
Kleinmann, Matthias ..... QI 12.4
Kleinschmidt, Lennart ..... BP 16.2
Kleinschmidt, Peter .....CPP 46.43, HL 26.5, HL 26.13, •HL 26.41, O 54.2
Klembt, Sebastian ..... HL 1.12
Klement, Philip .....DS 11.7, HL 23.8
Klempt, Carsten .....QI 15.3
Klenkert, Daniel .....•HL 24.3
Klenovský, Petr .....•HL 55.3
Klepetsanis, Ilias .....•TT 85.5
Klepetsans, Ilias ..... O 21.1
Kleppe, Annette ..... TT 80.3
Klett, Kolja .....•DY 33.7
Kleykamp, Olaf A. ..... O 61.4, O 69.7
Kliemt, K. .....MA 27.8, TT 25.6
Kliemt, Kristin .....MA 7.16, MA 7.56, MA 8.3, MA 8.5, MA 27.2, O 40.11, TT 25.10, TT 37.11, TT 62.2, TT 62.3, TT 62.4, TT 79.3, TT 93.1, TT 98.2
Klier, Jens ..... HL 52.5, AKPIK 5.3
Kliesch, Martin ..... QI 1.10
Kliewer, Thomas .. HL 39.3, •HL 39.4
Klimczuk, Tomasz ..... FM 9.2
Klimek, Justin ..... O 34.5
Klimmer, Sebastian HL 54.1, HL 54.2, HL 54.3
Kling, Matthias F. ..... MA 33.11
Klingel, Sophie ..... TT 92.6, TT 92.7
Klingel, Steffen ..... AKPIK 4.2
Klingeler, Rüdiger . MA 7.74, MA 7.75, MA 31.5, MA 42.6, MA 52.38, MM 19.13, TT 47.5
Klinger, Marvin .... MA 18.7, TT 30.7, TT 89.2
Klingner, Nico .....HL 38.3, HL 38.11, HL 40.5, •HL 56.2, QI 2.9
Klint, Niphredil ...•CPP 10.1, •DY 16.1
Klöffel, Tobias ..... MM 19.6
Klonz, Maximilian ..... HL 54.6
Klopf, J. M. .....O 57.6
Klopf, Michael .....AKBP 2.5
Klopotek, Miriam .... DY 6.2, •DY 6.3, DY 14.3
Kłos, Jarosław S. .....CPP 39.2
Klose, Daniel .....FM 11.12
Klose-Albinger, Martina .....UP 8.3
Klotz, Chistian .....BP 7.41
Klubertz, Sophia CPP 17.7, CPP 22.6, •FM 4.9, HL 53.4
Klug, Sebastian . •DS 20.22, MM 12.8
Kluge, Paul ..... DS 18.5
Kluge, Robert .....MA 7.28
Kluge, Thomas . AKBP 5.3, AKBP 5.4, AKBP 6.1, AKBP 6.2, AKBP 6.3, AKBP 6.5
Klumpp, Stefan .....BP 1.1, •BP 1.7, BP 7.15, BP 7.16, BP 12.4, BP 12.11, BP 14.2, BP 40.1, CPP 1.1, •CPP 1.7, CPP 17.3, DY 4.1, •DY 4.7, •DD 24.4, DD 26.3
Kluth, Elias ..... HL 57.1
Kluwe, Bruno ..... MA 49.4
Kluwe, Moritz ..... DY 19.10
Klyatskaya, Svetlana .....O 9.4
Kmječ, Tomáš ..... DS 7.5, MA 7.30
Knaak, Melanie ..... BP 14.34
Knabl, Wolfram .....MM 17.1
Knap, Michael .....DY 13.2, TT 2.3, TT 19.2, TT 72.1
Knap, Wojciech .... HL 52.2, HL 52.3
Knapman, Ross ...MA 7.38, MA 7.43, MA 7.72, •MA 58.7
Knapp, Marco ..... O 94.5
Knauer, Sebastian .....•MA 48.2
Knauft, Manuel .....•MA 48.5
Knaus, Philipp .....•MA 9.2
Knebel, G. ..... TT 29.1
Knebloch, Jakub .....•DD 20.1
Knebusch, Jules M. .. O 7.5, •O 71.19, TT 9.5, •TT 66.19
Knechtges, Matthias ....•CPP 17.23, CPP 53.4
Knechtges, Philipp ..... BP 14.57
kneissl, michael ... HL 26.6, HL 37.3, HL 37.4
Knekna, Chrystalla ... O 76.4, TT 27.4
Kneller, Omer .....•HL 8.1, MA 12.2
Kneschaurek, Ekatarina .... CPP 48.1
Kneschaurek, Ekaterina ... CPP 12.5, HL 4.1
Knewitz, Sophie .....•O 61.8
Knipšis, Ričards ..... O 59.5, TT 48.5
Knipšis, Ricards Kristers ..... O 71.1, •O 71.18, TT 66.1, •TT 66.18
Knispel, René .....•O 44.2
Knispel, Timo ..... O 64.3
Knížek, Karel ..... DS 7.5, •MA 7.64, MA 34.2, MA 57.5
Knobloch, Edgar .....DY 8.10
Knöckl, Ernst .....•HL 20.9, HL 30.6, TT 59.6
Knol, Marvin .....O 61.10
Knoll, Alexander L. ..... O 24.7
Knoll, Alexander L. M. ..... MM 19.1
Knolle, Johannes . DY 13.2, MA 19.11, MA 31.3, TT 2.3, TT 19.2, TT 31.11, TT 47.3, TT 64.6, TT 72.9, TT 79.1, TT 79.2, TT 98.8
Knolle, Wolfgang ..... QI 20.6
Knoop, Franz Niklas ..•O 58.6, O 83.9
Knopp, Tobias .... MA 49.4, SOE 10.1
Knorr, Andreas ....HL 20.3, HL 20.15, HL 26.48, HL 30.4, O 27.7, TT 59.4
Knorr, Matthias ..... HL 8.1
Knossalla, Florian ..... MA 7.54
Knothe, Angelika .....DS 8.3, DS 14.7
Knüpfer, Andreas ..... MA 49.5
Knüpfer, Fabian .....•BP 14.11
Kny, Anna J. .....O 46.5
Ko, Jacky ..... BP 14.42
Kobayashi, Kaito ..... TT 51.8
kobayashi, kaya ..... O 95.7, TT 96.7
Kobayashi, Ryo ..... FM 15.3
Kobayashi, Shingo .....•TT 6.5
Kobayashi, Yasuhito .....•FM 9.2
Kobayashi, Yohei .....O 60.7
Kober, Stefan ..... MA 35.6, TT 60.6
Kober, Steffen ....•MA 7.46, MA 12.4
Köbler, Sven .....•CPP 46.58
Koblmüller, Gregor .. FM 19.5, HL 8.7, HL 57.4
Kobus, Julia ..... CPP 19.4, DY 20.4
Kocer, Emir .....CPP 9.4, MM 19.1
Koch, Christiane .....HL 8.12
Koch, Christoph ..... FM 15.1
Koch, Christoph T. ..... HL 25.3
Koch, Elias .....•DY 6.5, DY 22.9
Koch, Elias R. .....DY 41.9, DY 48.4
Koch, Erik ..... TT 3.4, TT 23.21
Koch, Jennifer ....•TT 28.1, TT 28.12
Koch, Julian ..... DS 20.48
Koch, Juliane .. CPP 46.43, •HL 26.5, O 54.2
Koch, Leon .... TT 28.7, QI 2.7, QI 8.3
Koch, Leon M. ..... QI 11.6, QI 11.9
Koch, Martin .....HL 20.20
Koch, Norbert ..... HL 4.7
Köcher, Simone ..... FM 2.4, FM 5.5
Kochergov, Aleksandr ..... HL 33.5, •HL 42.5
Kochl, Robert ..... BP 14.42
Kochummachen Oommen, Joshy •TT 93.5
Kocsis, Vilmos .... MA 7.28, MA 17.4, TT 93.14
Koehler, Lara ....•BP 10.4, •CPP 18.4, CPP 20.2, •DY 18.4, DY 23.2
Koelpin, Nadja ..... CPP 17.19
Koenderink, Gijsje H. ..... BP 27.7
Köerner, Chris ..... MA 59.7
Koert, Ulrich ..... O 31.2, O 45.9
Kofler, Annalena .....BP 15.8
Koganti, Harsha .....BP 20.6
Kögel, Marco .....CPP 26.2
Köglmayr, Daniel ..... DY 6.8
Kohama, Yoshimitsu ..... MA 9.1
Kohl, Felix ..... MA 48.3, •MA 48.9
Kohl, Hagen P. ..... MM 33.1
Kohlbrecher, Joachim .... CPP 46.12, CPP 54.6
Köhler, Alexander .....AKBP 10.1
Köhler, Anna ... CPP 17.17, CPP 44.6, CPP 46.27, CPP 48.5, CPP 57.2, HL 15.5, HL 45.5, HL 53.3
Köhler, Anna Frederike ..... QI 18.6
Köhler, Annkathrin . HL 16.7, •HL 56.3
Köhler, Antonia .....•O 39.2
Köhler, Benjamin .....•DY 15.10
Köhler, Fabian .....•TT 86.1
Köhler, Jonas .....•MA 47.9
Köhler, Larissa ..... BP 9.5
Köhler, Laura .....•UP 6.3
Köhler, Robin ..... BP 14.51
Köhler Ruiz, Elena .....•CPP 23.3, •DY 24.3
Kohler, Sigmund .....HL 31.2
Köhler, Thomas ..... CPP 16.6, •CPP 17.36, CPP 17.39, •TT 56.9
Kohlfürst, Christian ..... TT 2.5
Kohlmann, Johannes ..... TT 22.7, TT 22.9, TT 28.9, TT 28.10
Kohlmann, Marcel ..... MA 39.7
Kohlmorgen, Paul ..... O 34.8, O 81.1
Kohlstedt, Raphael ..... MA 57.4
Kohn, Julia ..... O 77.4
Köhne, Finn ..... DY 15.11, •DY 15.12
Kohnen, Benedikt ..... FM 6.7
Kohout, Jaroslav ....DS 7.5, MA 7.30
Kohrmann, Andreas ..... •CPP 17.16, CPP 25.2
Kohrs, Daniel ..... O 3.1
Kojima, Keita ..... •FM 9.5
Kok, Karel .....DD 12.3
Kokalj, Jure ..... TT 23.2
Kokh, Konstantin ..... MA 12.2
Kokorin, Artem .....BP 14.63
Kokovin, Artem .....•TT 93.18
Koláček, Jan ..... TT 93.12
Kolasseri, Ihsan Ahmed .... •TT 72.8
Kolbe, Matthias ..... MM 21.9
Kolbe, T. ..... HL 37.6
Kolbe, Thomas ... •BP 36.6, •DY 57.6
Kölbl, Constanze .....•TT 23.6
Kole, Abhisek .....•O 63.9, •TT 55.9
Kolek Martinez de Azagra, Monica HL 20.32, •TT 92.15
Kolev, Svetoslav ..... MA 7.27
Koley, Anish .....•TT 72.2
Koliofoti, Christina ..... TT 53.7
Koliogiorgos, Athanasios ... •HL 39.1
Koll, Maximilian .....•MA 7.63
Kollàr, Alicia .....DY 2.2, TT 1.2
Kollar, Marcus .... MA 7.29, •TT 70.2, TT 94.9
Kollath, Corinna .... DY 59.9, TT 99.9
Kölle, Dieter ..... MA 49.3
Koller, Volkmar .....•DS 20.41, QI 6.5
Kolley-Köchel, Francine .... BP 14.62
Kollwitz, Leo .....•MA 39.21
Kolmer, Marek ..... O 63.11, TT 55.11
Kolodzinska, Wiktoria .....DS 11.5
Kolok, Baksa .....HL 38.6, •QI 6.3
Kolorenč, Jindřich .....•TT 25.4
Komar, Y. .....•BP 27.8, BP 37.2
Komarek, Alexander C. .....O 84.5, TT 5.10, TT 84.5
Komeda, Joe ..... O 9.4
Komesu, Takashi .....•O 60.6
Komissarova, Yana .....•TT 43.10
Komissinskiy, Philipp .....DS 11.6
Komiyama, Haruka ..... MA 59.4
Komori, Fumio ..... O 48.3
Kompa, Philipp J. .....•AKBP 8.9
Komsa, Hannu-Pekka •HL 16.3, O 7.6, TT 9.6
Konczykowski, M. .....TT 69.6
Konczykowski, Marcin ..... MM 40.2
Kondákor, Mark .....MA 8.9
Kondo, Takeshi .....O 60.7
Kondoh, H. ..... O 85.2
Kondovych, Svitlana .....•DY 43.19
Kondratenko, Serhiy ..... HL 1.4
Konermann, Beatrix ..... BP 14.14
Konermann, Lars .....•O 42.5
Kong, Dehao .....AKPIK 6.4
Kong, Fanpeng .....•O 88.1
Kong, Lingda .....TT 43.8
Kong, Yan Tung .....•QI 20.3
Kong, Yan-Tung .....QI 20.4
Könghofer, Bettina .....O 8.4
Konidena, Sudarshan .....•DY 19.5, DY 19.8
Konieczna, Amanda Anna ..•TT 72.5
König, Elio J. .....TT 6.4, TT 64.5, TT 83.12
König, J. ..... HL 17.7, HL 20.27
König, J. K. ..... HL 54.10
König, Janne Mattis .....•CPP 17.38
König, Jannis .....•DD 17.1
König, Jeniffer ..... HL 47.1
König, Jürgen .....HL 17.3, HL 20.43, MA 52.2, O 89.9, TT 18.6, TT 42.5
König, Lukas ..... DY 46.8, TT 75.8
König, M. .....TT 29.1
König, Markus .... FM 19.1, MA 42.11, TT 5.8, TT 17.2, TT 42.12, QI 4.2
Koniukov, Georgii .....BP 15.2
Konomaev, Feodor Svetlanov •MA 30.11
Konopko, Leonid .....•MM 19.15
Konovalov, Oleg .....BP 14.24
Konrad, Jens .....BP 40.1
Konrad, Paul .....HL 16.6, HL 20.61, HL 24.3, •HL 49.2
Konstantinou, Konstantinos .. O 47.2
Kontogeorgiou, Konstantinos HL 10.3, TT 20.3
Könye, Viktor ..... FM 22.6, •TT 98.4, AKPIK 5.12
Kooi, Bart .....FM 12.10
Koop, Thomas .....O 5.3
Kopelevich, Yakov ..... MA 13.8
Koper, Marc .....•O 39.3, O 87.9
Kopietz, Peter .....TT 13.12, TT 13.13
Köpke, Markus .....HL 26.17
Köpp, Sebastian ..HL 26.21, •HL 40.7
Kopp, Thilo .....TT 83.1

Koppenhöfer, Martin QI 13.3, •QI 16.9
Koppenhöfer, Simon . DD 7.1, DD 21.1, •DD 30.7, DD 30.8
Koppens, Frank H.L. . HL 10.1, TT 20.1
Koppitz, Boris . . . . . FM 12.2
Kops, Geert J.P.L. . BP 32.11, DY 52.11
Koraltan, Sabri . . •SYSD 1.2, MA 55.6, •MA 59.6
Körbächer, Christopher P. . . . . DS 8.2
Korbany, David . . . . . •QI 3.10
Korbel, Jan . . . . . •SOE 11.3, SOE 11.4
Körbel, Sabine . . . . . •FM 11.35
Körber, Lukas . . . . . MA 2.4
Körber, Rainer . . . . . TT 28.3
Korell, Konstanze . . . . . •MA 27.3
Korell, Lukas . . . . . MM 3.6
Koren, Gad . . . . . MA 27.10
Koren, Vladislav . . . . . BP 3.3
Kormos, Marton . . . DY 46.10, TT 17.7, TT 75.10, QI 4.7
Korn, Alexander . . . . . O 74.2, •O 74.3, TT 68.2, •TT 68.3
Korn, Tobias . . . . . HL 20.25, HL 24.9
Korneev, Kirill . . . . . •BP 7.20
Körner, Chis . . . . . MA 30.12
Körner, Chris . . . . . MA 52.16
Körner, Wolfgang . . . . . MM 14.3
Korneychuk, Svetlana . . . . . MM 3.6, MM 30.2, MM 34.2, MM 35.2, •MM 39.3
Kornich, Viktoriia . . . . . TT 89.3
Körnig, Andre . . . . . BP 14.43
Korniienko, Ievgeniia . . . . . •MA 9.6, MA 58.11
Kornilov, Grigory . . . . . FM 15.1
Kornyushchenko, Anna . . . . . •MM 3.5
Körösy, Caroline . . . . . BP 20.8
Korotyeyev, Vadym V. . . . . HL 52.2
Korshunov, Artem . . MA 7.2, MA 11.3, MA 16.1, TT 21.3, TT 81.6
Korte, Carsten . . . . . MM 27.4
Kortus, Jens . . . . . FM 7.5, HL 26.49, MM 13.3, MM 19.5, MM 19.46, O 18.6, O 50.2
Korzeb, Paweł . . . . . •BP 7.47
Kos, Šimon . . . . . •TT 62.11
Kosan, Malte Beran . . . . . DD 9.1
Kosari Mehr, Ali . . . . . •AKBP 3.6
Kosbahn, David P. . . . . CPP 12.4, •CPP 31.4
Kosheleva, Valeriia . . . . . O 49.1
Kosov, Daniel . . . . . TT 42.9
Kossert, Karsten . . . . . TT 82.3
Kostanovski, Ilya . . . . . DS 11.8
Kostarev, Aleksandr . . . . . •BP 9.4
Koster, Gertjan . . . DS 20.13, FM 12.10
Köster, Sarah . . . . . BP 7.14, BP 7.15, BP 7.17, BP 7.18, BP 12.4, BP 12.11, BP 14.30, BP 40.1, DY 44.17
Kostera, Zuzanna . . . . . MM 19.3, •MM 19.22
Kostka, Martin . . . . . FM 6.8, TT 23.9, •TT 81.8
Köstler, Stefan . . . •CPP 10.4, •DY 16.4
Kostur, Eray . . . . . CPP 39.3
Kostylev, Mikhail . . . . . MA 48.7
Kostyurina, Ekaterina . . . . . BP 26.3, •BP 26.4, CPP 43.3, •CPP 43.4
Kosub, Tobias . . . . . HL 23.1
Kot, Malgorzata . . . . . DS 11.5
Kotsugi, Masato . . . . . AKPIK 5.6
Kott, Viktor . . . . . •TT 23.5, TT 70.1
Kotte, T. . . . . MA 47.7
Köttgen, Jan . . . . . FM 11.2, FM 11.7
Kottmann, Jakob . . . . . QI 3.5
Kotyada, Chandra . . . . . TT 57.6
Kotyada, Chandra V . . . . . TT 23.31, •TT 71.1
Kotz, Maximilian . . •BP 36.2, •DY 57.2
Koujok, Abbas . . . . MA 9.3, •MA 9.10, MA 9.12
Koulas-Simos, Aris •HL 54.6, HL 54.7, HL 55.1
Koutsioumpas, Alexandros . . DS 21.4
Koutsostathis, Athanasios •AKBP 7.1
Koutzarova, Tatyana . . . . . MA 7.27
Kouyate, Maryke . . . . DY 6.12, •O 23.5
Kovacheva, Daniela . . . . . MA 7.27
Kovacs, Alexander . . . . . MA 50.2
Kovacs, Andras . . . . . •MA 38.10
Kovalchuk, Iryna . . . . . MM 40.4
Kovalchuk, Serhii . . . . O 41.4, •O 54.3, TT 38.4
Kovalenko, Maksym . . . . . HL 20.49, HL 45.4
Kovalev, Sergey . . MA 7.46, •MA 12.4, MA 25.8, TT 41.2
Kovtunovych, Vladyslav . . . . •FM 14.2
Kowalik, Malgorzota . . . . . MM 25.1
kowallik, verena . . . HL 26.6, •HL 37.3
Kowalska, Joanna . . •PSV IV, •PSV VI
Kowalski, Alexander . . . . . •TT 3.5
Kowalski, Hagen-Henrik . . . . . QI 16.7
Kowalski, R. A. . . . . O 57.6
Kowerko, Danny . . . . . BP 18.5
Koyiloth Vayalil, Sarathlal . . CPP 15.1, CPP 25.4, •CPP 41.4, CPP 44.5, CPP 46.51, CPP 58.2, CPP 59.1, CPP 59.3
Koziol, Jan Alexander . . . . . TT 23.5, TT 23.7, •TT 26.2, QI 14.17
Kozitsky, Yuri . . . . . DY 54.2
Kozlenko, Denis . . . . . MA 7.30
Kozlov, Dmitriy A. . . . . TT 97.2
Krabbe, Heiko . . . . DD 30.4, •DD 32.1, DD 37.2
Krack, Matthias . . . . . MA 11.7, TT 21.7
Kraemer, Atahualpa S. . . . . DY 47.3
Kraemer, Calvin . . . . . QI 14.17
Krafft, Christoph . . . . . BP 14.29
Kraft, Dennis . . . . . QI 17.2
Kraft, Florian . . . . . MA 9.4, •MA 52.3
Kraft, Louisa . . . . . CPP 46.2
Kraft, Louisa E. . . •CPP 27.4, •DY 26.4
Kraft, Markus . . . . . •DY 46.3, DY 46.4, •TT 75.3, TT 75.4
Kraft, Robert . . . . . •MA 7.41
Kraft, Ulrike . . . . . •HL 2.1
Kraft-Bermuth, Saskia . . . . . TT 22.35
Krage, Rainer . . . . . HL 26.9, HL 26.12
Krahn, Oliver . . . . . O 55.1
Kraiker, A. . . . . MA 27.8
Krajnik, Ziga . . . . . DY 46.10, TT 75.10
Krämer, Calvin . . . . . TT 23.7
Krämer, Christian . . . . O 62.8, TT 54.8
Krämer, Jakob . . . . . AKBP 8.6
Krämer, Marcel . . . . . •TT 13.4
Krämer, Michael . . . DY 58.8, SOE 17.8
Kramer, Robin . . . . . MA 13.1
Kramp, Jakob . . . •DY 58.5, •SOE 17.5
Krane, Nils . . . . . O 9.7
Krantz, Claude . . . . . AKBP 7.4
Křápek, Vlastimil . . . . . O 27.1, •O 96.7
Krapf, Leonard . . . . . CPP 44.6
Krasheninnikov, Arkady . . . . . O 84.10, TT 84.10
Krasheninnikov, Arkady V. . . . DS 12.5, FM 2.2, O 95.3, TT 96.3
Krasilnikov, M. . . . . BP 27.8, BP 37.2
Kraska, Richard . . . . . O 40.9, TT 37.9
Krasovskii, Eugene E. . . . . O 66.5
Kräter, Martin . . . . . BP 7.44
Kratzer, Markus . . . . . •MM 4.4
Kratzer, Peter . . . . . HL 24.2, •HL 35.8, HL 47.4, MA 42.3, O 61.6, TT 2.5
Kratzer, Veronika . . . . . AKBP 5.1
Kraus, Barbara . . . . . QI 1.9, QI 15.6
Kraus, Bastian K. . . . . •BP 7.37
Kraus, Marco . . . . . TT 28.10
Kraus, Martin . . . . . MM 24.1
Kraus, Stefan . . . . . •DD 4.2
Krause, Christoph . . . . . HL 12.1
Krause, Jens . . . . . BP 14.90
Krause, Marius . . . . . •MA 39.13
Krause, Matthias . . . . . •FM 11.24
Kraushofer, Florian . . O 23.10, O 94.3
Krauss, Falk . . . . . CPP 16.1
Krauss, Sebastian W. . . . . •BP 5.2
Krautloher, Max . . . . . TT 40.1
Kravchuk, Volodymyr . . . . . •MA 2.11, MA 7.49, MA 20.1
Kravikass, Mathar . . . . . •BP 14.64
Krawczyk, Maciej MA 16.11, MA 44.8, TT 76.8
Krebber, Sarah . . . . MA 7.56, TT 62.2, TT 62.3, TT 79.3
Krebs, Robin . . . . . •QI 15.8, QI 21.4
Krebs, Tobias . . . . . •HL 53.2
Krebsbach, Michael . •QI 16.7, QI 16.9
Kredel, Samuel A. . . . . MM 3.6
Kredl, Jana . . . . . •MA 39.7
Kreienkamp, Kim L. . . . . DY 34.9
Kreiger, Jonas . . . . . MA 8.3
Kreindler, Lior . . . . . BP 14.15
Kreis, Aaron . . . . . •BP 14.28
Kreisberger, Felix . . . . . TT 89.2
Kreisel, Andreas . . . MA 33.3, TT 29.9
Kreissl, Patrick . . . . . CPP 49.1
Krejci, Ondrej . . . . . •O 47.2
Krelle, Lukas . . . . . HL 20.5, HL 20.6, HL 20.13, HL 39.5, •HL 39.7, HL 39.11
Krellner, C. . . . . MA 27.8, TT 25.6
Krellner, Cornelius MA 7.16, MA 7.56, MA 8.3, MA 8.5, MA 27.2, O 40.11, TT 25.10, TT 37.11, TT 62.2, TT 62.3, TT 62.4, TT 79.3, TT 93.1, TT 98.2
Kremer, Kurt . •PRV II, BP 4.4, BP 31.5, CPP 50.5, DY 43.10
Kremer, Sascha . . . . . CPP 16.5
Krempaský, Juraj . . . . . MA 8.3
Krenner, Hubert . . . . . HL 3.11, HL 18.5, HL 20.19, HL 26.1, HL 36.1, HL 48.4, TT 32.5
Krenz, Marvin . . . . . •O 56.1
Kress, Holger . . . . . CPP 41.7
Kress, Katharina . . . . . MA 49.2
Kresse, Georg . . . . . HL 23.9, MM 22.6
Kretsch, Karin . . . . . BP 7.7, BP 7.21
Kretschmer, Andreas . •O 65.7, O 87.5
Kretschmer, Fred . . . . . •CPP 25.5, CPP 57.3
Kretschmer, Silvan . •O 59.4, •TT 48.4
Kreutz, Maike . . . . . •BP 14.38
Kreuzberger, D. . . . . TT 22.31
Kreuzberger, Daniel . . . . . •TT 22.27, TT 22.30, TT 82.2
Kreuzer, Alex . . . . •TT 22.14, TT 22.15, TT 43.7
Kreuzer, Lucas . . . . . •PSV III, PSV VI, •CPP 32.4, •DY 35.4
Kreuzer, Lucas P. . . . . CPP 46.45
Kreyßig, Andreas . . . . . MM 19.42
Kreysing, Eva . . . . . BP 7.46
Kreysing, Moritz . . . . . BP 33.3
Kreyssig, Andreas . . FM 6.8, MA 33.4, TT 5.6, TT 23.9, TT 23.10, TT 26.9, TT 81.7, TT 81.8
Krezhov, Kiril . . . . . MA 7.27
Krieg, Anna M. H. . . . O 89.7, •O 99.9
Krieg, Elisha . . . . . •CPP 54.4
Krieg, Kim . . . . . BP 26.8, CPP 43.8
Kriegel, Marko . . . . . •O 10.10, O 33.6, O 72.1, •TT 16.10, TT 67.1
Kriegel, Moritz . . . . . •DD 8.3
Krieger, G. . . . . TT 69.3
Krieger, Janis . . . . . AKPIK 4.2
Krieger, Jonas A. . . . TT 57.2, TT 57.3, TT 72.3
Krieger, Joshua . . . . . •CPP 17.35
Krieger, Lukas . . . . . TT 43.12
Krieger, Michael . . . . . AKjDPG 1.3
Kriegner, D. . . . . MA 47.7
Krien, Friedrich . . . . . TT 13.10
Krill III, Carl E. . . . MM 30.2, •MM 30.3
Krinitsin, Wladislaw . . . . . •DY 14.13
Krinninger, Matthias . . . . . O 23.10
Krischok, Stefan . . . DS 4.4, DS 20.23, DS 20.35, HL 31.3
Krishnaswamy, Suchitra . . . . . QI 5.9
Krishnia, Sachin . . . MA 21.1, MA 21.6, MA 29.9, •MA 29.10, MA 39.1, MA 55.3, MA 55.8, MA 55.9, TT 46.9, •TT 46.10
Krishtopenko, Sergey . . . . . HL 29.5, TT 58.5
Krisponeit, Jon-Olaf . . . . . HL 20.66
Kristen, Maximilian . . . . . TT 43.2
Kristina, Weinel . . . . MA 19.8, TT 31.8
Kritika, Kritika . . . . . •CPP 46.55
Krivanek, Ondrej . . . . . FM 15.1
Krivenko, Igor . . . . . TT 23.24
Krivkova, Anna . . . . . •AKBP 12.2, AKBP 12.4, AKBP 13.2
Křížek, Filip . . . . . MA 30.6
Krnel, M. . . . . TT 5.9
Kroesbergen, Max . . . . . •TT 51.5
Kröger, Jörg . . O 61.9, O 74.7, TT 68.7
Kröger, Sebastian . . . . . DD 32.1
Krogh Norrild, Rasmus . . . . . DY 44.19
Kroha, Johann . . . . . TT 94.2
Krohn, Corvin . . . . . •MA 38.2
Krohns, Stephan . . . . . MA 17.6
Kröll, Eva . . . . . FM 4.4
Kroll, Florian . . . . . AKBP 7.5
Kroll, Martin . . . . . MM 19.25
Kroll, Matthias . . . . . TT 81.8
Kroll, Tim . . . . . •DY 6.13
Kron, Michelle . . . . . •BP 14.83
Kronast, Florian . . . . . MA 38.4
Kronenberg, Samuel . . . . . •AKBP 2.4
Kroner, Martin . . . . . HL 13.4
Kronik, Leeor . . . . . MA 11.4, TT 21.4
Kronseder, Matthias . . . . . TT 73.7, TT 74.12, TT 97.1
Kroß, Leon . . . . . •HL 8.5
Kroy, Klaus . . . . . CPP 28.2, DY 29.2
Krsnik, Juraj . . . . . MA 11.6, TT 21.6
Krstić, Marjan . . . . . DS 21.2, O 46.3
Krueger, Manja . . . . . •MM 38.1
Krueger, Maximilian . . . . . O 4.6
krueger, michael . . . . . O 43.12
Krueger, Peter . . . . . O 64.7
Kruel, Emily . . . . . O 57.4
Krug, Joachim . . . . . •BP 21.4, BP 21.5, BP 21.7
Krug, Lisa-Marie . . . . . •MM 7.7
Krug, Malte . . . . . •QI 13.1
Krug von Nidda, Hans-Albrecht MA 31.2, MA 31.7, TT 47.2, TT 47.7
Krüger, Anton . . . . . HL 45.8
Krüger, David A. . . . . •TT 90.2
Krüger, Heidemarie . . . . . TT 5.2
Krüger, Janet . . . . . BP 7.34
Krüger, Jannis . . . CPP 7.4, •CPP 58.5
Krüger, Kerstin . . . . . O 11.2
Krüger, Lea Johanna . . . . . BP 7.48
Krüger, Lion . . . . . •HL 45.5
Krüger, Matthias . . . BP 7.30, BP 7.31, CPP 10.11, DY 16.11, DY 43.5, DY 54.3
Krüger, Peter •MA 2.10, O 60.4, O 60.7
Krüger, Severin . . HL 20.35, HL 20.44, •HL 20.47, HL 26.31
Kruklinskii, Daniil •O 84.10, •TT 84.10
Krumrey, Thilo . . TT 22.14, •TT 22.15, TT 43.7
Krupinski, Michal . . . . . MA 59.6
Kruppke, Iris . . . . . FM 19.4
Kruse, Niklas . . . . . O 44.13
Kruse, Niko . . . . . •O 34.5
Kruti, Daniel . . . . . •TT 43.1
Krychowski, Damian . . . . . •TT 42.1
Kryński, Marcin . . . •FM 2.3, FM 11.10
Krysiak, Olga A. . . . . FM 6.7
Krywka, Christina . CPP 4.6, CPP 16.2, CPP 17.27
Krzysteczko, Patryk . . . . . TT 28.3
Ksari, Younal . . . . . O 67.4
Ku, Yu C. . . . . MA 19.5, TT 31.5
Ku, Yu-Chieh . . . . . O 84.5, TT 84.5
Ku, Yu-Chih . . . . . TT 3.3
Kubala, Björn . . . . . TT 62.9, TT 82.5, TT 82.6, TT 85.4, TT 89.4
Kuban, Martin . . . . •FM 6.5, MM 22.3, AKjDPG 1.4
Kubánková, Markéta . . . . . •BP 7.44
Kübel, Christian . . . . MM 35.2, O 23.2
Kübelbäck, Florian . MA 7.5, MA 7.33, •TT 61.7
Kubetschek, Nico . . •O 58.8, TT 61.14
Kubicki, Milan . . . . . •O 58.2, O 58.3
Kubíčková, Lenka . . . . . DS 7.5
Kubis, Jessica . . . . . CPP 49.1
Kubitschke, Hans . . . . . DD 25.2
Kubitza, Niels . . . . . MA 52.26
Kübler, Felix . . . AKPIK 4.4, AKPIK 5.8
Kübler, Michael . . . . . QI 20.1
Kublitski, Jonas . . . . . CPP 40.6
Kubo, Mihiro . . . . . •O 82.6
Kubo, Taisei . . . . . TT 49.8
Kubsch, Marcus . . . . . DD 37.1
Kucera, Stephan . . . . HL 11.6, HL 31.5
Kuch, Wolfgang . . MA 7.47, MA 36.10, •MA 38.4, MA 38.6
Küchemann, Stefan . . . . . DD 9.2
Küchenmeister, Jens . . . . . DD 30.5
Kuchkin, Vladislav . . . . . MA 7.4
Kuchkin, Vladyslav M. . . . . •MA 37.1
Kuechle, Theresa . . . . . •HL 4.4
Kuehl, Kristin . . . . . MA 52.39
Kuenze, Georg . . . . . DS 18.5
Kugler, David . . . . . •O 5.6, O 55.4
Kugler, Fabian B. . . . TT 13.1, •TT 13.11
Kugler, Nils . . . . . DD 30.7, DD 30.8
Kugler, Paul . . . . . •TT 22.12
Kühl, Kristin . . . . . TT 24.3
Kuhl, Santiago . . . . . •BP 7.42
Kühl, Thomas . . . . . AKBP 7.3
Kuhlemann, Eike F. . . . . MA 36.10
Kühlkamp, Maximilian . . . . . •DD 23.1
Kuhlke, Jakob . . . . . O 12.4, •O 12.7
Kuhlmann, Gerrit . . . . . UP 3.1
Kühn, Danilo . . . . . •TT 14.5
Kühn, Franziska •MA 48.8, MA 52.20
Kuhn, Jochen . . . . . DD 9.2
Kuhn, Marcel . . . . . DY 58.3, •DY 58.4, SOE 17.3, •SOE 17.4
Kühn, Stefan . . . . . QI 3.7
Kuhn, Tilmann . . . . . HL 3.6
Kuhn, Tobias . . . . . •TT 78.2
Kühne, Alexander JC . . . . . HL 45.5
Kühne, H. . . . . TT 80.6, TT 93.7
Kühne, Julius . . . . . •HL 12.7, MM 4.2
Kühne, Sune . . . . . •DY 60.7
Kühne, Thomas . •CPP 34.1, •DY 36.1

Kühne, Thomas D. ..... FM 11.37
Kühnhammer, Matthias .... CPP 26.4
Kuhnhold, Anja ..... DD 17.1
Kuhnke, Klaus .. O 9.8, O 12.6, O 95.6, TT 96.6
Kühnle, Angelika ..... O 5.3, O 36.3, O 36.6, O 39.2
Kühnlenz, Kai ..... •FM 7.1, HL 31.3
Kuibarov, Andrii ..... •O 2.3, TT 5.7
Kuimov, Anatolii ..... •CPP 17.17
Kujur, Milli Suchita ..... MM 19.48
Kukharchyk, Nadezhda .... TT 22.25, TT 22.26, TT 22.33, QI 2.4, QI 14.21
Kukharenko, Oleksandra .... BP 31.5, CPP 50.5
Kukhtaruk, Serhii ..... HL 52.2
Kuklinski, Lennart J. ..... DY 8.3
Kulbakov, Anton ... •MA 7.2, MA 19.3, MA 19.6, TT 31.3, TT 31.6
Kulbakov, Anton A. MA 31.8, TT 47.8, TT 72.3
Kulic, Igor ..... BP 12.2
Kulkarni, Omkar ..... TT 14.9
Kulkarni, Ruta ..... TT 25.1
Kullick, Tim ..... •O 71.13, •TT 66.13
Kullig, Julius ..... DY 59.4, TT 99.4
Külper, Phillip ..... HL 38.10
Kultaeva, Anastasiia ..... FM 11.12, •FM 11.20, HL 26.24, MA 13.8
Kumar, Abhinav ..... BP 14.62
Kumar, Abhishek ..... TT 5.4
Kumar, Aditya ... MA 39.2, •MA 43.4, •O 88.3
Kumar, Ajay ..... HL 20.28, •O 44.12
Kumar, Ajeet ..... CPP 44.3
Kumar, Ajesh ..... TT 61.11
Kumar, Amit FM 18.8, O 63.4, TT 55.4
Kumar, Ankit ..... •TT 11.2
Kumar, Ashwani ..... MA 36.1
Kumar Dey, Jayjit ..... •MA 39.18
Kumar, Dhaneesh ..... O 35.7
Kumar, Durgesh ... MA 39.1, MA 39.2
Kumar, Gaurav ..... MA 7.26
Kumar, Hitesh ..... •HL 48.1
Kumar, Kavya Harsha ..... O 31.1
Kumar, M Maneesh ..... •MM 19.35
Kumar, Manohar ..... TT 83.4
Kumar, Manoranjan ..... MA 7.84
Kumar, Mohit ..... •HL 1.5
Kumar N M, Anjan ... O 41.3, TT 38.3, TT 49.2
Kumar, Palani Muthu ..... •O 94.7
Kumar, Rajendra ..... HL 57.3
Kumar, Rohan ..... •MM 19.17
Kumar Samal, Pankaj ..... O 65.12
Kumar, Saravana ..... O 36.4
Kumar, Sourabh ..... •FM 9.4
Kumar, Surender CPP 22.4, •CPP 26.2
Kumari, Anjali ..... MA 19.9, TT 31.9
Kumari, Pallavi .... •BP 7.15, BP 12.11
Kumawat, Sagar Mal ..... •MA 31.10, •TT 47.10
Kumberg, Ivar ..... MA 38.4
Kumbhakar, Shreya ..... •TT 49.2
Kümmel, Simon ..... •MM 19.38
Kümmel, Stephan ..... BP 2.11
Kummer, K. ..... MA 23.5, MA 27.8, TT 35.5
Kummer, Kurt ... MA 33.11, MA 52.27, TT 25.10, TT 62.4
Kümper, Verena ..... AKBP 8.6
Kuna, Pierre ..... •QI 20.6
Kundi, Ilona ..... •DY 44.19
Kundu, Asish K. ..... HL 24.10
Kundu, Mayukh CPP 46.55, •DY 41.16
Kundu, Moumita ..... •MA 33.1
Kundys, Bohdan ..... FM 9.3, TT 5.11
Kuneš, Jan ..... MA 8.13
Kunisch, Nils ..... •DD 26.5, DD 39.1
Kunjwal, Ravi ..... QI 12.3
Kunkel, Christian ..... O 23.4
Kunst, Flore ..... MM 25.4
Künstle, Kevin ..... MA 9.4, •MA 9.5, MA 52.9, MA 52.11
Kuntscher, Christine MA 11.2, TT 21.2
Kunz, Yannik ..... •MA 9.4, MA 9.5, MA 48.7, MA 52.11
Kunze-Liebhäuser, Julia ..... O 13.10
Kunzelmann, Julia ..... QI 18.8
Kunzelmann, Viktoria ..... HL 40.3
Kunzmann, Susanne ..... FM 6.8
Kunz-Schughart, Leoni A. ... BP 33.5, BP 33.6
Kuo, Chang Y. ..... MA 19.5, TT 31.5
Kuo, Chang-Yang .... TT 3.3, TT 25.2
Kuo, Liang-Yin ..... •MM 8.7
Kuo, Pang-Shun ..... TT 93.8
Kupenko, Ilya ..... FM 15.2
Küpper, Jochen ..... BP 33.10
Kurebayashi, Hidekazu ..... MA 9.10
Kurfman, Seth ..... MA 7.8, MA 9.8, MA 52.17, MA 52.21
Kurfman, Seth W. ..... •MA 48.10
Kurihara, Takayuki ..... MA 38.8
Kurilovich, Pavel D. ..... QI 6.10
Kurizki, Gershon ..... QI 7.5
Kurkowski, Moritz ..... CPP 59.1
Kurleto, Rafal ..... HL 24.10
Kuroda, Kenta ..... O 60.7
Kuroda, Yuta ..... •CPP 11.2, •DY 17.2
Kurowska, Anna ..... O 69.1
Kürpick, Ulrike ..... •TT 61.14
Kurschat, Timo A. HL 26.9, •HL 26.12
Kurt, Aulenbacher ..... •AKBP 15.1
Kurtanidze, A. .... •MA 23.5, •TT 35.5
Kurtanidze, Ana ..... MA 52.27
Kurths, Jürgen ..... DY 8.2
Kurtz, Felix .. O 22.2, •O 22.3, O 86.2, O 86.7
Kurtze, Hannes ..... MM 21.6
Kurz, Thomas ..... AKBP 10.1
Kurzmann, A. ..... HL 20.27
Kurzmann, Annika ..... HL 47.1
Kurzthaler, Christina .. BP 1.2, BP 1.5, •BP 36.1, CPP 1.2, CPP 1.5, DY 4.2, DY 4.5, DY 44.13, •DY 57.1
Kurzweg, Lucas ..... CPP 41.7
Küß, Matthias ..... DS 20.17, MA 9.4
Kusari, E. ..... DS 3.4
Kusari, Endrit ..... O 19.2, O 93.2
Kusber, Anncharlott ..... •CPP 57.3
Kusche, Ralph ..... HL 26.28
Kuschel, Olga ..... DS 6.5
Kuschel, Timo ..... DS 6.5, MA 2.8, MA 5.1, MA 29.10, •MA 35.1, MA 39.6, MA 39.13, MA 51.2, MA 54.11, O 28.7, TT 7.1, TT 46.10, •TT 60.1, TT 88.2
Kushch, Natalia ..... TT 23.17
Kushwaha, Naina ..... O 66.8, O 76.5
Kushwaha, Niraj ..... SOE 6.7
Küster, Kathrin O 19.1, O 33.3, O 62.6, O 74.5, TT 54.6, TT 68.5
Kusters, Guido ... •BP 32.2, CPP 10.4, DY 16.4, •DY 52.2
Kusumaatmaja, Halim ..... CPP 5.1, CPP 8.1
Kutas, Mirco ..... HL 52.5, AKPIK 5.3
Kutnyakhov, D. ..... O 59.2, TT 48.2
Kutovy, Yurii ..... TT 73.6
Kutovyi, Yurii . HL 12.1, HL 38.1, QI 6.2
Kuttner, Christian ..... •PSV III
Kutz, Tim ..... •BP 7.27
Kutzner, Jacob ..... O 40.17, TT 37.17
Kuvezdic, Marko ..... FM 18.6
Kuwano, Taro ..... •FM 22.8
Kužel, Petr ..... MA 25.8
Kuzmenko, Alexey B. ..... O 52.3
Kuzmenko, Artem M ..... MA 17.11
Kuznetsov, Alexander ..... •HL 55.2
Kuznetsov, Andrej ..... HL 40.5
Kuznetsov, Andrey CPP 20.7, DY 23.7
Kuznetsova, Tatiana ..... HL 23.6
Kuznetzov, Andrey ..... DY 44.22
Kvaratskheliya, Askar ..... •MM 18.2
Kvashnina, Kristina O. ..... TT 25.8
Kvitnitskaya, Oksana ..... •TT 93.3
Kvitnitskaya, Oksana E. ..... TT 5.7
Kwoka, Krzysztof ... HL 18.3, TT 32.3
kwon, yong seung ..... TT 25.11
Kyoseva, Hristiyana ..... O 57.5
Kyriienko, O. ..... HL 54.10, HL 54.12
L. Doltsinis, Nikos ..... FM 15.2
L. Lado, Jose ..... MA 5.9, TT 7.9
L. Portalupi, Simone ..... HL 34.5
L. Schmidt, Thomas ..... TT 83.4
La Berge, Maxwell ..... AKBP 10.2
La Mattina, F. ..... TT 5.9
Laakso, Jarno ..... HL 4.6
LaBerge, Maxwell ..... AKBP 10.1, AKBP 11.4, AKBP 12.5, AKBP 13.3
Labonté, Laurent ..... QI 18.1
Lacerda-Santos, Antonio ... •HL 29.2, •TT 58.2
Łach, G. ..... CPP 32.3, DY 35.3
Lach, Mareike ..... QI 18.7
Lach, Stefan ..... O 61.7, O 83.10
Lacmann, T. ..... O 19.10
Lacmann, Tom ..... TT 14.4
Ladecký, Martin ..... CPP 8.2
Ladewig, Björn •DY 58.10, •SOE 17.10
Ladines, A.N. ..... AKPIK 6.5
Ladines, Alvin N. MM 22.3, AKPIK 6.3
Lädke, Sarah Louisa BP 7.30, •BP 7.31
Lado, Jose ..... MA 17.5
Lado, Jose L. ..... O 59.7, TT 48.7
Ladovrechis, Konstantinos . •TT 41.11
Lafeld, Dennis ..... •DD 30.9
LaFleur, Alexander ... O 42.3, O 44.3, TT 22.3, •TT 92.19
Laforsch, Christian ..... CPP 41.7
Lägel, Bert ..... O 57.4
Lagemann, Kai ..... •MM 19.47
Lagemann, Kai Stefan ..... MM 35.2
Lagnese, Gianluca ..... QI 17.8
Lagoin, Marc ..... DY 21.2
Laguta, Hanna ..... •O 28.4
Laha, Sudarshana ..... BP 5.6
Lahabi, Kaveh ..... TT 28.4, TT 57.9, QI 20.8
Lähnemann, Jonas ..... •TUT 1.1, •TUT 1.2, DS 20.18, •FM 1.1, •FM 1.2, FM 7.8, HL 23.10, HL 33.4, HL 57.5
Lai, King Chun ..... O 55.5, O 88.3
Lai, Samuel ..... O 71.11, TT 66.11
Laible, Dominik ..... MA 36.9, O 61.7
Laird, Diana J. ..... BP 3.11
Lak, Aidin ..... BP 20.8
Lake, Bella TT 26.7, TT 26.8, TT 26.10
Lake, Stephanie ..... MA 52.21
Lakhara, Aarti ..... HL 10.4, TT 20.4
Lakkis, Ali . •DY 19.9, DY 25.2, DY 41.2
Lakshmi Nilayam, Ajai Raj .... O 23.2
Lambers, Hendrik .. •HL 3.6, HL 13.2, HL 20.17
Lambert, Sascha ... •BP 1.1, BP 12.11, BP 40.1, •CPP 1.1, •DY 4.1
Lamers, Christina ... DS 18.1, DS 18.2
Lammel, M. ..... MA 48.11, MA 52.8, MA 59.8
Lammel, Michaela . HL 18.1, MA 7.52, MA 29.8, MA 39.7, MA 39.24, •MA 52.10, MA 52.33, MA 59.5, TT 32.1, TT 46.8
Lämmerhofer, Michael ..... DS 20.44
Lammerskötter, Tom P. ..... •O 59.2, •TT 48.2
Lamon, Denny ..... HL 17.1
Lamsal, Bidit ..... CPP 54.1
Lan, Qianqian ..... MA 46.5
Lan, Wenze .... •HL 26.36, HL 26.39, HL 39.11
Landaeta, Javier ..... TT 94.5
Landaeta, Javier F. ..... TT 29.5
Landeros, Pedro ..... MA 57.2
Landers, Joachim ..... MA 36.1, •MA 52.26
Landmark, Solveig ..... UP 7.5
Landwehr, Felix ..... O 46.2
Lane, Ch ..... MA 19.7, TT 31.7
Lane, Harry ..... O 80.3
Lang, Felix ..... HL 4.7, HL 4.8
Lang, Johannes ..... DY 9.8
Lang, Julia ..... HL 26.51
Lang, Julia A. ... •DY 22.10, HL 26.56
Lang, Martin ..... MA 34.4, MA 50.2, MA 58.1
Lang, Michael . CPP 39.2, CPP 46.10, CPP 54.4, •CPP 54.5
Lang, Simon ..... QI 11.10
Lang, Thomas C. ..... TT 62.12
Lange, Colin ..... •MA 2.7
Lange, Jan ..... •HL 20.35, HL 20.36
Lange, Regina .... BP 14.25, BP 33.9, O 68.6
Lange, Steffen .... •BP 33.5, BP 33.6
Lange, Zoë ..... •BP 37.5
Langendorf, Mattis O 40.18, •O 40.21, TT 37.18, •TT 37.21
Langenohl, Lena ..... MM 15.5
Langer, Jürgen ..... MA 21.4
Langer, Marc ..... •QI 1.9, QI 15.6
Langer, Marcel ..... MM 17.3
Langer, Marcel F. ..... •MM 9.2
Langer, Moritz ..... HL 55.7, HL 56.4, •HL 56.5, •DD 28.4
Länger, Patrick ..... MM 12.4
Langfeld, Benedikt ..... AKBP 7.3
Langguth, Inga ..... O 16.2
Langhammer, Christoph ... MM 39.3
Langheld, Anja ..... TT 2.6, TT 23.7, QI 14.17
Langhoff, Arne ..... CPP 60.3
Längle, Manuel ..... DD 18.1
Langlotz, Nils ..... O 10.9, TT 16.9
Lansalot, Muriel ..... DY 62.5
Lanz, Amon. P ..... TT 23.31, TT 71.1
Lanzer, Michael ..... BP 15.5
Lapertot, G. ..... TT 29.1
Lapertot, Gérard ..... O 62.2, TT 54.2
Lapkin, Dmitry .. CPP 12.3, •CPP 12.5, CPP 48.1, HL 4.1, AKPIK 6.6
Laplanche, Guillaume ..... MM 11.4
Lapp, Clara Johanna ..... TT 15.9
Laquai, Frédéric ... CPP 57.5, HL 15.1
Lardet, Eloise .... •CPP 11.9, •DY 17.9
Larhrissi, Khadija ..... •BP 14.41
Larocque, Hugo ..... HL 34.4
Larrazabal, Maialen ..... TT 73.1
Lars, Rodewald ..... •BP 14.8
Larusch, Jan-Hendrik ..... HL 25.2, HL 39.2, •HL 39.3, HL 39.4, HL 39.6
Lasagni, Andrés ..... DS 21.9
Laschewsky, André ..... CPP 31.4, CPP 46.31, CPP 46.37
Lasinger, Katharina . MA 9.5, MA 52.3
Lass, J. ..... TT 25.9
Lastres, Marco ... •DY 32.8, •TT 45.8
Lászlóffy, András •TT 15.12, TT 15.13
Latour, Julia ..... •TT 22.33
Latus, Annamaria ..... O 36.3
Laubrock, Paul . O 5.5, O 36.2, O 44.5
Läuchli, A. M. ..... TT 25.9
Lauditi, Clarissa ... DY 45.5, SOE 14.5
Lauer, Kevin ..... FM 7.1, •HL 31.3
Lauer, Maximilian ..... •HL 48.2
Laufer, Sarah ..... •O 67.5
Läuger, Jörg ..... CPP 15.2
Lauhoff, Christian ..... MA 13.4
Laumann, Daniel .. DD 12.1, •DD 15.2, DD 26.2
Launois, Pascale ..... •CPP 26.1, •CPP 36.1
Lauritsen, Jeppe Vang ..... O 34.5
Lausch, K. Nikolas ..... MM 19.1
Lautenschläger, Franziska .. BP 7.20, BP 12.6, BP 40.2
Lauter, V. ..... MA 3.8
Lauterbach, Stefan ..... O 54.5
Lauth, Jannika ..... CPP 26.2
Lavagna, Enrico ..... •BP 15.2
Law, Chun Kit Dennis ..... •QI 13.10
Lawes, Patrick . •O 9.4, O 45.4, O 78.3
Lawrenz, Dominic ..... MA 38.2
Laxhuber, Kathrin S. ..... •BP 10.11, •CPP 18.11, •DY 18.11
Lazareva, Sofiya ..... DS 14.6
Lazarova, Katerina ..... DS 20.3
Lazdans, Ernests ..... •O 18.4
Lazzaroni, Paolo ..... DY 14.9
Lazzeri, Michele ..... MM 41.9
Le Berre, Martine ..... FM 4.1
Le Cardinal, Ariane ... UP 6.2, •UP 8.4
Le, Congcong ..... TT 39.7
le Coutre, Nils ..... •BP 14.82
Le, David ..... •O 46.7
Le, Doan ..... CPP 17.42
Le, Doan Duy Ky ..... •CPP 17.15
Le Du, Hugo ..... •TT 49.4
Le Du, Morgan ..... CPP 12.4
Le Dû, Morgan P. ..... CPP 31.4
Le Guyader, L. ..... MA 7.14
Le, Hoang-Anh ..... O 89.2
Le, Isabel Nha Minh ..... •QI 5.8
Le, Khoa ..... O 7.2, TT 9.2
Le Mardelé, Florian MA 23.2, TT 35.2
Le Merrer, Marie .. CPP 20.9, DY 23.9
Le Roy, Hugo ... •BP 39.5, •CPP 55.5
Le Tacon, M. O 19.10, O 59.2, TT 48.2
Le Tacon, Matthieu .. O 22.3, TT 14.4
Le Verge-Serandour, Mathieu •BP 8.4
Lea, Klausfering ..... •O 5.2
Leandersson, Mats ..... O 76.7
Lebs, Roman ..... •QI 14.22
Lechermann, Frank MA 8.12, MM 8.3, •TT 69.7, TT 69.9
Lecheval, Valentin ..... •SOE 9.5
Lechler, Rochus ..... •QI 14.4
Lechner, Barbara A. J. ..... HL 12.5, O 23.9, O 23.10
Lechner, Klemens •MM 17.1, MM 21.5
Lecuyer, Sigolène ..... BP 11.6
Ledentsov Jr., Nikolay ..... HL 26.46
Ledentsov, Nikolay ..... HL 26.46
Lederer, Jonas ..... O 61.10
Ledesma Martin, Jose Omar •MA 39.1
Ledesma-Martin, Jose Omar •MA 29.9, •TT 46.9
LeDuc, Henry G. ..... QI 11.8
Ledwith, Patrick ..... TT 4.5
Lee, Byeongin ..... TT 4.10, TT 78.5
Lee, Chanhyeon ..... TT 72.7
Lee, Chul-Ho ..... TT 93.14

Lee, Edward .•SOE 6.7
Lee, Hankyu .TT 78.5
Lee, Hannarae .BP 16.9
Lee, Hojun .MA 29.4, TT 46.4
Lee, Hyun-Woo .MA 29.4, TT 46.4
Lee, Jaehyun .O 64.2
Lee, Ji Eun .MA 7.34
Lee, Jinjoo .O 89.10
Lee, Jong Yeon .TT 4.5
Lee, Junho .BP 9.6
Lee, K. .TT 69.6
Lee, Kyoung P. .O 95.5, TT 96.5
Lee, Kyu-Myung .O 82.2
Lee, Mal-Soon .O 65.10
Lee, Nien-Hsuan .•HL 31.5
Lee, Oliver .CPP 17.17
Lee, Patrick .TT 71.3
Lee, S.-E. .MA 27.8
Lee, Sang-Eun .MA 7.16
Lee, Sangwon .MM 36.1
Lee, Sangyun .DY 49.10
Lee, Seungjae .DY 8.3, DY 51.2, SOE 15.2, SOE 16.1
Lee, Seung-Sup B. .TT 13.11
Lee, Soonhyung .MA 43.5
Lee, Subin .MM 7.8, •MM 36.1
Lee, T. .O 59.2, TT 48.2
Lee, T.-L. .O 93.9
Lee, Tien-Lin .HL 48.5, O 83.1
Lee, Yejin .MA 6.12, TT 5.3, TT 17.2, TT 22.23, TT 40.1, •TT 57.10, QI 4.2
Lee, Ying-Je .HL 20.55
Leeb, Valentin .•SYSD 1.3
Leemans, Wim .AKBP 13.1
Leemans, Wim P. .AKBP 8.4
Leffell, Alex .•SOE 4.1
Legenstein, Lukas .MM 22.5, •MM 31.4
Legeza, Örs .QI 3.1
Legrand, William .MA 52.10
Legut, Dominik .DS 7.2, MA 9.6, MA 34.3, •MA 58.11
Lehmann, Carl .•TT 10.4
Lehmann, Florian .MM 3.9
Lehmann, Katrin .MA 52.17
Lehmann, Louis .CPP 23.3, DY 24.3, O 25.2, O 87.3, •O 87.7
Lehmann, Marinus .•MM 19.41
Lehmann, Michael .FM 19.5
Lehmann, Natalie .•O 42.1, O 70.7, TT 65.7
Lehmann, Sebastian .DS 20.28, HL 20.23, HL 20.24, HL 26.10, HL 26.23
Lehmkühler, Felix .CPP 27.5, •CPP 46.5, DY 26.5
Lehnen, Jonas Hans .•BP 31.3, •CPP 50.3
Lehner, Jennifer .HL 3.8
Lehnert, Ulf .AKBP 2.1, AKBP 8.2
Lehtinen, Janne .HL 17.2
Lei, Hechang .TT 57.6
Lei, Shan .HL 31.4
Lei, Wenjing .O 26.1
Lei, Yang .•MM 35.1
Lei, Yong .CPP 4.5, FM 5.1, MM 4.8, O 97.5
Lei, Zijin .HL 48.1
Leibfarth, Katharina .•DD 27.7
Leibig, Jonas .•TT 2.6
Leibnitz, Oskar .•FM 7.7
Leibold, Joachim P. .HL 26.34
Leiderer, Paul .MA 27.10
Leiprecht, Phillip .MA 27.10
Leiser, Harald .•TT 23.8
Leisgang, Nadine .•TT 12.3
Leisner, Thomas .UP 8.3
Leist, Justus .O 24.2, •O 97.4
Leistner, Karin .CPP 46.47, MA 57.4, MA 57.6, MM 39.1
Leite Gomes, João Pedro .•MA 37.5
Leitenstorfer, A. .MA 52.8, MA 59.8
Leitenstorfer, Alfred .MA 38.8
Leithäuser, Jan .•DS 11.7
Leithe-Jasper, A. .TT 5.9
Leithe-Jasper, Andreas .FM 9.3, TT 5.8, TT 5.11, TT 17.2, TT 25.8, QI 4.2
Leitherer, Andreas .•QI 12.3
Leitmann, Katharina .•TT 91.4
Leitner, Erich .CPP 6.4
Leitner, Matthias .O 13.10
Leiva–Leroy, Catalina .MA 36.1
Leiva-Montecinos, Sergio .•MA 51.3, •TT 88.3
Lelek-Greskovic, Sara .BP 14.38
Lemay, Serge .O 87.9
Lemke, Robert .•O 27.7
Lemmens, Peter .FM 22.9, MA 8.9, •MA 40.8
Lemmer, Uli .HL 45.8
Lemperle, Anna .•O 94.8, O 94.10
Lemut, Gal .MA 27.1, •O 63.6, TT 41.10, TT 50.5, •TT 55.6
Lenarcic, Zala .QI 17.8
Lendínez, José Miguel .MA 38.4
Lenger, Malik .•TT 24.6, TT 92.5
Lenhard, Philipp .TT 22.12
Lenk, Katharina .TT 4.12
Lenke, Nadine .•QI 9.6
Lenschen, Jakob .TT 22.16, •TT 43.3, TT 43.4
Lenski, Diana .•BP 7.23
Lentz, Adrian Maximilian Roda •BP 14.72
Lentz, Florian .HL 26.33
Lenz, Corvin .•QI 14.13
Lenz, Kilian .•MA 44.8, MA 45.4, MA 51.1, MA 57.2, •TT 76.8, TT 88.1
Lenz, Martin .BP 14.89, •CPP 20.2, •DY 23.2, DY 33.6
Lenz, Philip .CPP 46.5
Lenzeder, Stefanie .BP 7.12
Lenzen, Stefanie .•BP 33.10
Leo, Karl .CPP 15.6, CPP 17.20, CPP 17.24, CPP 22.3, CPP 25.5, CPP 38.5, CPP 40.1, CPP 40.4, CPP 40.6, CPP 57.1, CPP 57.3, CPP 57.6, DS 16.5, HL 1.12, HL 2.6, HL 2.7, HL 22.1, HL 22.2, HL 22.4, HL 22.5, •HL 53.1
León, Carlos .MA 3.1
Leon, Dario .MM 37.4
Leonardo, Aritz .HL 8.11
Leone, Grace .CPP 17.42
Leone, Luca .DY 14.12
Leong, Shu Yao .BP 9.4
Leonhardt, Christopher M. .CPP 22.5
Leppert, Linn .HL 45.6
Lerch, Michael .MA 7.3
Lerch, Nikolas .•BP 14.35, BP 36.7, DY 57.7
Lerner, Rom .BP 30.2, CPP 47.2
Lerner, Sören .DS 20.33
Lesko, Daniel .SYFC 1.5
Leßmeister, Jannis .•O 9.1, O 27.5, O 41.1, O 42.2, O 83.4, TT 38.1
Lesne, Edouard .DS 4.1, DS 20.51, MA 7.36, MA 24.2, •MA 33.5, MA 52.29, TT 36.2, TT 40.3, TT 57.10
Lesniewski, Maria C. .CPP 24.1
Lesnyak, Vladimir .HL 20.48
Lesovský, Tadeáš .O 6.1, O 8.2
Lessing, Daniel .•QI 14.17
Letrou, Mathieu .•BP 11.6
Lettau, Thomas .HL 1.11
Lettermann, Leon .•BP 1.4, BP 14.67, •CPP 1.4, •DY 4.4
Lettieri, Mariateresa .O 80.3
Lettinga, Mathilde G. .•BP 37.7
Letzer, Simon .•HL 20.48
Leu, Ariana .•BP 11.11
Leubner, Nathan CPP 17.39, •FM 23.6
Leucke, Moritz .•O 37.5
Leumer, Nico .•TT 42.2
Leung, Kevin .O 36.1
Leutner, Kilian .•MA 55.3, MA 55.9
Levantino, M. .HL 46.6
Levashov, Sergej .DS 9.3, DS 12.3, O 97.8
Levchenko, Khrystyna .MA 9.9
Leven, Richard .•MA 30.9, O 84.4, TT 84.4
Levichkova, Marieta .CPP 17.9
Levinský, Petr .DS 7.5, MA 57.5
Levitin, Lev .TT 22.17
Levy Yeyati, Alfredo .TT 73.7
Levytskyi, Mykhailo .DS 21.4
Levytskyi, Volodymyr FM 9.3, TT 5.11, TT 25.8, •TT 42.12
Lewenstein, Maciej .DY 53.5, TT 87.5
Lewera, Adam .O 93.3
Lewin, Daniil .FM 11.18
Lewis, Alan .O 59.8, TT 48.8
Ležaic, Marjana .MA 51.7, TT 88.7
Lezuo, Luca .O 80.1
Lhotzky, Johannes .DD 14.2
Lhuissier, Henri .DY 19.1
Li, An-Ping .O 73.1
Li, B. .BP 27.8, BP 37.2
Li, Bingxin .MM 39.6, •O 65.9
Li, Boxi .QI 8.5, QI 8.6, QI 11.3, QI 13.7
Li, Chao .TT 85.3
Li, Chuan .TT 6.1, TT 41.1, TT 57.9
Li, Danfeng .•TT 39.1
Li, Dongzhe .MA 16.7
Li, Feitao .MM 21.2
Li, Fen .BP 7.10
Li, Fu .FM 6.4, MA 2.12, MA 8.7, •MA 33.7
Li, Guanyi .•HL 9.2
Li, Haobo .•FM 6.9
Li, Hongshuai .•MM 18.1
Li, Jennifer M. .BP 14.68
Li, Jia-Cheng .•HL 20.55
Li, Jian .QI 7.2
Li, Jing .MA 51.3, TT 88.3
Li, Jingrui .HL 4.6
Li, Jinzhao .HL 4.4
Li, Junqi .MM 4.8
Li, Lang .•O 65.3
Li, LI .BP 7.9
Li, Linge .•BP 14.92, BP 14.93
Li, Lixing .CPP 17.18, CPP 17.42, CPP 44.5, CPP 48.2, •CPP 53.6, CPP 58.2, CPP 59.3
Li, Longlong .•BP 2.7
Li, Nicky Kai Hong .TT 17.9, QI 4.9, •QI 16.10
Li, Ning .CPP 17.19
Li, Pengji .DS 20.21
li, qiwei .•TT 56.7
Li, Qixuan .•CPP 30.3
Li, Shanlong .BP 39.1, CPP 55.1
Li, Shuo .TT 69.1
Li, Tong .MM 11.1
Li, Wangtao .O 55.6, •O 81.4
Li, Weibin .O 10.2, O 84.9, TT 16.2, TT 84.9
Li, Weizhe .SYFC 1.5
Li, X. .BP 27.8, BP 37.2
Li, Xiaocui .•MM 23.4
Li, Xiaohan .AKPIK 6.4
Li, Xiaoqin .O 95.5, TT 96.5
Li, Xinyu .•DS 12.1
Li, Xinzhi .HL 26.10
Li, Xiyang .•MA 31.4, •TT 47.4
Li, Yahui .•DY 13.8, •TT 19.8
Li, Yiheng .•MA 43.2
Li, Ying .TT 98.3
Li, Yingxin .TT 42.6
Li, Yong .MM 3.2, •MM 15.6, MM 15.7
Li, You-Sheng .TT 25.7
Li, Yue .MM 11.1
Li, Yungui .HL 15.4, HL 15.6
Li, Zelong .CPP 37.2
Li, Zerui .CPP 44.5, CPP 48.2, CPP 57.5
Li, Zhangtao .MM 23.5
Li, Zhiyuan .•MM 15.3
Li, Zhongyang .•MM 21.10
Liang, Feng .FM 5.1
Liang, Shiling .•DY 21.5
Liang, Yien .•QI 18.4
Liang, Yuxin .•CPP 4.6, CPP 16.2, CPP 17.27, CPP 17.33
Liao, Menghan .MA 49.2
Liao, Shansi .•MM 18.4
liao, tianhui .•DY 19.3, DY 41.1
Liberal, Lucas .•HL 47.2
Libisch, Florian .O 93.1
Liborius, Lisa .HL 26.5
Libuda, Jörg .O 13.12, O 65.12, O 94.4
Lichtenberg, Kurt .•O 12.3, O 43.11
Lichtenstein, Alexander .TT 53.5
Lichtenstein, Alexander I. .TT 53.1
Lichtl, Henrik .O 15.7, •O 89.1
Lidberg, Hermann .•DD 15.1
Lie, Fabian .HL 45.6
Liebald, Christoph .TT 79.4
Liebchen, Benno CPP 28.1, CPP 28.3, DY 14.6, DY 27.3, DY 29.1, DY 29.3, DY 34.2, DY 44.3, DY 49.10, DY 62.2
Lieberich, Francisco .•TT 57.12
Lieberwirth, Eric .•BP 14.25
Liebich, Marlene .HL 39.8, O 38.6
Liebig, Alexander .TT 74.12
Liebig, Bernd .TT 22.32
Liebing, Simon .•O 50.2
Liebmann, Marcus .HL 20.40
Liebscher, Christian MM 34.7, TT 5.6
Liebscher, Christian H. .MM 15.5
Liedke, Maciej Oskar .DS 20.22, •MM 12.8
Liedl, Tim .BP 9.5
Liemann, Gerhard .TT 22.32
Lienau, C. .HL 54.10
Lienau, Christoph .HL 46.2, HL 46.3, O 44.6, O 79.2, DD 33.1
Lienhard, Benjamin .•QI 2.1, QI 2.7
Liese, Julia .AKBP 10.4, AKBP 11.1
Liese, Susanne .BP 26.4, •BP 29.1, CPP 43.4, •CPP 45.1
Liesenfeld, Jürgen .O 19.7
Lieske, Leonard-Alexander .O 3.2, O 9.12
Lietz, Haiko .SOE 5.3
Lighthart, Rian A.M. .TT 92.19
Ligthart, Rian .O 44.3, TT 22.3
Ligthart, Rian A.M. .•O 42.3
Lihm, Jae-Mo .TT 13.11
Lilensten, Lola .•MM 10.1
Lilienkamp, Thomas .DY 22.6
Liljeroth, Peter .O 59.7, TT 48.7
LILLEPÄG, Jelena .MM 16.4
Lima, Irlan S .FM 2.6
Limame, Imad .HL 54.6, HL 54.7, •HL 55.1
Limberg, Ulrich .•HL 20.11
Limot, Laurent .•O 64.6
Lin, Chi-Chia .•MA 50.9
Lin, Haicheng .TT 95.3
Lin, Jinghan .•CPP 17.12
Lin, Kun-Han .CPP 57.2
Lin, Peize .O 12.3
Lin, Rong-Zhu .TT 2.1
Lin, Sheng-Hsuan .QI 15.6
Lin, Tzu Yen .•MM 36.4
Lin, Yayi .TT 5.2
Lin, Zijing .O 70.6, TT 65.6
Lindblad, Andreas .TT 14.5
Linden, Stefan .O 26.3
Lindenau, Anja .•BP 14.39
Lindenmeir, Christoph .CPP 17.42
Lindenmeir, Christoph G. .CPP 17.5, •CPP 53.2
Lindenmeir, Christoph Gernot CPP 44.2
Lindenthal, Jakob .•DS 16.5, HL 1.12
Linder, Markus B. .BP 26.5, CPP 43.5
Lindfors-Vrejoiu, Ionela .MA 27.10
Lindhorst, Thisbe .CPP 27.2, DY 26.2
Lindner, Aleksandra .MA 35.6, MA 57.2, TT 60.6
Lindner, Anke .CPP 20.4, DY 23.4
Lindner, Benjamin .•DY 33.1, DY 33.7, DY 33.8, DY 63.1
Lindner, Florian .MM 19.36
Lindner, Javed .DY 58.5, •DY 58.8, SOE 17.5, •SOE 17.8
Lindner, Jürgen .MA 12.4, MA 35.6, MA 44.8, MA 45.4, MA 51.1, MA 57.2, TT 60.6, TT 76.8, TT 88.1
Lindner, Patrick .HL 20.41
Lindorff-Larsen, Kresten .BP 39.1, CPP 55.1
Lindström, Tobias TT 22.12, TT 22.17
Ling, Zhitian .FM 10.4, MA 36.8, MA 39.3
Link, Julia Monika .TT 15.9
Link, Valentin .QI 7.3, QI 17.4
Linnala, Tatu .•MM 19.9
Linnér, Erik .•TT 13.9
Linnerud, Marthe .MA 6.11
Linnhoff-Popien, Claudia .QI 1.11
Linscott, Edward .MM 12.2, MM 17.5
Linz, Scott Daniel .•DY 59.10, •TT 99.10
Linzen, Sven TT 5.1, TT 64.2, TT 93.6
Liou, Yi-Ting .HL 18.9, TT 32.9
Lipavský, Pavel .TT 93.12
Lipfert, Jan .•BP 9.3, BP 14.80, BP 20.8
Lipika, Lipika .TT 61.4
Lipilin, Fedor .HL 35.6
Lipp, Hansjoerg .O 29.3
Lipp, Hansjörg .O 29.1, O 94.11
Lippitz, Markus .BP 14.78, O 26.2, O 27.6, O 57.2
Lippmann, Otto .CPP 19.4, DY 20.4
Lippmann, Stephanie .MM 19.31, MM 33.1
Liscak, Stefan .•MA 7.4
Lischner, Johannes .O 71.7, O 95.10, O 96.10, TT 66.7, TT 96.10
Lisenfeld, Jürgen TT 22.13, TT 22.14, TT 22.16, TT 43.3
Lisinetskii, Victor .HL 8.8
Lisjak, D. .MA 36.3
Liška, Jiří .O 96.7
Lissel, Franziska O 6.5, O 45.5, O 58.4
List, Ilja .•QI 9.5
Litman, Yair .O 9.2
Littek, Carsten .•CPP 11.4, •DY 17.4,

DY 44.5
Litterst, F. Jochen .. TT 57.2, TT 57.3
Littlehales, Matthew ..... •MA 16.6
Littmann, Jan-H. ..... HL 26.28
Littmann, Jan-Heinrich ..... •HL 23.8
Litvinov, Sergey ..... AKBP 7.4
Litzba, Lukas ..... •TT 18.6
Litzius, Kai ..... HL 38.8, MA 7.35, MA 7.40, •MA 16.3, MA 37.8
Liu, Bing ..... DS 20.43
Liu, Chang ..... MM 7.5
Liu, Chun-Xiao ..... TT 15.3
Liu, Danyang ..... FM 11.23
Liu, Dongdong ..... O 46.7
Liu, Dongmei ..... MM 33.1
Liu, Enke .. MA 24.6, TT 29.6, TT 36.6
Liu, En-Pei ..... MA 31.10, TT 47.10
Liu, Fang ..... •MA 19.8, •TT 31.8
Liu, Fupin ..... MA 36.12
Liu, Hao ..... CPP 41.7
Liu, J. ..... O 93.9
Liu, Jialiang ..... FM 2.4
Liu, Jianqiang ..... O 64.5
Liu, Junde ... •O 14.3, O 38.1, O 40.18, O 40.20, O 40.21, O 98.10, TT 37.18, TT 37.20, TT 37.21
Liu, Jung-Ching ..... •O 69.10
Liu, Liangzhen ..... CPP 16.2
Liu, Ming-Hao . DS 8.3, •TT 4.1, TT 4.6
Liu, Renxiang ..... O 6.2
Liu, Shi-Hui ..... •DS 20.26, HL 40.1
Liu, Shiqiang ..... AKPIK 6.4
Liu, Shuheng ..... QI 10.11
Liu, Sichen ..... O 23.3, O 88.9
Liu, Tsai-Ling .... MA 31.10, TT 47.10
Liu, W. .... MA 18.1, MA 18.5, TT 30.1, TT 30.5
Liu, Wei . MA 18.2, MA 52.23, TT 30.2
Liu, Wenchuan ..... •MM 19.4
Liu, Wentao ..... HL 4.7
Liu, Xiaojiao ..... TT 80.3
Liu, Xiaojing ..... •O 76.4, TT 27.4
Liu, Xiaoling ..... TT 12.3
Liu, Xingchen ..... CPP 17.32
Liu, Xinyang ..... TT 29.6
Liu, Yaowu ... O 15.6, •O 15.9, O 64.2, TT 95.3
Liu, Ye ..... •O 9.10, O 69.5, O 77.3
Liu, Yebin ..... QI 8.5
Liu, Yifeng ..... •CPP 17.29
Liu, Yizhi ..... CPP 27.4, DY 26.4
Liu, Yu ..... TT 52.3
Liu, Yuefei ..... •MA 45.3
liu, yuqi ..... •FM 5.2
Liu, Yuqian ..... CPP 37.2
Liu, Zhengyuan ..... •O 99.3
Liu, Zhongkai ..... •O 62.11, •TT 54.11
Liu, Zihao ..... •SOE 4.7
Liubchenko, Oleksii ..... MM 19.3
Liubimtsev, Nikolai ..... •CPP 31.5
Lively, Kevin .... QI 3.2, •QI 3.8, QI 5.5
Liyanage, Gayani ..... O 46.3
Lizárraga, Kevin ..... O 15.2
LLorca, Javier ..... MM 36.5
Lloyd, Lawson ..... O 40.11, TT 37.11
Lloyd, Lawson Lloyd ..... MA 7.18
Lloyd, Lawson T. ..... •O 38.4, O 38.7, O 71.10, TT 66.10
Lo Gullo, Nicola ..... MA 7.59
Lo Sardo, Flavia ..... •TT 4.11
Lobe, Elisabeth ..... •QI 5.2
Lobo, Ricardo P. M. S. ..... DS 20.30
Locatelli, Andrea .... O 10.3, O 88.10, TT 16.3
Loch, Maximilian ..... •DD 22.2
Loche, Philip ..... MM 9.2, •MM 17.3
Locmelis, Sonja ... HL 20.10, HL 24.5
Lodewijks, Bas ..... TT 70.2
Löffler, Lorenz ..... •HL 1.12
Löffler, Markus .... •FM 19.4, HL 22.6
Löffler, Rebecca ..... •MA 7.73
Löfgren, Joakim ..... MM 19.9
Lofink, Fabian ..... MA 52.17
Lögl, Anton ..... HL 26.36, •HL 26.39
Loh, Hannah ..... •O 45.6
Loh, Teemu ..... DD 6.1
Loisch, Gregor AKBP 12.4, AKBP 13.2
Lojewski, T. ..... MA 7.14
Lokamani, Mani ... MM 22.7, •O 71.6, •TT 66.6
Loke, Rajendra . •MA 23.6, MA 52.34, MA 52.36, •TT 35.6
Lombardi, Enrico ..... MM 40.8
Lombardi, Juan Manuel ..... DY 6.12, •MM 8.9, MM 22.1
Lomeli, Eder G. ..... MA 33.11
Long, Daniel ..... QI 11.7
Long, Mengmeng ..... TT 23.15
Long, Tianyun ..... AKBP 12.2
Lönnecke, Katharina ..... BP 33.5
Lonnes, Julius ..... •O 97.7
Löns, Christian ..... •UP 3.4, UP 3.5
Loosdrecht, Paul H. M. van . MA 27.5
Lopes, J. Marcelo J. ..... DS 20.18
Lopes, Joao M. J. .. HL 18.9, TT 32.9
Lopes, João Marcelo DS 11.3, HL 24.6
Lopes, Joao Marcelo Jordao DS 12.9
Lopes, Thiago ..... CPP 2.3, SOE 3.3, UP 1.3
Lopez, Francisco Cardenas ... QI 13.7
López Páramo, Santiago ..... BP 2.9
Lopez, Rafael Rojas ..... MA 30.9
Lopez, Ruben ..... O 87.8
López- Salas, Nieves ..... O 23.1
Lopez-Richard, Victor ..... HL 29.5, TT 58.5
Łopion, Aleksandra ..... •HL 25.2, HL 39.3, HL 39.4, HL 39.6, HL 39.9
Lorch, Simon ..... •DS 20.15
Lord, Oliver ..... TT 80.3
Lorenceau, Elise ..... CPP 58.4
Lorente, Nicolas ..... O 35.1, O 35.2, O 35.3, O 69.3, O 77.1, O 99.4
Lorentz, Bernd ..... AKBP 7.4
Lorenz, Alena ..... •TT 23.23
Lorenz, Charlotta ..... •BP 20.6
Lorenz, Florian ... •DY 59.2, •TT 99.2
Lorenz, Janine ..... O 31.3, •TT 93.6, QI 6.9
Lorenz, Thomas . TT 23.13, TT 23.14, TT 61.2
Lorenz-Spreen, Philipp .... •SYTP 1.5
Lorke, A. HL 17.7, HL 20.27, HL 20.39
Lorke, Axel HL 17.3, HL 17.8, HL 20.12, HL 47.1, HL 55.5, HL 55.6, O 68.2
Lorke, Michael ..... HL 47.1, O 61.6
Löser, Robert ..... •MM 4.7
Lotfi, Z. ..... BP 27.8, BP 37.2
Loth, Sebastian ..... O 12.3, O 15.7, O 43.11, O 89.1, O 89.5, O 99.1, •O 99.8
Lotkhov, Sergey ... •TT 22.8, TT 43.5
Lotsch, Bettina ..... HL 15.1
Lotsch, Bettina V. ..... MM 5.4
Lott, James A. ..... AKPIK 3.4
Lottenburger, Ben ..... O 44.12
Lottermoser, Thomas ..... MA 7.32, MA 27.9, O 98.2
Lotze, Christian O 9.9, O 43.6, O 43.9, O 80.4, TT 73.3
Lou, Jun ..... MM 32.6
Lou, Rui ..... TT 5.7
Lou, Zekun ..... •O 59.8, •TT 48.8
Louafi, Widad ..... TT 71.6
Lounis, Samir ..... MA 6.7, MA 7.57, MA 33.6, MA 38.12, MA 54.9, O 17.1, •O 64.9, TT 85.5
Lovejoy, Tracy ..... FM 15.1
Lovrinčević, Bernada ..... MM 19.30
Low, Jonathan Z. ..... TT 90.6
Löwen, Hartmut . CPP 11.5, CPP 20.3, CPP 30.2, DY 17.5, DY 21.9, DY 23.3, DY 27.3, DY 27.4, •DY 49.8, DY 49.9, DY 49.10, DY 49.11, DY 62.3
Lowengrub, John ..... BP 37.8
Loy, Sebastian ..... HL 13.5
Loyola, Tobias Huber ..... QI 18.7
Lozano-Gómez, Daniel ..... TT 26.5
Lozovanu, Valeria ..... BP 37.7
Lu, Bo ..... TT 98.5
Lu, Haichang ..... •MA 34.7
Lu, Hanqian ..... MA 27.2
Lu, Haoran ..... TT 43.8
Lu, I-Te ..... DS 20.52, O 49.4, O 79.3
Lu, Jia G. ..... O 63.9, TT 55.9
Lu, Jiong ..... O 95.10, TT 96.10
Lu, Tiemei ..... BP 29.1, CPP 45.1
Lu, Wenjun ..... •MM 23.1, MM 23.2
Lu, Yan ..... •CPP 4.1
Lu, Yang ..... MM 23.4
Lu, Yao ..... QI 14.13
Lu, Yifan ..... CPP 41.7
Lu, Yuan ..... TT 73.9
Luan, Tangdi ..... •BP 14.94
Luber, Leo ... HL 4.2, HL 4.3, HL 45.2
Luber, Mattias ..... BP 7.43, BP 7.49, BP 37.1
Lubig, Kevin ..... DS 13.2
Lubk, Axel FM 11.15, FM 19.9, MA 7.17, MA 19.8, MA 27.4, MA 30.6, MA 44.6, O 70.2, TT 31.8, TT 65.2, TT 76.6
Lübkes, Christof ..... UP 6.3
Lubomirsky, Igor ..... MA 52.32
Lucas Fagundes, Renan .... •SOE 6.1
Lucas, Maxime ..... •TT 4.2
Lucht, Jens ..... CPP 27.4, DY 26.4
Lucibello, Carlo ... DY 45.2, SOE 14.2
Lücke, Marvin ..... SOE 8.3
Ludacka, Ursula ..... FM 18.8
Lüdge, Kathy ..... QI 10.4, AKPIK 4.3
Ludt, Christian .. CPP 17.36, •FM 12.8
Ludwig, A. ..... HL 17.7, HL 20.39
Ludwig, Alfred ..... FM 6.7, FM 6.8, FM 6.10, MM 11.3
Ludwig, Arne ..... HL 17.8, HL 20.35, HL 20.36, HL 20.41, HL 20.44, HL 20.47, HL 26.7, HL 26.9, HL 26.12, HL 26.31, HL 55.4, HL 55.5, HL 55.6, HL 55.8
Ludwig, Michael ..... CPP 21.2
Ludwig, Stefan ..... HL 25.4
Luetkens, Hubertus . MA 8.3, MA 8.5, TT 57.2, TT 57.3
Lühken, Arnim ..... DD 31.1
Lühmann, Thomas ..... TT 29.5
Lührs, Lukas ..... MM 21.10
Lui, Fang ..... O 71.11, TT 66.11
Lui, Ming Hong ..... •BP 14.48
Luigs, Marie ..... •O 36.6
Luitz, David DY 32.1, TT 17.3, TT 44.6, TT 45.1, TT 53.6, QI 4.3, QI 9.4
Luitz, David J. ..... DY 42.1, TT 63.1
Lukács, Árpád ..... QI 20.5
Luke, D. Russel .... O 40.19, TT 37.19
Luke, D. Russell ..... O 14.10
Lüke-Mense, Thorben ..... UP 3.5
Lukin, Jana ..... •DY 43.21
Lukin, Mikhail ..... TT 12.3
Lukose, Rasuole .... DS 14.8, HL 23.3
Lukosius, Mindaugas ..... DS 14.8, HL 23.3
Lülff, Martin ..... •O 40.14, •TT 37.14
Lundemo, Sondre Duna ..... •TT 56.6
Lundwall, Marcus ..... DS 3.3
Luneau, Jacquelin ..... TT 43.11
Lünemann, Daniel ..... HL 46.3
Lunkad, Raju ..... •CPP 21.3
Lunkenbein, T. ..... O 88.11
Lunkenbein, Thomas ..... O 85.6
Lunova, Veronika ..... •HL 26.22
Lünser, Klara ..... •MM 21.8
Luo, C ..... MA 19.7, TT 31.7
Luo, Chen .DS 12.9, MA 7.47, MA 16.4
Luo, Chengjie ..... •BP 7.6, DY 49.2
Luo, Haixuan ..... •FM 11.5
Luo, Jun ..... •TT 69.1
Luo, Xiangyu ..... HL 24.10
Luo-Hofmann, Jinji ..... TT 43.4
Luoma, Kimmo ..... O 57.7
Luong, Minh-Anh ..... HL 25.3
Luonis, Samir ..... O 21.1
Lupascu, Andrian ..... QI 11.3
Lupascu, Doru ..... FM 4.4, FM 11.18, •FM 11.32
Lüpke, Anne ..... O 61.7, O 83.10
Lüpke, Felix . MA 43.3, O 31.3, O 41.4, O 54.3, O 63.9, •O 63.11, O 86.5, O 95.8, TT 38.4, TT 55.9, •TT 55.11, TT 93.6, TT 96.8, QI 6.9
Lupo, Elena ..... •QI 11.7, QI 13.6
Luppi, Eleonora ..... HL 35.9
Lupuleasa, Andrei ..... O 26.1
Lurz, Yannic ..... BP 12.2
Lustemberg, Pablo G. ..... O 23.3
Luther, S. ..... TT 80.6
Luther, Sven ..... TT 23.1
Lüttig, Julian ..... HL 46.4
Lutz, Eric ..... O 99.1, O 99.8
Lutz, Matthew ..... MA 25.6
Lutz, Wolfgang ..... DD 24.3
Lützenkirchen-Hecht, Dirk . MM 19.30
Luu, Thomas ..... TT 17.3, QI 4.3
Lux, Christine ..... DD 10.3, DD 26.4
Luxa, Jan ..... HL 35.6
Luyckx, Adrien ..... •DY 19.4
Lygouras, Chris ..... TT 41.4
Lykhach, Yaroslava . O 13.12, O 65.12, •O 94.4
Lynch, Lindsey ..... FM 11.16
Lynch, Ronan ..... FM 12.5
Lynch-Gonzalez, Alejandro ... O 69.13
Lysne, Erik ..... MA 37.6
Lysogorskiy, Yury ..... MM 19.10
Lytvynenko, Y. ..... O 19.10, O 59.2, TT 48.2
Lytvynenko, Yaryna ..... TT 14.4
Lyu, Lu ... •O 8.1, O 9.1, O 42.2, O 83.4
Lyu, Meng ..... MA 31.4, TT 47.4
Lyu, Yuanqi ..... FM 10.5
M. Aladdin, Omar ..... •TT 28.9
M. Andersen, Brian ..... MA 33.3
M. Eremin, Ilya ..... TT 71.2
M. Etchells, Isaac ..... CPP 48.5
M Fathabad, Sobhan ..... FM 11.18
M. Fernandes, Rafael ..... TT 14.10
M. Kennes, Dante ..... O 49.5
M. Murphy, Bridget CPP 27.2, DY 26.2
M. Oppeneer, Peter ..... MA 12.5
M. Rogers, David ..... BP 2.10
M. Schneider, Jochen ..... DS 7.5
M. Ugeda, Miguel ..... TT 14.10
M. van der Veen, R. ..... HL 46.6
M. Vicente-Arche, Luis ..... TT 69.4
ma, boyang ..... •O 43.12
Ma, Chenxi ..... DS 20.21, HL 20.50, HL 20.51
Ma, He ..... HL 9.2
Ma, Ji ..... O 6.2
Ma, Yan ..... FM 5.8, MM 15.4
Ma, Zihao ..... •TT 93.2
Maas, Christian .. HL 48.2, •MA 39.16
Maas, Hendrik ..... •DD 26.1
Maass, Philipp .... DY 41.3, DY 43.20, DY 61.5
Mabrouk, Youssef ..... CPP 14.4, •CPP 21.5
Maccari, F. ..... MA 50.3
Maccari, Fernando ..... MA 50.4
Maccari, Ilaria ..... TT 64.2
Macêdo, Rafael ..... QI 12.6
Macháček, Jan ..... O 72.4, TT 67.4
Machado Charry, Eduardo ... CPP 6.4
Machado Pérez, David .... •DY 33.12
Machchhar, Shachi ..... HL 13.1
Mächtel, Kevin ..... •CPP 46.52
Machtl, Leon ..... O 38.6
Mäck, Martin ..... •TT 42.10
Mackenzie, A. P. ..... TT 69.6
Mackenzie, Andrew . MM 40.2, O 76.7
Mackenzie, Andrew P. ..... MA 8.8, MM 19.43, TT 41.5
MacKintosh, Fred C. ..... BP 27.7
MacManus-Driscoll, Judith L. FM 18.5
Madadi, Mahkam ..... •MM 19.25
Madalaimuthu, Jose Prince •CPP 17.25, CPP 48.4
Madani, Mahnoush ..... BP 39.4, CPP 55.4
Madhusudan Rao, Prajwal Rigvedi TT 22.2
Mädrich, Jan ..... O 19.6
Madrigal Solis, Erick A. ..... DY 6.7
Madsen, Anders ..... O 40.15, O 98.3, TT 37.15
maeda, tomoki ..... O 95.9, TT 96.9
Maehl, S. ..... O 85.2
Maehrlein, Sebastian ..... MA 25.3, AKBP 2.5
Maehrlein, Sebastian F. .... MA 35.6, O 49.2, TT 60.6
Maeland, Kristian .... MA 7.51, O 2.5, •TT 11.5
Maeng, Min-Jae ..... O 82.2
Maes, Michael ..... SOE 10.3
Magagnin, Gregoire ..... FM 4.1
Magalhaes Braga, Ian ..... •DY 33.11
Magalon, Axel ..... BP 41.1
Magan, Devika ..... BP 15.5
Mager, Carlotta ... CPP 27.2, DY 26.2
Magerle, Robert .... BP 7.3, BP 14.34, •BP 26.6, •CPP 43.6
Magin, Nils ..... •CPP 42.5
Magnabosco, Giulia ..... HL 39.9
Magrez, Arnaud ..... HL 8.10
Mahadevan, Lakshminarayanan BP 37.11
Mahadevan, Sudhi ..... •HL 26.18
Mahajan, Anima •HL 26.14, •MM 30.5
Mahajan, Avinash .. MA 31.7, TT 47.7
Mahajan, Vaibhav •BP 27.10, BP 37.7
Mahajan, Ved ..... •CPP 46.56
Mahanoglu, Cagla TT 22.28, TT 22.29
Mahdavi, Esmaeil ..... SOE 8.4
Mahdi Syed, Luqman ..... O 73.5
Mahendru, Bharti ..... TT 50.8
Mahmood, Ather ..... O 60.6
Mahmoudi, Samad ..... CPP 28.3, DY 29.3, •DY 44.14
Mahmudul, Hasan ..... MA 52.31
Mährlein, Sebastian ..... AKBP 2.1
Mai, Han ..... MM 5.5
Mai, Han Lin ..... •MM 25.2
Maiberg, Matthias ..... DS 8.5
Maier, Alexander ..... •DY 21.6

Maier, Alexander M. ..... DY 7.4
Maier, Andreas R. ..... AKBP 8.4, AKBP 11.2
Maier, Berenike .... BP 11.5, BP 11.11, BP 14.16
Maier, Christian ..... MM 4.4
Maier, Florian .. O 4.2, O 87.1, •O 87.6
Maier, Paul .....•TT 73.10
Maier, Philipp .....•TT 85.4
Maier, Philipp E.J. ..... O 44.3
Maier, Sabine .MA 5.4, O 35.1, O 35.2, O 35.3, O 77.1, TT 7.4
Maier-Kiener, Verena ..... MM 32.3, •MM 36.2
Maignan, Antoine ..... TT 3.3
Maile, Dominik .....QI 14.4, QI 20.2
Mailly, Dominique .....HL 20.54
Mair, Georg .....TT 22.25, TT 22.26, •QI 2.4, QI 14.21
Maire, Raphael .....•DY 62.7
Maisi, Ville ..... TT 78.1
Maisuls, Ivan ..... FM 15.2
Maiti, Abhishek .....•O 63.1, •TT 55.1
Maiti, Prabal ..... MM 31.6
Maitra, Toulik ..... HL 15.4
Maity, S. ..... TT 24.7
Maity, Sandip .....•TT 92.2
Majee, Arghya ...•BP 31.4, •CPP 50.4
Major, Márton ..AKBP 9.3, •AKBP 9.4
Majumdar, Atreya ...•DY 6.6, DY 61.4, FM 12.4, MA 7.38, MA 58.7, AKPIK 5.2, AKPIK 5.4
Majumdar, Satya .....•DY 7.6
Majumdar, Satya N. .. DY 7.7, DY 49.7
Majumder, Mayukh .MA 31.2, TT 47.2
Majumder, Suman .....CPP 38.6
Mak, Kin Fai .....•TT 27.1
Makarov, Denys .... FM 6.11, HL 23.1, MA 7.20, MA 30.8, MA 44.6, MA 44.7, MA 49.1, MA 49.5, MA 49.6, MA 49.7, TT 76.6, TT 76.7
Makarov, Dmitrii E. .....SOE 9.3
Makarov, Oleg Yu. ..... HL 26.46
Makhdoumi Kakhaki, Zahra ..•TT 5.4
Makino, Hitoshi ...•MA 3.11, MA 7.61
Makk, Péter .....HL 30.2, TT 59.2
Makowski, Wiebke ..... O 45.8
Makris, Grigorios ....•TT 2.4, TT 2.10
Makushko, Pavlo .. HL 23.1, MA 7.20, MA 30.8, •MA 49.1, MA 49.7
Malachias, Angelo ...O 95.2, TT 96.2
Malakhova, Iuliia .....CPP 17.13
Malatesta, Enrico . DY 45.5, SOE 14.5
Malcangi, Francesco ..... •DY 61.2
Malcherek, Kyra .....•HL 26.8
Maldonado, Ana ..... TT 29.2
Maldonado, Cintli Aguilar ....TT 26.8
Maletinsky, Patrick MA 43.4, •TT 24.1
Malgaretti, Paolo ... DY 61.6, DY 62.8
Mali, Ankur ..... SOE 4.3
Malic, E. ..... HL 54.10
Malic, Ermin . HL 3.7, O 98.9, O 98.10
Malica, Cristiano ..... MM 8.1
Malik, Bilal .....HL 26.35
malik, harshita .....•O 46.8
Malik, Mohammad .....•HL 38.7
Malis, Oana .....HL 57.3
Maliyov, Ivan ..... O 7.2, TT 9.2
Mallada, Benjamin .....•O 69.13
Mallet, Pierre . O 15.1, O 62.2, TT 54.2
Malova, Polina .....•BP 7.49, BP 37.1
Maltitz, Jeremy ..... DS 20.25
Malyuk, Andrey ..... TT 26.7
Mamiev, Zamin .....O 33.4
Mamiyev, Zamin .....O 62.7, O 66.2, O 74.9, •O 79.6, O 84.2, TT 54.7, TT 68.9, TT 84.2
Manacorda, Alessandro .....DY 49.4
Mañas-Valero, Samuel .....FM 11.23
Manchini, Andrea .....O 57.3
Mandal, Debottam ..... HL 23.1
Mandal, Haraprasad .....•O 43.3
Mandal, Prabhat ..... TT 79.5
Mandal, Pranay .....BP 27.11
Mandal, R. ..... HL 46.6
Mandal, Sagarmoy .....MM 19.6
Mandal, Soham .....•MM 31.6
Mandal, Souraj ..... CPP 46.18
Mandal, Suvendu ....BP 1.2, CPP 1.2, DY 4.2, DY 14.6, DY 34.2, DY 44.3
Mandalaparthy, Varun .....•CPP 13.2
Mandjes, Michel .....DY 7.8
Mañes, Juan L. ..... HL 8.11
Manganelli, Costanza Lucia . HL 38.9
Mangeat, Matthieu .....•CPP 11.1, •DY 17.1
Mangeolle, Léo .... TT 79.1, •TT 79.2
Mangin, Stéphane MA 27.11, TT 14.12
Mangini, Edoardo •MA 21.6, MA 55.5
Mangold, Florian ..... O 57.3, O 79.5, •O 85.7
Mangold, Maximilian .....•TT 97.1
Mania, Felix .....•DS 20.33
Mankovsky, Sergiy MA 14.3, •MA 17.1, MA 35.7, MA 35.8, TT 60.7, TT 60.8
Mankowsky, R. ..... MA 25.6
Manmana, Salvatore . O 86.7, TT 70.3
Manmana, Salvatore R ..... TT 44.9
Mann, Gerrit Johannes •O 7.3, •TT 9.3
Mann, Riley .....•TT 62.7
Manna, Kaustuv ..... TT 61.4
Manna, Poulami ..•TT 64.3, TT 93.16
Mannel, H. .....•HL 17.7, HL 20.27, HL 20.39
Mannel, Hendrik ... HL 17.3, HL 55.5, HL 55.6
Mannhart, Jochen ..... DS 11.3
Mannini, Matteo .....O 42.4
Mannsfeld, Stefan C. B. ..... DS 13.1
Mannteuffel, Lennart .....AKPIK 4.4, AKPIK 5.8
Manoharan, Hajaani .....BP 40.1
Manoharan, Pavithira .... CPP 46.43, •O 54.2
Manoharan, Yanisha .....UP 6.1
Manor, Ofer .....CPP 21.2, •O 13.5
Manske, Dirk .....•TT 14.7
Mansky, Maximilian Balthasar •QI 1.11
Mansour, Ahmed E. .....•AKjDPG 1.1
Mansouri, Miad ....MA 35.2, TT 60.2
Mansuroglu, Refik .....•QI 1.1, QI 1.2
Manten, Maja .....•O 26.4
Manthe, Uwe ..... DY 46.12, TT 75.12
Manthei, Tobias .....•HL 20.28
Manucharyan, Ani ..... FM 11.30
Manzano Diosdado, Daniel ..QI 14.19
Mao, Ning .....DS 20.51, TT 44.2
Mao, Qian ..... MM 25.1
Mao, Zhiqiang ..... MM 40.5
Maouene, Djamil A. A. ...•CPP 46.54
Maradan, Dario .....HL 25.1
Maranzana, Luca .....•MA 16.2, MA 30.10, MA 37.7
Marbach, Sophie .. CPP 11.6, DY 17.6, DY 61.3
Marbini, Arwin .....•UP 8.6
Marcel, Mokbel .....•BP 5.5
Marcelli, Claudia .....•BP 7.18
Marcelli, Giorgia .....•DY 61.7
Marchand, Halima Alem ..... BP 7.1
Marchant, Georgia A ..... MA 58.1, •MM 41.3
Marchetti, Lucca ..TT 29.7, •TT 56.12
Marchetti, M. Cristina ..... BP 37.10
Marcks, Christian ..... O 68.2
Marczak, Malwina A. .....HL 55.4
Marek, Andreas .....MA 58.1
Marganska, Magdalena ....TT 56.13, •TT 74.12
Margraf, J. T. ..... O 57.6
Margraf, Johannes ..... O 34.2
Margraf, Johannes T. .....CPP 15.7, MM 13.5, MM 19.8, MM 22.9, O 34.1, O 34.3, •O 96.8
Margraf, Jonas .....HL 54.1
Marín Boyero, Adrián .....•QI 14.19
Marin Ramirez, Juan Marcos DY 60.4
Marini, Giovanni .... HL 46.7, TT 49.4
Marinkovic, Marina ..... QI 3.4
Marino, Marco .....O 84.4, TT 84.4
Marino, Vito .....TT 95.5
Markham, Damian ..... QI 18.9
Markham, Matthew ..... QI 13.5
Markina, Daria ..... HL 13.7, HL 20.5, HL 20.6, HL 20.13, HL 20.22, •HL 39.5, HL 39.7
Marklund, Mattias .....AKBP 4.5
Markmann, Jürgen ..... MM 30.3, MM 30.4, MM 39.2
Markó, István .....•TT 41.9
Markou, Anastasios .....•MA 57.3
Markov, Anton .....TT 10.3
Marković, Toni ..... O 44.15
Marks, Joshua .....•UP 7.1, UP 7.3
Marmasse, Aurélien .....QI 18.6
Marmodoro, Alberto .....•MA 35.7, •TT 60.7
Marocko, Marina ... HL 30.2, TT 59.2
Maroutian, Thomas .....FM 4.5
Marpe, Moritz .....•SOE 12.2
Marquardt, Christoph .....QI 14.1
Marquardt, Florian ..QI 12.1, QI 14.20, AKPIK 3.1
Marquardt, Lina ..... O 88.6
Marque, Clément ..... BP 16.10, CPP 46.23
Marques, Carolina A. O 44.3, TT 29.2
Marques, Joao C. ..... BP 14.68
Marques Salvador, Helder CPP 46.51
Marqués-Marchán, Jorge ..•MA 7.79
Márquez, J.A. .....AKPIK 6.5
Márquez, José A. .....AKPIK 6.3
Marrazzo, Antimo .....MA 2.1
Marré, Daniele ..... MM 40.4
Marschall, Katja ..... MM 40.7
Marschall, Paul .....•MA 7.13
Marsili, Margherita ..... DS 13.4
Marsman, Martijn HL 23.9, MA 34.13
Marszal, Philip .... •DY 51.1, SOE 6.5, •SOE 15.1, SOE 16.1
Marszalek, Tomasz .....•FM 10.4, MA 36.8, MA 39.3
Martens, Thore .....•TT 72.6
Mårtensson, Nils ..... TT 14.5
Marthaler, Michael ...MA 6.8, QI 14.4
Marthelot, Joël ..... DY 19.1
Martin, Anthony ..... QI 18.1
Martin, Carmen San ..... BP 2.4
Martin, Dennis ..... BP 14.74
Martin, Jens .....DS 20.25
Martin, Kévin ..... O 69.10
Martín Merodio, Alejandro ...•MA 3.1
Martin, Nora ..... BP 21.2, BP 21.6
Martín Salamanca, Fernando •CPP 46.10
Martina, Riccardo .....CPP 9.5
Martinek, Jan ..... O 99.4
Martinelli, Alessandro .....CPP 35.2, DY 37.2
Martinetto, Vincent .....•MM 41.4
Martinez, Biel ..... QI 2.10
Martinez de la ossa, Alberto AKBP 12.3
Martinez, Pablo ..... O 87.8
Martinez, Pablo M. .....•MM 31.2
Martínez, Patricia ..... O 67.3
Martínez-Carracedo, Gabriel MA 42.2
Martinez-Castro, Jose MA 43.3, O 3.7
Martínez-Galera, Antonio J. ..•O 33.5
Martínez-García, Andrés ...•HL 30.7, MM 40.8, •TT 59.7
Martinez-Garcia, Ricardo ...•BP 32.9, DY 22.8, •DY 52.9, SOE 4.7
Martínez-Rojas, Patricia .....•O 67.11
Martin-Fabiani, Ignacio .....DY 62.5
Martini, P. ..... TT 22.31
Martinis, John M. ..... QI 16.2
Martín-Mayor, Víctor .....DY 15.5
Martino, Francesca .....•TT 62.4
Martinuzzi, Francesco .....•DY 6.4
Martis, Joel ..... FM 15.1
Marukara, Hashima ..O 14.3, •O 38.1, O 40.20, TT 37.20
Marx, Achim ..QI 2.4, QI 14.7, QI 14.8, QI 18.2, QI 18.3
Marx, Dominik .....TT 91.4
Marx, Dorian .....•BP 7.39, DY 43.5
Marx-Glowna, Berit DS 13.2, DS 20.16
Maryshchak, Nick .....•QI 10.5
Maryshev, Ivan ..... BP 12.5
Marzari, Nicola ..... MM 8.1, MM 8.2, MM 12.2, MM 17.4, MM 17.5, MM 41.5, O 97.10
Marzouk, Mostafa .....•DS 11.8
Masa, Ilke .....•TT 23.13
Maschmann, Luis ...•O 14.11, O 38.5, O 66.5
Mascio, Paolo ..... BP 33.12
Masell, Jan .....MA 16.10, MA 33.2, MA 37.4, MA 37.6, •MA 54.1
Mas-Garcia, Josep .•O 59.3, •TT 48.3
Mashkovich, Evgeny A. ..... MA 27.5
Masilamani, Muthu .....O 80.5
Masis, Sergei ..... TT 22.16, TT 43.3, TT 43.4
Masiuta, Nazar .....•HL 9.3
Maskanaki, Katerina .....•DS 20.5
Masliuk, L. .....O 88.11
Mason, Philip ..... CPP 19.5, DY 20.5
Massee, Freek ..... MM 40.5, O 63.1, TT 55.1
Masuda, Hidetoshi MA 17.8, MA 30.1
Maßwohl, Markus .....MM 21.5
Mateo, Luis M. ..... O 83.5
Mateos, Oscar .....•O 87.8
Matera, Sebastian ..DY 6.9, DY 41.15, DY 43.4, DY 43.7, MM 31.10, O 55.5, O 81.7, O 88.3
Materne, Anne .....•BP 3.3
Materska, Joanna M. .....DY 33.2
Matestskii, Andrei ..... O 83.2
Matetskii, Andrei C. ..... O 45.9
Mathe, Julia .....•TT 17.9, •QI 4.9
Mathes, Lucian .....MM 7.7
Mathew Roy, Renjith ..... MA 7.34, MA 33.4
Mathews, Prince .....•MM 25.3
Mathey, Ludwig ..... TT 56.2
Mathias, Stefan ...MA 7.10, MA 55.6, O 14.3, O 14.10, O 19.6, O 38.1, O 40.17, O 40.18, O 40.19, O 40.20, O 40.21, O 66.9, O 98.10, TT 37.17, TT 37.18, TT 37.19, TT 37.20, TT 37.21, TT 44.9
Mathisen, Anders C. ..... •MA 24.3, •TT 36.3
Mathisen, Anders Christian ....O 2.1, O 2.5, O 76.6
Matiash, Oleksandr .....CPP 57.5
Matin Javid, Amin .....AKBP 9.3
Matković, Aleksandar ..... HL 20.17
Matsidik, Rukiya .....O 82.5
Matsumoto, Yuta ..... HL 38.4
Matsuyama, Naofumi ..... MA 9.1
Matsuzawa, Takumi ..... BP 20.6
Matta, Bharti O 62.6, •O 74.5, TT 54.6, •TT 68.5
Mattern, Maximilian .....MA 7.19, O 40.15, •O 98.3, TT 37.15
Matthäus, Franziska ..... BP 37.5
Matthäus, Lisa .....MM 33.1
Matthias, Dana ..... BP 20.6
Matthias, Rebecca .....BP 11.6
Matthies, Mailin .....MA 55.6
Matthies, Tim .... MA 7.68, MA 30.7, •MA 55.7
Mattiroli, Cesare ..... TT 22.33
Mattoso, Samuel .....•O 13.3, O 48.1
Mattoso, Samuel H. ..... O 65.7
Matukhno, N. ..... HL 54.12
Matusche, Johanna ....O 3.3, O 15.4, O 17.7, •O 99.10
Matute-Cañadas, Francisco Jesus TT 73.7
Matyšek, Richard . MA 3.3, MA 52.35
Matzdorf, René .....O 58.8, TT 61.14, TT 92.9
Mauch, Tim .....•SOE 16.4
Mauer, Alsu ..... UP 3.5
Maueröder, Christian .....BP 14.50
Maunz, Teresa M. .....•BP 14.23
Maur, Moritz ..... TT 22.18
Maurand, Romain .....QI 2.10
Maurer, Felix .....BP 14.35, BP 14.41, •BP 36.7, •DY 57.7
Maurer, Reinhard .....O 31.3, •O 86.1
Maurer, Reinhard J. ...MM 9.4, O 4.1, O 33.7, O 50.6, O 62.4, O 66.10, O 80.2, O 86.3, O 98.8, TT 54.4
Maurizot, Victor .....O 45.4
Mauro, Lorenzo .....QI 2.10
Maurya, Krishna .....QI 13.9
Maus, Holger .....DD 37.1
Mauser, Hans .....CPP 48.1
Mauz, Philipp ..... DD 30.7, DD 30.8
Mavrikakis, Manos .....O 65.10
Max, Herzog ..... MA 19.8, TT 31.8
Maximov, Leo .....MA 7.5, •MA 7.33, TT 23.3, TT 61.7
May, Falk .....CPP 48.3
Mayer, Alexandre ..... AKPIK 5.10
Mayer, Benjamin ... HL 3.11, •HL 36.1
Mayer, Thomas ..... TT 74.12
Mayr, Sina ..... MA 8.13
Mayr, Thomas .....•BP 2.2
Mayrhofer, Christian ..... TT 10.1
Mayrhofer, Leonhard .....O 31.4
Mazarov, Paul .....HL 56.2
Mazibrada, David ..•O 19.7, TT 22.22
Mazin, Igor I. ..... MA 33.10
Mazinchenko, Igor .....DS 11.8
Maznichenko, Igor .....•MA 7.57
Mazo, Juan ..... DY 62.8
Mazur, Greg ..... TT 15.3
Mazur, Michal ..... DS 11.5
Mazza, Federico ... MA 19.3, TT 31.3
Mazza, Leonardo ....TT 17.11, QI 4.11
Mazza, Marco ...•CPP 11.8, •DY 17.8
Mazzocchi, Francesco ..... FM 7.3
Mazzola, Federico .....MA 33.12
Mazzolini, P. .....O 57.6
Mazzone, D. G. .....TT 25.9
Mbognou, Florette C. F. .....MA 54.6
McCall, Patrick M. .....•BP 39.3,

•CPP 55.3
McCann, Edward .....•TT 70.4
McCauley, Mairi .....•FM 15.1
McClarty, Paul .....MA 47.4
McCluskey, Conor .....•FM 12.5
McClusky, Conor .....FM 12.6
McCord, Jeffrey .....MA 21.3
McDonald, Alexander ..... QI 17.7
McDowell, Curtis .....TT 4.6
McFarlane, Emily C. .....•O 42.9
McGraw, Joshua .....•CPP 20.4, CPP 20.9, •DY 23.4, DY 23.9
McGuinness, Philippa .....MM 40.2
McIver, James ..... O 98.5
McNeely, Paul ..... O 78.1
McNeill, Christopher R. .....HL 53.5
McQuaid, Raymond FM 11.16, FM 12.5
McRoberts, Adam . MA 23.3, TT 35.3
Mead, Monica . MM 19.45, •MM 35.4, MM 35.5
Mearini, Simone ..... O 61.1, O 69.2, O 69.6, O 83.4
Mears, Laura ... BP 14.91, MM 19.20, O 87.2
Mears, Laura L.E. .....O 87.5
Mechnich, Annika ..... FM 23.5
Mechtcherine, Viktor ..... DY 19.10
Mecke, Joscha .•CPP 28.2, •DY 29.2, DY 34.1
Meckenstock, Ralf ..... MA 50.8
Meddas, Amir .....MM 40.5
Medrano Sandonas, Leonardo BP 2.10, BP 14.63, •CPP 7.5, CPP 26.3
Meel, Hamza .....•MA 42.5
Meerovici Goryn, Alexandra ... O 17.2
Meffert, Matthias ..... FM 15.1
Mehboodi, Sina .....•MA 16.4
Mehdipour, Hamid ..... HL 47.4
Mehdizadehlima, Mahnaz .. MM 13.3
Mehlich, Kai ..... O 95.3, TT 96.3
Mehmandous, Mohammad .. TT 74.6
Mehring, Michael ..... DS 18.1
Meibohm, Jan .....•DY 27.2
Meienburg, Florian ..... UP 7.3
Meier, Andreas .....FM 7.2
Meier, Dennis DY 6.6, FM 4.6, FM 11.4, FM 11.34, FM 12.4, FM 18.7, FM 18.8, MA 37.6, MA 55.5, O 45.4, •O 81.2
Meier, Lorenz Friedrich ... •CPP 22.6
Meier, Louis .....•HL 26.24
Meier, M. ..... AKBP 1.1
Meier, Matthias ..... O 55.4
Meier, Maximilian ..... AKBP 4.4
Meier, Quintin ..... O 98.2
Meier, Thomas N.G. ..... TT 97.1
Meier, Tommy ..... HL 22.3
Meier, Torsten DY 59.8, HL 1.3, HL 1.5, TT 99.8
Meierhofer, Manuel ..... SYFC 1.1, MA 12.2, O 38.6
Meijer, Gerard ..... O 85.4
Meijer, Jan .....HL 26.32
Meijer, Yasjka ..... UP 3.1
Meindlhumer, Michael ..... MM 24.1
Meineke, Nicklas .....•QI 6.8
Meinel, Melissa Kim .....•HL 53.6
Meinert, Christina ..... O 68.2
Meinert, Helmut ..... HL 26.46
Meinert, Sophia-Marie ..... CPP 46.5
Meinhold, Tim Arniko .... •AKPIK 5.3
Meißner, Moritz ....HL 40.2, HL 40.6, •HL 46.6
Meissner, Moritz ..... HL 35.1
Meissner-Oszer, Laura ..... DY 34.4, •DY 34.5
Meister, Michael ..... DS 14.9
Meitzner, Josephine ..... BP 14.54, BP 18.2
Meixner, Michael ... TT 13.4, •TT 13.7
Mejuto-Zaera, Carlos ..... HL 35.2, TT 13.2, TT 13.8
Melalkia, Mohamed Fauzi .... QI 18.1
Melchioni, Nicola ..... O 57.3
Melde, Kai ..... CPP 46.20
Meledam, Geethu P. ..... CPP 46.31
Meléndez Sans, Anna .....•HL 42.4
Meléndez-Sans, Anna ..... TT 25.2
Melis, Gianfranco .....•CPP 12.3
Melix, Patrick ..... O 11.8
Melles, Jannis ..... DY 49.10
Melles, Jannis Michael .....•DY 27.3
Melnikov, Alexey ..... DS 20.37
Melson, Tobias .....MM 19.12
Meltschoch, Mona .....•CPP 5.5
Memon, Ayaz Ali .....FM 2.6
Menacho, Willy .....BP 18.6
Mena-Osteritz, Elena .....HL 46.3
Mendes da Silva, Rita ..... BP 14.30
Mendl, Christian B. .....QI 5.8
Mendoza Sosa, Alan Rodrigo DY 47.3
Mendozza, Raffaele BP 7.18, BP 7.39, •DY 44.17
Meneghini, Giuseppe ..... O 98.10
Menei, Tom .....•TT 61.9, TT 83.4
Meng, Kuan .....•CPP 15.5
Meng, Sheng ..... O 12.3
Meng, Xiangzhi .....O 83.8
Mengel, Lucia .....•O 65.6, O 94.10
Menges, Fabian ..... O 43.5
Menguelti, Kevin ..... HL 31.5
Menke, Henri ..... O 71.13, O 84.3, TT 66.13, TT 84.3
Menon, Sarath .... MM 5.5, •MM 5.7, MM 7.2
Mense, Cornelis .....•DY 49.6
Menteş, Tevfik Onur . O 10.3, O 88.10, TT 16.3
Mentink, Johan .. •SYBT 1.1, MA 27.6
Mentink, Johan H. .....MA 55.2
Menzel, Andreas .....CPP 12.2
Menzel, Andreas M. ..... BP 16.7, CPP 20.8, •CPP 42.6, DY 23.8, MM 3.3
Menzel, D. ..... MA 7.21
Menzel, Dirk .....TT 23.1, TT 57.2, TT 57.3, TT 81.5
Menzel, Ferdinand .....O 38.4
Menzler, Heiko Georg ..... •TT 44.3
Meraldi, Patrick ..... BP 2.3
Merboldt, Marco ....O 14.10, O 40.18, O 40.19, O 40.21, O 66.9, O 98.10, TT 37.18, TT 37.19, TT 37.21, TT 44.9
Mercadier, Laurent ..... MA 42.3
Mercebach, Phillip .....•TT 42.11
Mercurio, G. ..... MA 7.14
Merdon, Christian ....HL 38.9, O 81.7
Meretska, Maryna L. ..... BP 14.38
Merger, Claudia ..•DY 58.7, •SOE 17.7
Merkel, Konrad .....HL 40.3
Merkel, Konrand .....CPP 40.3
Merkel, Milena ... •CPP 17.21, O 72.3, TT 67.3
Merkel, Rudolf ..... BP 40.1
Merkoulidi, Eleftheria .....•DS 16.9
Merkwitz, Luise .....•DS 20.28
Merle, Benoit ..... MM 32.6
Merritt, Adrian .....•TT 95.2
Merschjann, Christoph ..... •HL 23.4
Merstorf, Marc ..... TT 71.6
Mert Iyiisler, Harun ..... MA 27.10
Mertelj, Tomaz ..... O 64.4
Merten, Pascal .....CPP 17.6
Mertig, Ingrid .... MA 29.5, MA 38.11, MA 38.12, MA 51.3, MA 54.9, MA 55.1, TT 46.5, TT 88.3
Mertsch, Philipp .....DD 10.1
Merzoni, Giacomo .....O 67.10
Mesaros, Andrej .....DS 12.4
Meseck, Atoosa .....AKBP 8.2
Mesple, Florie ..... O 62.2, TT 54.2
Messmer, Thomas .....•DY 8.4
Mester, Lars .....•HL 10.3, •TT 20.3
Metelmann, Anja ..... QI 11.2, QI 17.3
Meth, Michael ..... QI 15.2
Metje, Josefin .....•DD 30.4
Metson, Jakob .....•DY 27.6
Metternich, Daniel .MA 7.67, MA 37.8
Mettler, Jens ..... MA 3.7
Mettus, Denis ..... MA 37.7, MA 46.2
Metuh, Pietro ..... HL 54.6
Metz, Volker ..... MM 36.4
Metzen, Christian .....CPP 58.6
Metzkes-Ng, Josefine ..... AKBP 7.5
Metzler, Markus .....BP 7.44
Metzler, Ralf ..... O 44.12, SOE 12.1
Metzner, Walter ..... TT 94.1
Mewes, Jan-Michael ..... HL 26.16
Mey, Oliver .....AKPIK 3.3
Meyberg, Ellen .....•DY 43.11
Meyer, Bernd ...•MM 19.6, MM 19.10, O 94.5
Meyer, Carola .....BP 20.9
Meyer, Dirk C. ... CPP 16.3, CPP 16.6, CPP 17.36, CPP 17.39, FM 12.8, FM 23.6
Meyer, Hendrik .....•CPP 56.3
Meyer, Jannik C. .....CPP 26.2
Meyer, Julia S. .....•TT 50.1
Meyer, Lorenz .....•O 61.9
Meyer, Manuel ..... HL 29.5, TT 58.5
Meyer, Marcel .....QI 16.1
Meyer, Maximilian Tim ....•HL 26.38
Meyer, Nathan .....BP 41.1
Meyer, Nina ..... MA 39.7
Meyer, Noah .....O 84.8, TT 84.8
Meyer, Ralf ..... MM 19.39
Meyer, Ruth .....BP 7.14, BP 40.1
Meyer, Sabrina ... •HL 30.4, •TT 59.4
Meyer, Tobias ..... DS 16.10, O 40.21, TT 37.21
Meyer zu Heringdorf, Frank .. O 26.4, O 96.2, TT 6.6
Meyer zu Heringdorf, Frank-J. O 10.10, TT 16.10
Meyer zu Heringdorf, Frank-Joachim O 33.6, O 72.1, TT 67.1
Meyerbröker, Nikolaus ..... CPP 3.4
Meynard, Adrien .....DY 21.2
Mezger, Florian ..... TT 43.2
Mezger, Lara ..... O 89.5
Mezger, Markus .. CPP 23.6, DY 24.6
Miao, Bing .....BP 31.1, CPP 50.1
Miao, Guangyao O 7.6, O 10.5, O 59.1, •O 62.8, TT 9.6, TT 16.5, TT 48.1, •TT 54.8
Miao, Tingwen .....•O 44.10
Michael, Liron B. .....DS 20.30
Michael, Marios .... TT 4.12, •TT 71.3
Michaela, Arnold ..... AKBP 14.1
Michaela Braun, Franziska . DY 44.14
Michaelis de Vasconcellos, Steffen CPP 17.46, FM 15.2, MA 9.13, MA 12.1, MA 52.5
Michałek, Grzegorz .....•TT 90.4
Michalicek, Gregor .MA 16.12, O 37.3, O 50.1, O 71.6, TT 66.6
Michel, Thomas ...•DY 13.6, •TT 19.6
Michele Guerrini, Michele ..... HL 1.8
Michels, Andreas ...MA 7.4, MA 37.1, MA 46.1
Michels, Jasper .CPP 17.4, •CPP 38.3
Michelsen, Mona B. ..... •BP 14.19
Michely, Thomas ..... O 7.6, •O 10.1, O 10.5, O 10.8, O 15.4, O 17.7, O 17.12, O 59.1, O 62.8, O 64.3, O 72.1, O 89.8, O 99.10, TT 9.6, •TT 16.1, TT 16.5, TT 16.8, TT 48.1, TT 54.8, TT 67.1
Michen, Benjamin .....•TT 83.7
Michez, Lisa .....MA 7.52
Michl, Johannes ..... HL 34.2
Michler, P. .....HL 55.9
Michler, Peter ... HL 20.37, HL 20.38, HL 20.42, HL 31.4, HL 34.1, HL 34.2, HL 34.4, HL 34.5, QI 18.6
Michlíková, Soňa ... BP 33.5, BP 33.6
Michon, Adrien ..... O 62.3, TT 54.3
Michon, Bastien .....•MM 40.5
Mickiewicz, Konrad ...QI 9.5, •QI 17.4
Micklitz, Tobias ..... DY 13.9, TT 19.9
Miclot, Tom ..... BP 15.3
Micoloi, Magdalena ..... DD 14.1
Mier, Christina ..... O 17.2
Mietke, Alexander .....DY 34.6
Mignani, Niccolò ..... TT 49.7
Mihailova, Boriana ..... FM 4.4
Miháliková, Ivana .•TT 17.10, •QI 4.10
Mihatsch, Jakob .....•BP 16.7
Mihlan, Levin .....•MM 14.2
Mihm, Maximilian ..... MA 52.33
Mijowska, Ewa ..... MM 19.13
Mikadze, Luca ... MA 14.3, MA 40.10
Mikhailau, Uladzislau .....•O 93.5
Mikhalev, Daniil .....•DY 19.10
Mikosch, Jochen ..MA 39.22, O 70.4, O 70.5, TT 65.4, TT 65.5
Mikuni, Kouki .....MA 45.2
Milchev, Andrey ..... CPP 56.4
Miler, Lena .....HL 26.37
Miles, Adam C. .....FM 2.1
Miles, Sebastian .... HL 17.4, TT 15.3
Milewska, Anna .....CPP 16.4
Milinkovitch, Michel ..... •BP 3.1
Milivojević, Marko ..... DS 12.7
Millard, Toby ..... O 96.10
Millek, Vojtech .....DS 13.1
Miller, Cornelius .....•BP 15.10
Miller, Morgan .....BP 16.9
Milles, Sigrid .....•BP 14.55, BP 18.3, BP 20.7
Millis, Andrew J. .....TT 12.7
Milosevic, Nikola ..... DY 14.7
Mimani, Krishnam .....•TT 22.22
Min, Chul Hee ..... O 2.1, O 2.5
Min, Chul-Hee ..... MA 24.3, O 76.6, •TT 25.11, TT 36.3
Minakova, Olga .... •MA 25.3, O 49.2
Minár, J. ..... O 93.9
Minar, Jan HL 1.10, MA 13.6, MA 17.1, MA 35.7, O 2.4, O 21.2, •O 67.1, O 67.6, O 76.2, O 93.6, TT 60.7, TT 62.11
Minkov, Vasily .....•TT 80.4
Minoguchi, Yuri .....QI 13.8
Minola, Matteo .... MA 48.5, TT 39.6, TT 39.7
Minotakis, Michail ..... •MM 22.2
Mir, Mashood Tariq MA 39.22, O 70.4, O 70.5, TT 65.4, TT 65.5
Mir, Showkat H. .....CPP 17.47
Miranda, Henrique ..... HL 23.9
Mirasso, Claudio .....SOE 10.2
Mirau, Luca .... •CPP 26.4, CPP 49.5
Mirelmi, Pouria .....•SOE 5.3
Mirian, Najmeh .....AKBP 8.2
Mirkes, Holger ..... TT 74.4
Mirlin, Alexander D. ..... QI 21.6
Miroshkina, Olga . •MA 13.2, MA 13.5
Mirzajani, Nasim .... •O 61.3, O 95.5, TT 96.5
Misbah, Chaouqi .....BP 27.5
Mischke, Maximilian .....•DS 14.6
Mischke, V. ..... O 85.2
Mischo, Johannes ..... •BP 7.41
Mischok, Andreas . BP 14.39, HL 15.3
Mishra, Ashutosh ..... QI 13.6
Mishra, Monalisa ..... BP 14.49
Mishra, Prabuddha Kant ....MA 7.26, TT 41.7
Mishra, Priya ..... TT 64.3, TT 93.16
Mishra, Priyanka ... MA 44.7, TT 76.7
Mishra, S .....MA 19.7, TT 31.7
Mishra, Seemant ..... •DY 61.5
Mishra, Soumitree . BP 1.11, CPP 1.11, DY 4.11
Mishra, Swarnamayee .....•TT 4.8, TT 5.7, TT 61.5, TT 62.6
Mishra, Ujjval ..... •MA 39.20
Mishra, Vipin ..... CPP 17.47
Misios, Stergios .....UP 5.2
Misra, Abhishek ..... HL 20.28
Missaoui, Ghada .... O 52.2, •O 52.5, O 55.2
Misselwitz, Adrian Paul ....•TT 43.11
Misselwitz, Erik ..... O 46.3
Missirlis, Dimitris .....•BP 30.2, CPP 46.20, •CPP 47.2
Mistonov, Alexander .. TT 4.8, TT 5.7, •TT 62.6
Mitchell, Andrew ..... TT 90.5
Mitchell, Polly ..... •MA 6.4
Mitra, Arkadeep ...•DY 13.5, •TT 19.5
Mitra, Asimpunya .....TT 57.11
Mitra, Debarshi .....•BP 2.1
Mitra, Gautam ..... TT 90.6
Mitra, Souvik .....•FM 2.4
Mitra, Subhankur ..... CPP 7.2
Mitrenga, Dennis ..... DS 20.49
Mitscherling, Johannes ... •MA 29.7, MA 33.13, TT 41.3, •TT 46.7
mitsuishi, natsuki .... O 95.7, O 95.9, TT 96.7, TT 96.9
Mitsumata, Chiharu .....AKPIK 5.6
Mittag, Tanja ..... BP 39.1, CPP 55.1
Mittal, Rohan .....•DY 9.8
Mittelberger, Andreas ..... FM 15.1
Mittendorfer, Florian ... O 5.6, O 55.4, O 80.1
Mittendorff, Martin •HL 52.2, HL 52.3, HL 52.4
Mittenzwey, Henry HL 20.3, HL 20.15, HL 26.48
Mittermair, Gabriel ..... HL 13.2
Mittmann, Maarten .....•HL 22.2
Miwa, Jill A. ..... MA 33.12, O 95.11, TT 96.11
Miyagawa, Takeru ..... MM 12.6, •MM 22.8
Miyamachi, Toshio ..... O 48.3
Miyar, Rebeca .....•FM 2.1
Mizani, Sakineh .....•DY 47.4
Mizuguchi, Masaki ..... O 48.3
Mlkvik, Peter .....FM 7.7
Mo, Shu ..... O 76.7
Moca, Cătălin P. ..... TT 41.9
Moca, Catalin Pascu .....DY 46.10, TT 75.10, QI 21.9
Moca, Pascu ..... TT 17.7, QI 4.7
Mocatti, Stefano ..... HL 46.7
Mocatti, Stefono ..... HL 8.2
Möckl, Leonhard ..... BP 7.50
Mockute, Aurelija ..... FM 6.8
Modak, Ishita ..... •DY 13.3, •TT 19.3
Modak, Ranjan .....DY 47.8

Moderer, Tim ..... BP 20.3
Modes, Carl .....BP 12.9, BP 14.49, BP 14.52, DY 51.5, SOE 15.5
Modes, Carl D. ..... BP 3.3
Modregger, Peter .BP 14.44, •FM 19.2
Moebus, Finn .....HL 17.5
Moessner, Roderich •PRV IV, DY 13.7, DY 53.3, MA 31.12, TT 19.7, TT 40.1, TT 44.7, TT 47.12, TT 57.7, TT 79.4, TT 86.1, TT 86.2, TT 86.6, TT 87.3, TT 98.7
Moghadas, Emin .....TT 62.8
Moghaddam, Ali .....FM 22.6
Mogharehabed, Negin ..... •HL 12.4, HL 26.11
Mognetti, Bortolo Matteo ... BP 36.6, DY 57.6
Mohamed, Ahmed .....CPP 17.16, •CPP 25.2
Mohamed, Hamza .....•CPP 2.4, •SOE 3.4, •UP 1.4
Mohamed, Shaimaa El-saied . BP 7.2
Mohamed, Zakaria ..... TT 22.17
Mohammad, Amir .....CPP 16.3, CPP 16.6, CPP 17.39
Mohammad, Sajjan .....O 35.1
Mohammadi, Mahdieh ..... •DY 25.3
Mohammadian, Mahsa ....•BP 14.26
Mohammed, Hussen Oumer •CPP 13.4
Mohanakumar, Shilpa ..... O 36.4
Mohanty, Smruti ... O 10.10, TT 16.10
Mohanty, Smruti Ranjan .....•O 33.6, O 72.1, TT 67.1
Mohapatra, Sumit .. HL 15.3, •HL 15.7
Moharana, Ashish ..... MA 29.2, •MA 36.8, MA 36.9, MA 39.3, O 61.8, TT 46.2
Mohelsky, Ivan .....MA 23.2, TT 35.2
Mohite, Atul Tanaji ..... •DY 21.3
Mohr, B. ..... AKPIK 6.5
Mohr, Bernadette ..... MM 22.3
Mohr, Jan-Niklas ...•O 72.6, •TT 67.6
Mohrhusen, Lars .....•O 81.5
Mohylna, Mariia ..... MA 34.1
Moitra, Saranyo .... TT 72.2, TT 83.5, •TT 83.11
Moitzi, Franco ... MM 21.4, •MM 41.6
Mokbel, Dominic ..... BP 37.3
Mokrousov, Yuriy .. MA 5.8, MA 20.5, MA 29.4, MA 29.9, MA 29.10, MA 39.1, MA 51.4, MA 51.7, TT 7.8, TT 46.4, TT 46.9, TT 46.10, TT 88.4, TT 88.7
Moldovan, Grigore ..... FM 19.1
Molenda, Janina .....CPP 16.4
Molina, Rafael A. ..... TT 15.8
Molina-Luna, Leopoldo .....DS 7.5, MA 50.4, MA 50.5
Molinari, Elisa .....TT 10.6
Molinaro Guerra, Beatriz ... CPP 37.5
Molina-Sánchez, Alejandro ...HL 8.3, MA 7.31, •O 7.2, O 59.3, O 71.2, •TT 9.2, TT 48.3, TT 66.2
Molkenthin, Nora .....•SOE 6.6
Moll, Alexander .....HL 26.46
Moll, Philip .TT 17.2, TT 57.7, TT 97.5, QI 4.2
Mölleken, Andre .....•O 19.4, O 19.5
Mollenhauer, Doreen ... O 3.1, O 58.1, O 69.7
Möller, Angela .....MA 40.8
Möller, Anna ..... BP 14.50
Möller, Christian .....HL 31.3
Möller, Johannes .. O 40.15, TT 37.15
Möller, Jonathan ..... DD 18.1
Möller, Lea ..... BP 37.5
Möller, Marius .....•TT 33.2
Möller, Milan ..... O 45.6
Möller, Rolf .....O 19.4, O 19.5
Möller, Samuel ..... HL 10.3, TT 20.3
Möllers, Paul valerian O 42.8, •O 93.4
Molnár, András .....QI 1.2
Molter, Daniel .... HL 52.5, AKPIK 5.3
Momeni, Narges ..... TT 73.7
Monaico, Eduard HL 20.23, HL 20.24, •HL 26.10
Monaico, Elena ..... HL 26.10
Monchietti, Elisa ...•QI 14.28, QI 15.9
Monclús, Miguel A. ..... MM 36.5
Mondal, Debashish .....•TT 43.12
Mondal, Priyanka . HL 20.13, HL 39.5, HL 39.7, •HL 39.11
Mondal, Ritwik .... MA 12.3, MA 45.2
Mondal, Suchanda ..... TT 79.5
Mondal, Suman ..... TT 44.3
Mondal, Vivek .....O 71.18, TT 66.18
Monfared, Mohammad .....HL 35.6
Mönig, Harry ..... CPP 17.21, O 23.1, O 72.3, TT 67.3
Monje, Viviana .....CPP 41.2
Monney, Claude ..... O 67.6
Mönnich, Marco ..... O 43.11
Monroy-Villa, Ricardo .....AKBP 9.1, •AKBP 14.3
Montalvo, Galia ..... BP 40.2
Montemore, Matthew M. ..... O 81.2
Montenegro-Pohlhammer, Nicolas O 9.4
Montes, Luis ..... O 44.11
Montoto, Ana Vera ...O 59.7, TT 48.7
Montoya-Soto, G. ...BP 27.8, BP 37.2
Monz, Thomas .....QI 16.1
Moody, Meghan .....•TT 93.17
Moody, S. ..... TT 25.9
Mook, Alexander .•SYQF 1.2, MA 2.3, MA 2.4, MA 2.5, MA 2.7, MA 9.7, MA 12.3, MA 39.23, •MA 40.6, TT 79.1
Moon, Seawoo ...•O 71.10, •TT 66.10
Moorlag, Martijn ..... BP 14.38
Moortgat-Pick, Gudrid .... AKBP 13.2
Moos, Aaron ..... O 96.11
Moos, Eduard .....•O 66.4
Moos, Katja Sophia .....•MA 38.13
Mooshammer, Fabian HL 8.1, HL 39.8
Mora, Thierry ..... BP 32.5, DY 52.5, •SOE 2.1
Moradimehr, Shiva CPP 10.2, DY 16.2
Morales, A. ..... TT 24.7
Morales, Andrea .... MA 6.2, MA 6.9, DD 7.2
Morales, Carlos .....DS 9.4, DS 11.5, O 23.3, •O 88.7, O 96.6
Morales Cocera, Miguel ..... •HL 3.4
Morales, Miguel ..... TT 27.2
Morales, Siddhartha .....DY 28.2
Morales-Fernández, Pamela MA 7.79
Morando, Vincent ..... TT 94.3
Morawe, Elise .....•HL 26.20
Morawski, Irek ..... O 41.4, TT 38.4
Morawski, Ireneusz .....O 54.3
Mørch Nielsen, Carl Emil ..... HL 3.4, HL 13.6
More-Chevalier, Joris .....DS 7.5
Morée, Jean-Baptiste .....•TT 56.10
Moreira, José .....O 26.1
Moreno, Luis .....FM 18.6
Moresco, Francesca .... O 6.2, O 6.5, •O 45.5, O 58.4
Morgenstern, Karina MM 11.3, O 16.2
Morgenstern, Markus ..... HL 20.40, O 44.8
Morhbach, Hevré .....BP 12.2
Morhusen, Lars ..... O 34.5
Morice, Corentin TT 23.34, •TT 74.10, TT 83.13
Morigi, Giovanna .....DY 49.10
Morimoto, Takahiro ..... TT 44.1
Morin, Mathieu ..... O 56.6
Moritz, Susanne .....•HL 1.7
Morosan, Emilia ...MA 16.1, MA 19.7, TT 31.7
Morpurgo, Alberto .....MA 49.2
Morral-Yepes, Raúl ... QI 1.9, •QI 15.6
Morrow, Ryan .....MA 7.28, MA 19.5, TT 31.5
Mors, Dennis Heinz Bruno •HL 20.58
Mors, Mira .....•CPP 14.7
Mortada, Hanadi ..... MA 9.3
Mortazavi, Bohayra .....CPP 26.3
Mortensen, Anders ..... O 66.8
Mortensen, Anders S. ..... O 76.5
Mortensen, Anders Sandermann •O 85.3
Mortezapour, Behzad .....O 45.7
Morvan, Tangi .....TT 17.11, QI 4.11
Moseler, Michael ..... O 31.4
Moser, S. ..... O 85.2
Moser, Simon .....DS 14.3, DS 20.43, O 63.8, O 74.4, TT 5.6, TT 55.8, TT 68.4
Möseritz-Schmidt, Jan .... •DY 42.11, DY 59.2, •TT 63.11, TT 99.2
Moshnyaga, Vasily .....DS 16.10
Mosina, Kseniia . HL 20.13, HL 20.22, HL 39.5, HL 39.7, HL 39.8, HL 39.11, O 38.4
Moske, Leonhard ..... •QI 9.4
Mosko, Timon .....•DS 14.2
Moskorz, Wiebke ..... BP 14.56
Mößle, Michael ..... PSV IV
Moss, Megan Schuyler .....DY 58.1, SOE 17.1
Mossa, Alessandro .....CPP 29.6
Mostarac, Deniz .....CPP 20.7, •CPP 24.3, DY 23.7
Mostofi, Arash ....CPP 46.61, O 50.7, O 71.7, TT 66.7
Mostofi, Arash A. .. O 95.10, TT 96.10
Mostovoy, Maxim ... MA 4.5, MA 4.6, MA 16.2, MA 17.2, MA 29.11, TT 46.11
Mothe, Raphaël ..... QI 15.9
Mothes, Nico .....DS 21.4
Moth-Poulsen, Kasper .....O 35.2
Motome, Yukitoshi .....MA 8.1
Motrunich, Olexei ... DY 13.8, TT 19.8
Motrunich, Olexei I. . DY 32.8, TT 45.8
Mottamchetty, Venkatesh ...MA 12.6
Motti, Federico .....O 38.2
Möttönen, Nea B. . BP 26.5, CPP 43.5
Motzny, Kathrin .....BP 18.3, BP 20.7
Motzoi, Felix ....QI 8.2, QI 8.5, QI 8.6, •QI 11.3, QI 13.7, QI 13.10, QI 16.5, QI 17.6
Mou, Lizhong ..... •BP 14.45
Moudgalya, Sanjay . DY 13.8, DY 32.8, TT 19.8, TT 45.8, TT 53.3
Mouhoub, Asma .....MA 9.3
Moulding, Owen .....TT 80.3
Mounir, Muhammad .....BP 26.2, CPP 43.2
Mousa, Marwan .....MM 16.5
Moussa, Tarek .....MA 9.5
Moya, Jaime .....MA 16.1
Moynihan, Eoin ..... FM 12.3
Mozo, Edwin .....DS 1.1
Mozumber, Rubel ..... MM 22.3
Mráz, Stanislav .....DS 7.5
Mrenca- Kolasinska, Alina .... DS 8.3
Mrenca-Kolasinska, Alina ....•TT 4.6
Mrezguia, Hela ..... O 67.4
Mrovec, Matous .... MM 3.8, MM 9.1
Mrowiński, Paweł .....HL 20.34
Mrudul, MS ..... MA 14.3, MA 40.10
Mu, Guannan .....•MA 49.5
Much, Alexander .....•CPP 59.2, CPP 59.6, MA 39.15
Mudassar, Javed ..... DY 41.15
Muehlebach, Michael ..... SOE 4.5
Mueller, F ..... BP 37.2
Mueller, Lukas ..... AKPIK 4.2
mueller, melanie .....O 43.12
Mueller, N. S. ..... O 57.6
Mueller, Niclas S. ..... O 95.5, O 96.8, TT 96.5
Muenker, Till .....BP 7.25, BP 37.1
Muenzenberg, Markus .....MA 39.7
Mugele, Frieder ... CPP 17.49, O 36.4
Mühl, Thomas .....MA 6.3
Muhler, Martin .....MA 36.1
Mühlhauser, Matthias .....TT 23.5, TT 70.1
Mühlpointner, Morris E. L. .... O 46.5, •O 46.6
Mühlschlegel, Lena ..... •BP 14.53
Muhr, Andreas .....MM 19.20
Mukatayev, Iskander ..... •MM 41.9
Mukenhirn, Markus ..... BP 27.10
Mukharjee, Prashanta .....TT 72.6, TT 72.7
Mukherjee, Anamitra TT 25.1, TT 86.5
Mukherjee, Pratyay ..... MA 45.2
Mukherjee, Shantanu ..... TT 29.9
Mukherjee, Tania ... •O 38.7, O 71.10, TT 66.10
Mukhin, Alexander A ..... MA 17.11
Mukhina, Anna .... BP 7.49, •BP 37.1
Mukhopadhyay, Aritra ..... DY 14.6
Mukhopadhyay, Aritra K. ..•CPP 28.1, CPP 28.3, •DY 29.1, DY 29.3, DY 44.3, DY 62.2
Mukhopadhyay, Soham .....•BP 14.7
Mulder, Menno .... DY 45.3, SOE 14.3
Müllen, Klaus ..... MA 5.9, TT 7.9
Müller, Anke-Susanne ..... AKBP 4.2, AKBP 7.1
Müller, Arnold ..... O 96.12
Muller, C. ..... MA 47.7
Muller, David A. ..... TT 43.8
Müller, F. ..... BP 27.8
Müller, Fabio .....CPP 38.6, DY 43.12
Müller, Fabio A. .... •O 40.2, •TT 37.2
Müller, Felix ..... •O 42.2
Müller, Frank ..... O 54.1
Müller, Heiko ..... O 65.4, DD 42.1
Müller, Jens ..... MA 7.70, TT 23.17, TT 42.6, TT 62.2, TT 62.3
Müller, Jonas Maximilian •AKPIK 5.9
Müller, Judith ..... BP 26.3, CPP 43.3
Müller, Kai .....•O 57.7
Müller, Katharina ..... •MA 30.5
Müller, Klaus-Robert ..... O 61.10
Müller, Leon .....•MM 19.14
Müller, Louis ..... •O 42.7
Müller, Lukas .....AKBP 13.2
Müller, M. ..... DS 3.4
Müller, Mahni ..... HL 23.6
Muller, Marcus ..... BP 16.8, CPP 3.2, CPP 20.1, CPP 21.3, DY 23.1, DY 60.7
Müller, Markus ..... QI 16.1
Müller, Martin .....•CPP 13.6
Müller, Martina .....FM 4.2, •FM 17.1, FM 23.4, O 19.2, O 93.2, QI 6.5, QI 14.23
Müller, Matthias .....QI 10.6, •QI 13.2
Müller, Maximilian ..... AKBP 6.1
Müller, Melanie O 22.1, O 43.4, O 43.8, O 43.10, O 66.3
Müller, Michael ..... CPP 46.19
Müller, Niclas S. ..... O 98.7
Müller, Rainer ..... DD 30.1, DD 30.10
Müller, Rolf .....UP 5.3
müller, simon .....TT 25.11
Müller, Thomas ..... CPP 46.37
Müller, Thorge ..... QI 3.6
Müller, Tim .....MA 7.1
Müller, Tobias ... •BP 26.8, BP 26.10, •CPP 43.8, CPP 43.10
Müller, Toni .....CPP 54.4
Müller, Verena ..... MM 14.2, •O 54.7
Müller-Bender, David .....•DY 41.7, DY 43.23
Müller-Buschbaum, Peter ... •PLV IX, CPP 4.2, CPP 4.6, CPP 12.4, CPP 15.1, CPP 16.2, CPP 17.5, CPP 17.15, CPP 17.18, CPP 17.26, CPP 17.27, CPP 17.28, CPP 17.29, CPP 17.31, CPP 17.32, CPP 17.33, CPP 17.37, CPP 17.42, CPP 25.4, CPP 31.4, CPP 44.2, CPP 44.3, CPP 44.5, CPP 46.17, CPP 46.48, CPP 46.51, CPP 48.2, CPP 53.2, CPP 53.6, CPP 57.5, CPP 58.2, CPP 59.3, FM 11.5, MM 19.16
Müller-Schüssele, Stefanie .. TT 24.3
Mummadavarapu, Ram .... •TT 83.8
Mun, B. S. ..... O 85.2
Munawar, Muhammad .....•O 11.3
Münch, Alexander ..... CPP 13.6
Münch, Alexander S. ..... CPP 12.1
Münch, Lukas .. •TT 22.20, TT 22.21, TT 22.22, TT 28.2
Mundy, Julia A. ..... MA 27.7
munir, Akhtar .....BP 14.13
Münker, Till ..... BP 7.49, DY 43.5
Münker, Till Moritz . BP 7.30, BP 7.31, BP 7.39
Munkhbat, Battulga ..... HL 54.6
Munne, Sophia ..... O 76.1
Munnik, Frans .....FM 11.24, HL 42.5
Münning, Felix .....O 63.9, TT 55.9
Muñoz, Christian ..... •DY 43.5
Munoz, Gustavo Gabriel Moya BP 20.8
Muñoz-Arias, Manuel ..... QI 16.10
Münster, Florian ..... O 68.1
Münster, Lambert ..... •DY 15.4
Münster, Lasse ..... O 38.6
Munteanu, Valentin ..... DS 21.4, AKPIK 6.6
Münz, Kilian .....•TT 62.9
Münzenberg, Markus .....MA 21.3, MA 39.12, MA 54.11
Muradov, Mustafa .....FM 11.1
muramatsu, haruki .•O 95.7, •TT 96.7
Muras, Laura .....BP 12.2
Murat, Kamila .....•FM 11.26
Muravev, Viacheslav HL 10.5, TT 20.5
Murawski, Caroline •HL 2.5, •HL 15.9, HL 20.48, HL 20.57, HL 22.6, HL 26.18
Murayama, Kantaro .....FM 22.9
Murcek, Petr ..... AKBP 2.2
Murdin, Ben N. ..... HL 11.6
Mureşan, Alex ..... DS 18.7
Murillo Vilella, Elena ..... BP 11.6
Murphy, Bridget ..... CPP 46.4
Murphy, Bridget M. CPP 19.4, DY 20.4
Murray, Sean ..... BP 14.51
Mursalin, Mubarrat .....•CPP 17.3
Murta, Bruno .....•QI 1.10
Murugan, Arvind ... BP 32.5, DY 52.5
Musacchio, Marco .....•CPP 11.5,

•DY 17.5
Musiał, Anna ..... HL 20.34
Musiienko, Artem ..... HL 4.7
Musiol, Lukas ... •MM 14.4, MM 14.4
Musta, Alexander ... HL 3.9, HL 18.8, TT 32.8
Mustafa, Luqman ..... FM 6.8
Muth, Dominik .... HL 20.20, HL 45.8
Mutlay, Zehra Gizem .... •CPP 46.62, FM 19.3
MUTLU, Saliha . •CPP 17.30, FM 19.6, MM 16.4
Mütschele, Jeremias ..... •MA 39.24
Mutschler, Thomas ..... MA 7.68
Mutter, Daniel ..... •MM 8.3
Mygind, Jon Bjarke Valbaek .. O 97.9
Myin, Charlotte •CPP 11.10, •DY 17.10
Mysliveček, Josef .. •O 13.12, O 65.12
N. Anisimov, Andrey ..... HL 11.7
N. Gastiasoro, Maria ..... TT 14.10
N M, Anjan ..... TT 74.6
N, N .....•AKBP 15.2, •AKBP 15.3
Naber, Nicole ..... MA 47.1
Nacci, Christophe .... O 69.12, O 73.6
Nachtnebel, Kara .....•BP 14.50
Nadas, Rafael ..... HL 47.2, O 95.2, TT 96.2
Nádasi, H. ..... MA 36.3
Nadazdy, Vojtech ..... CPP 57.5
Nadler, Elke ..... HL 4.1
Naduvile Thadathil, S. ..... TT 29.1
Naduvile Thadathil, Sajal ...•MA 47.7
Naeimi, Moha ..... O 27.2, •O 46.9
Naert, Antoine .....•DY 21.2
Nag, Shankha .... MM 5.5, •MM 34.7
Naga, Abhinav ..... CPP 5.1, CPP 8.1
Nagaosa, Naoto ... MA 16.2, MA 16.6
Nagashima, Raigo .....•TT 95.4
Nagel, Katrin .....•DD 33.1
Nagel, Sören ..... •SOE 8.3, SOE 9.1
Nägele, Maximilian .....•AKPIK 3.1
Nähle, Ole ..... TT 82.3
Naidyuk, Yurii ..... TT 93.3
Naimer, Thomas .....•DS 12.2
Nair, Akhil S. ..... MM 13.6
Nair, Nisanth N. ..... MM 19.6
Nair, Rakesh ..... BP 41.2, CPP 38.5
Nair, Rakesh R. ..... HL 22.5
Najafishirtari, Sharif ..... O 34.8
Nakajima, Makoto ..... MA 38.8
Nakamura, Atsutomo ..... MM 23.3
Nakamura, Junji ..... O 61.11
nakamura, yuiga ..... O 95.9, TT 96.9
Nakanishi, Takeshi .....•HL 3.12
Nakano, Akitoshi .. FM 9.2, •FM 22.3, FM 22.8
Nakatsuji, Satoru ..... TT 41.4
nakazawa, ryotaro .....•O 67.7
Nakerst, Goran .....•JOB 2.1
Nakhaie, Siamak ..... AKjDPG 1.1, •AKjDPG 1.2
Nam, Kyeonghyeon .....•O 88.11
Nam, Shinjae .. O 3.5, O 17.4, •O 56.2, O 77.6
Nambisan, Ameya ..... TT 14.2
Namisi, Mwanaidi Mauwa ...•FM 4.8
Namy, Olivier ..... BP 9.2
Nan, Lin ..... O 57.3
Nandakumar, Nirbhika .... •HL 20.57
Nandakumar, Shweta ..... BP 40.2
Nandi, Saikat ..... MA 31.7, TT 47.7
Nandi, Sunny .....•FM 5.9
Nandy, Ashis Kumar ..... TT 25.1
Nandy, Snehasish . •MA 2.2, TT 92.11
Nandy, Sourav ..... DY 46.4, TT 75.4
Nandy, Subhajit ..... MA 39.18
Naralapura Manohara, Anjan Kumar •TT 49.5
Naraschkewitz-Epp, Dennis AKBP 9.6
Narasimhan, Shobhana .... MA 51.4, TT 88.4
Narayanan, Rajesh .. DY 13.3, TT 19.3
Nardin, Alberto ..... TT 17.11, QI 4.11
Nardini, Cesare ..... DY 15.7, DY 43.1
Narducci, Alessandra ..... BP 20.8
Narita, Akimitsu ..... MA 5.9, TT 7.9
Naritsuka, Masahiro .. O 80.3, O 95.9, TT 96.9
Narkowicz, Ryszard MA 44.8, TT 76.8
Nascimento, Von Braun ..... MA 4.1
Naseeb, Noor ..... BP 14.77
naskar, moumita ..... •TT 72.3
Naskar, Supriyo . •BP 31.5, •CPP 50.5
Nassif, Nadine ..... •SYGF 1.1
Näsström, H. ..... AKPIK 6.5
Näsström, Hampus ..... AKPIK 6.3
Nast-Kolb, Timon ..... BP 12.8
Nastos, Panagiotis ..... UP 3.3
Nasuti, Giacomo ..... DY 7.2
Nataf, Guillaume F. ..... FM 4.5
Natal, Joseph ..... AKBP 8.3
Nathan, Yarden .....•MM 3.1
Natterer, Fabian D. . FM 11.23, O 42.3, O 44.3, O 44.7, TT 22.3, TT 92.19
Natusch, Lars .....•BP 2.12
Naujok, Antonius ... O 14.2, •O 40.16, •TT 37.16
Naujoks, Dirk ..... O 78.1
Naumann d'Alnoncourt, Raoul O 23.4
Naumann, Tim ..... O 61.4, O 69.5, •O 69.7, O 77.3
nava mireles, abraham .....•HL 54.5
Nava Sedeño, Josué Manik . DY 33.9
Navarrete, Catalina ..... CPP 33.4
Navarrete, Nuria ..... MM 21.1
Navarrete-Vera, Catalina ...•BP 26.1, •CPP 43.1
Navarro, Juan ..... O 65.5
Navia Rafide, Simon .....•DY 22.3
Nawrath, Cornelius ..... HL 34.1
Nawrodt, Ronny ..... DD 7.1, DD 21.1, DD 30.7, DD 30.8
Nayak, Ankita ...•MA 29.11, MA 51.6, •TT 46.11, TT 88.6
Nayak, Kapil ..... DS 6.6
Naydenov, Boris ..... FM 11.28
Nayir, Nadire ..... HL 24.4, •MM 25.1
Nazari Pour, Ali Reza ..... UP 8.5
Nazarov, Yuli V. ..... TT 50.1
N'Diaye, Alpha ..... O 60.6
Neat, Matthew ..... TT 29.2
Neaton, Jeffrey .....MA 11.4, TT 21.4
Neb, Sergej ..... O 66.5
Nederstigt, Max ..... O 36.4
Neef, Alexander ..... O 38.4
Neehus, Avedis .....•TT 98.8
Neel, Ambar .....•BP 14.52
Néel, Nicolas O 61.9, •O 74.7, •TT 68.7
Neelissen, Ruben ..... HL 12.3
Neethijaran, J. ..... MA 50.3
Neethirajan, Jeffrey MA 6.4, MA 6.10, TT 40.1
Nefedov, Alexei O 55.6, O 81.4, O 88.5
Negi, Devesh ..... MM 21.7
Negi, Rajendra Singh ..... SYGF 1.5
Neher, Dieter ... CPP 40.2, •CPP 53.1
Neils, Will ..... O 44.11
Neiman, Alexander B. ..... DY 33.1
Neipel, Jonas ..... BP 3.9, BP 14.11, •BP 32.6, •DY 52.6
Neiß, Christian ..... MA 5.4, TT 7.4
Neis, Marc .... TT 93.6, QI 6.9, QI 8.5
Neisser, Claudia .... HL 18.4, TT 32.4
Nell, Hannah .....•HL 12.3
Nell, Sebastian ..... DD 30.6
Nelson, Jenny ...•BP 35.4, •CPP 51.4
Neme, I. .....•TT 62.5
Neme, Isadora ..... TT 61.3
Nemes, Norbert Marcell .... MA 16.8
Nemeth, Gergely ..... CPP 46.17
Nemmaier, Alexandra V. ..... HL 8.7, •HL 57.4
Neplyak, Gleb ..... TT 92.19
Neplyakh, Gleb ..... O 42.3, •O 44.3, O 44.7
Neri, Silvia .....•TT 71.4
Nerl, Hannah ..... •TUT 1.4, •FM 1.4
Nerl, Hannah C. ..... TUT 1.1, FM 1.1
Nerreter, Svenja ..... O 12.5
Nessem, Romany ..... MA 7.24
Nestler, Sandra .... DY 58.7, HL 56.5, SOE 17.7
Nettersheim, Kai •HL 18.10, •TT 32.10
Nettuno, Beatrice ..•BP 12.8, DY 22.4
Netz, Roland ..... BP 2.12, CPP 23.3, CPP 27.1, DY 24.3, DY 26.1, DY 54.4, DY 54.9, O 25.2
Netz, Roland R. ..... O 87.3, O 87.7
Neu, Elke ..... MA 6.1
Neu, Volker ..... MA 6.3, •MA 7.80, MA 39.17
Neubert, Julia ..... DD 26.4
Neubert, Sebastian ..... DS 3.1
Neufeld, Ofer ..... SYFC 1.5
Neufischer, Annika ..... O 97.4
Neugebauer, Joerg ..... SYAI 1.3
Neugebauer, Jörg .•TUT 6.1, •MM 1.1, MM 5.5, MM 9.1, MM 13.4, MM 22.4, MM 25.2, MM 25.3, MM 26.3, MM 32.2, MM 39.6, MM 39.7, O 13.6, O 48.1, O 65.7, O 65.9
Neugum, Michael .....•MA 7.86
Neuhaus, Alexander .. O 26.4, O 85.5, •O 96.2, TT 6.6
Neuhaus, Josefine .....•DD 25.3
Neuhaus, Leonard ..... O 8.7, O 31.5, O 35.4, O 35.5
Neuhaus, Marcel ..... MA 33.11
Neukirchen, Alexander ..... O 50.1
Neuman, Christof .... O 72.4, TT 67.4
Neuman, Tomas ..... O 12.4, O 12.6, O 12.7, •O 43.13, O 43.16
Neumann, Bruno ..... MM 21.8
Neumann, Christof . HL 20.14, O 10.6, O 10.7, O 54.7, O 73.2, TT 16.6, TT 16.7
Neumann, Friedrich .....•O 18.6
Neumann, Joanne ...•BP 7.9, BP 11.2
Neumann, Justus .. QI 10.10, •QI 14.9
Neumann, Marc ..... FM 4.2
Neumann, Paula .... •O 81.6, O 94.10
Neumann, Robin R. ..... •MA 2.5
Neupane, Mohan Bikram .... TT 72.4
Neupert, Titus ..... O 63.3, TT 55.3, TT 57.7, TT 83.1
Neureuther, Ilenia .... HL 34.1, QI 18.6
Neurohr, Jens ..... •O 54.1
Neu-Ruffing, Elke .....•TT 24.3
Nevermann, Daniel Henrik . •DY 45.6, •SOE 14.6
Ney, Andreas .... •MA 45.4, MA 48.2, MA 51.1, TT 88.1
Ney, Verena ..... MA 45.4, •MA 51.1, •TT 88.1
Neyman, Konstantin ..... O 81.1
Ng, Dr. Marcus Tze-Kiat .... •SYAI 1.1
Nghiem, Hoa ..... TT 90.5
Ngo, Cong ..... HL 1.3
Ngo, Huu Thoai ... DS 20.48, •O 62.7, •TT 54.7
Ngoi, Kuan Hoon ..... HL 4.1
Ngueldjou Tahabo, Cyrille . •BP 14.27
Nguyen, Anh T. ..... O 71.10, TT 66.10
Nguyen, Bich ..... DS 20.32
Nguyen, Chung ..... MM 14.1
Nguyen, D.-H.-Minh ..... TT 4.4
Nguyen, Dan Chi ..... O 89.10
Nguyen, Hai-Chau ..... •QI 15.7
Nguyen, Hong Dong ..... MA 17.3
Nguyen, Minh-Toan DY 58.9, SOE 17.9
Nguyen, Q. ..... MA 25.6
Nguyen, T. N. Ha ..... •DS 18.2
Nguyen, Thi Ngoc Ha ..... DS 20.47
Nguyen, Xuan T. ..... FM 18.5
Ni, Lingli ..... CPP 21.5
Nic Chormaic, Síle ..DY 59.3, TT 99.3
Nicholls, Rebecca ..... TT 97.5
Nickel, C. M. ..... AKBP 1.1
Nickel, Clemens M. ..... AKBP 4.4, AKBP 14.1
Nickel, Daniel .....•HL 23.3
Nickel, Felix ..... •TT 6.3
Nickel, Rachel ..... MA 33.11
Nicklas, Michael ..... TT 25.7
Nicolai, Hendrik ..... DY 28.3
Nicolaï, Laurent ..... O 76.3, •O 93.6, TT 52.5
Nicolas, Chistophe CPP 23.2, DY 24.2
Nicolas, Christophe ..... CPP 27.3, DY 26.3
Nie, Weijie ..... HL 34.1
Nie, Y. F. ..... TT 69.6
Niebojewski, Heimanu ..... QI 2.10
Niebuhr, Janus F. .....•TT 97.3
Niebur, André ..... CPP 26.2
Nieder, Clara Marie ..... •O 44.17
Niederbudde, Nathalie ..... •QI 14.23
Niehoff, T. .....•MA 52.22, MA 52.24
Niehues, Iris ..... HL 20.4, HL 20.8, HL 20.58, HL 26.37, •HL 35.7
Niehues, Sven .... MA 9.13, MA 52.5, •MA 52.14
Nielsch, Kornelius ..... DS 20.28, DS 20.51, FM 11.14, FM 22.5, HL 20.23, HL 20.24, HL 26.10, HL 26.23, MA 13.3, MM 19.44, TT 4.11, TT 49.2, TT 73.11
Nielsen, Thomas ... O 66.8, •O 95.11, •TT 96.11
Niemann, R. ..... O 57.6
Niemczyk, Raffael ..... AKBP 2.1, AKBP 2.2, AKBP 2.5, AKBP 8.2
Niendorf, Thomas ..... MA 13.4
Nienhaus, Hermann ... O 19.4, O 19.5
Nienhaus, Stefan .....•BP 7.51
Niermann, Laura ..... FM 19.5
Niermann, Tore ..... FM 19.5
Nieschwitz, Paul ..... BP 1.3, •BP 7.4, CPP 1.3, DY 4.3
Nievergelt, Adrian ..... BP 7.28
Nieves, Pablo ..... MA 9.6, MA 58.11
Niggas, Anna .....•O 93.1
Nihei, Anastasiia .... FM 6.2, •O 95.4, •TT 96.4
Nii, Yoichi ..... MA 17.8
Nikitin, Stanislav ..... MA 17.2
Niklowitz, Philipp ..... TT 95.7
Nikodem, Ella ..... TT 15.4, •TT 15.5, TT 15.6
Nikolaev, Kirill O. . MA 9.13, MA 52.14
Nikolaeva, Albina ..... MM 19.15
Nikolic, Branislav K. ..... MA 58.3
Nikolić, Danilo .....•TT 73.8, TT 97.3, TT 98.6
Nikoubashman, Arash ..... CPP 17.1, CPP 17.2, CPP 24.1, CPP 41.1, CPP 46.44, CPP 46.55, CPP 54.3
Nikulina, Alyona ..... •CPP 46.15
Nilforoushan, Niloufar HL 8.1, HL 39.8
Nilius, Niklas .O 52.2, O 52.5, •O 55.2, O 55.7
Nilsson, Rasmus Väinö Erik .... O 5.3
Nimmrichter, Stefan ..... QI 14.6
Nimtz, Pauleo ..... PSV I, PSV VI
Nimtz, Pauleo R. ..... •UP 5.4
Ninkovic, Jelena ..... TT 22.32
Nippert, Felix ..... HL 40.6, HL 55.11
Niquet, Yann-Michel ..... QI 2.10
Nisar, Amjad ..... MM 4.9
Nishiguchi, Daiki ..CPP 28.5, DY 29.5
Nitsch, Paul-G. ..... •O 96.6
Nitschke, Jonah ..... O 71.3, TT 66.3
Nitschke, Jonah Elias O 84.4, TT 84.4
Nitta, Shugo ..... HL 57.1
Nitu, Ioana-Alexandra .....•TT 22.28, TT 22.29
Nitz, Florian .....•O 11.5
Niu, Jiasen .....•TT 73.1
Niu, Ran ..... CPP 28.1, DY 29.1
Niu, Wenhui MA 35.4, O 46.1, TT 60.4
Niwata, Issei .....•MA 31.8, •TT 47.8
Nixon, R. .....•TT 5.9
Nizovtsev, Anton ..... O 69.7
Noack, Philipp ... HL 20.37, HL 20.42
Noack, Reinhard ..... TT 70.3
Noad, Hilary ..... TT 25.7
Noad, Hilary M. L. ... MA 8.8, TT 41.5
Nochowitz, Sam S. ... O 44.6, •O 79.2
Nöcker, Selina ..... SYFC 1.5
Nöding, Lukas .... MA 39.22, O 70.4, •O 70.5, TT 65.4, •TT 65.5
Noé, Frank ..... DY 14.2
Noé, Jonathan ..... DS 21.8
Noe Ladines, Alvin ..... FM 6.5
Noël, Paul ..... MA 29.3, TT 46.3
Noettger, Yannick .....•O 17.3
Nogueira, Flavio S. ..... DY 43.19
Noguera, Claudine ...•O 52.2, O 52.5, O 55.2
Noh, Jae Dong •CPP 11.11, CPP 11.12, •DY 17.11, DY 17.12, DY 44.9
Noh, Rang .....•CPP 46.9
Noheda, Beatriz .....DS 6.3, FM 12.9, FM 12.10
Nöhl, Felix ..... •DS 20.31
Noid, W. G. ..... CPP 24.1
Nojiri, H. ..... MA 23.5, TT 35.5
Noll, Marvin-Dennis .....AKBP 4.2
Nolte, Gustav F. ..•BP 1.10, •CPP 1.10, •DY 4.10, O 11.4
Nolte, Stefan .....•MM 33.1
Noman, Kawa .....•MA 52.13
nomoto, takuya ..... O 95.9, TT 91.1, TT 96.9
Nomura, Kentaro ..... TT 83.6
Nomura, Toshihiro ..... MA 9.1
Nonaka, Andrew ..... DY 6.10
None, Meera .....•HL 38.9
Nonnon, Pierre ..... O 14.1
Nord, Ashley .....•BP 41.1
Nord, Magnus ..... TUT 1.1, •TUT 1.5, FM 1.1, •FM 1.5, MA 6.11
Norden, Caren ..... BP 3.6
Nordlander, Peter ..... O 96.10
Nørskov, Jens ..... O 50.3
Nørskov, Jens Kehlet ..... O 88.8
Nosraty Alamdary, Daryoush .•O 56.4
Notarangelo, Adriano ..... •DS 4.5, HL 57.5
Nothhelfer, Jonas .....•MA 7.43
Novak, Ekaterina . CPP 20.7, DY 23.7, •DY 44.11, DY 44.22
Novák, Petr ..... FM 5.11
Novko, Dino ..... O 71.8, TT 66.8

Novotný, O. ..... TT 22.31
Novotný, Tomáš ..... QI 9.2
Nowak, Carsten ..... DD 17.3
Nowak, Domenic . MA 47.11, MA 54.7
Nowak, Ulrich .....MA 7.68, MA 12.5, MA 14.3, MA 33.1, MA 38.7, MA 38.8, MA 39.11, MA 40.10, MA 47.9, MA 48.6
Nowbagh, Abhimanyu .....DY 62.3
Nufer, Paul ..... •MA 7.48
Nugroho, Agustinus Agung ..MA 3.6, MA 52.34, MA 52.36, TT 23.13
Nugroho, Augustinus Agung . MA 3.7
Numrich, Luca ..... •MM 13.2
Nunes Ferreira, Pedro ..... •TT 80.9
Nunez, Alvaro ..... MA 7.58
Nunnenkamp, Andreas ..... DY 53.4, TT 87.4
Nurak, Ingrit .....•MM 3.6
Nurekeyev, Zhangatay .... •CPP 23.1, •DY 24.1
Nutz, Manuel .....DS 21.8
Nwemadji, Gibbs •DY 45.5, •SOE 14.5
Nyári, Bendegúz ..MA 58.5, TT 15.12, •TT 15.13
Nygard, Jesper .....TT 50.6
Nyman, Mathias .....CPP 25.5
Nysten, Emeline ...HL 3.11, HL 20.19, HL 26.1, HL 36.1
Nysten, Emeline Denise Sophie HL 18.5, TT 32.5
O. Alves, Gabriel .....•QI 7.1
O.Balayeva, Narmina ..... O 79.6
O. Demokritov, Sergej .....MA 52.5
O. Fumega, Adolfo .....MA 7.85
O. Nikolaev, Kirill ..... MA 52.5
Oakes, Patrick W. .....BP 3.11
Obczovsky, Markus ..... •DD 38.3
Oberdisse, Julian .....CPP 31.2, •CPP 36.1, •CPP 42.1, CPP 42.2, CPP 46.33, CPP 46.38
Oberer, Louis .....DY 44.16
Oberhofer, Harald ... DS 8.4, HL 15.8, HL 24.7, HL 53.3, MM 8.7, MM 12.4, MM 26.1
Oberle, S. ..... HL 55.9
Oberle, Simon ....HL 20.42, •HL 34.4
Oberleitner, Thomas ..... HL 20.38
Oberndorfer, Marie ..... •DD 28.3
Obrock, Tim .....TT 94.7
Obst, M. .....O 57.6
Obwaller, Barbara ..... DD 18.1
Ochmann, Migel .....BP 9.6
Ocker, Michelle ..... MA 8.5
Odenbach, Stefan ..... CPP 42.5
Odobesko, Artem ..... O 17.3, O 56.4, •O 63.3, •TT 55.3, TT 85.2
Oehler, Elias .....•DD 17.2
Oehrl, Patricia ..... MA 37.7, TT 43.9
Oel, Thomas .....CPP 17.8
Oelschläger, Anne ..... O 38.3
Oelsner, Gregor ..... TT 93.6
Oenes, Onur .....DD 4.1
Oestreich, Michael HL 38.10, HL 55.8
Oeter, Anne-Catherine ..... •O 44.16
Oettel, Martin ..... DS 1.1, •DY 14.1, DY 41.14, DY 47.4
Oettgen, Niklas ..... •MA 7.71
Oezkent, Maximilian ..... QI 6.5
Offermann, Katharina O 62.8, TT 54.8
Ogata, Shigenobu ..... •MM 20.1
Ogata, Shuji .....FM 15.3, FM 18.4
Ogawa, Tomohiro ..... FM 15.3
Oguchi, Tamio ..... MA 8.11
Oğuz, Erdal C. .....DY 47.3
Oh, Dongjin ..... HL 24.10
Oh, Haneol ..... BP 9.6
Oh, Jeongmin .. O 15.6, O 15.9, O 17.1
Oh, Soyoung ..... O 89.10
Oh, Woi Sok .....SOE 6.7
Ohad, Guy ..... MA 11.4, TT 21.4
Ohanyan, Vadim .. MA 36.2, •TT 94.9
Ohashi, Ryoi ..... TT 83.6
Ohe, Jun-ichiro ..... MA 30.1
Ohl, Claus-Dieter •BP 30.5, •CPP 47.5
Ohland, Jonas Benjamin ..AKBP 11.3
Ohlendorf, Rahel ....MA 8.5, •MA 8.8
Ohmann, Robin .....•O 71.8, •TT 66.8
Ohnesorge, Esther ..... •CPP 29.4
Ohnishi, Kazuki .....HL 57.1
Ohnmacht, David C. ..... TT 22.1
Ohnmacht, David Christian . •TT 50.7
Oing, Oliver ..... •HL 20.43
Ojaghi Dogahe, Badrosadat .. O 70.1, O 95.12, TT 65.1, TT 96.12
Ojha, Brindaban ..... •MA 39.8
Oka, Takashi ..... TT 57.7
Okabayashi, Norio ..... •O 3.4
Okada, Hajime .... BP 32.11, DY 52.11
okada, kazuki ..... O 95.9, TT 96.9
Okamoto, Yoshihiko ..... FM 9.5
Okasha, Nagwa .....MA 7.76
Okay, Cihan ..... QI 12.5
Okotete, Eloho ..... •MM 7.8
Okrugin, Kirill ..... DY 25.2
Okukura, Andrew-Hiroaki ..AKBP 11.3
Okuma, Ryutaro .....FM 9.5
Okumura, Shun ..... •MA 8.1
Okumus, Yigitalp ..... CPP 39.3
Olaf, Krey ..... DD 15.3
Olamaei, Bita ..... •QI 21.5
Olaniyan, Ibukun ..... HL 25.3
Olbrich, Eckehard SOE 11.5, •SOE 12.3
Olbrich, Johann ..... CPP 53.4
Olbrich, Markus ..... •DS 21.9
Oldenburg, Kevin ..... O 27.2
Oldenstaedt, Jonas A. .....•MM 9.5
Olejník, Kamil ..... MA 30.6
Oleynik, Paul ..... O 96.6
Olgiati, Matteo ..... O 87.5
Olguin, Yusser ..... CPP 41.5
Oliveira, Thales .... MA 7.46, MA 12.4
Oliver-Bonafoux, Sara .....•DY 33.10, DY 60.1
Olivier, Ségolène ..... QI 18.1
Ölke, Dominik .....HL 26.46
Ollefs, K. ..... MA 7.14, MA 50.3
Ollefs, Katharina ..MA 13.2, MA 50.8, MA 52.27
Ollier, Alexina ..... MA 43.5, MA 49.8
Ollivier, Jacques ..CPP 32.4, DY 35.4
Olsen, Christian .....QI 14.25
Olsen, Kristian .....•DY 21.9
Olsson, Henrik ..... SOE 2.8
Olszewski, Maciej W. ..... TT 43.8
Olszowska, Natalia ..... HL 24.10
Oluwabi, Oluwaseyi ..... MM 19.42
Omambac, Karim .... O 10.10, O 72.1, TT 16.10, TT 67.1
Omar, Ahmad ..... MA 7.37, •MA 13.1
Omar, Ali .....HL 26.41
Omelchenko, Oleh ..... •DY 8.5
Omidvarnia, Amir •TUT 3.3, •TUT 3.4, •AKPIK 1.3, •AKPIK 1.4
Omranpour, Amir ... MA 36.1, •O 39.5
O'Neil, Caitlin I. .... TT 25.7, •TT 41.5
O'Neill, Shane ..... O 44.15
Onishi, Tomoko .....•O 67.9
Ono, Teruo ..... MA 52.13, MA 59.4, MA 59.9
Onose, Yoshinori .. MA 17.8, MA 30.1
Opel, Matthias ..... MA 30.5
Opelt, Konrad ..... MA 50.9
Opfermann, Malte .....•O 11.2
Opitz, Andreas .....•CPP 22.2
Oppelt, A. ..... BP 27.8, BP 37.2
Oppen, Dominic .....CPP 15.2
Oppeneer, Peter M. MA 7.11, MA 12.6, MA 14.3, MA 38.6, MA 40.10, O 40.15, TT 37.15
Opper, Manfred ..... DY 55.2
Oppermann, Malte ..... HL 8.10
Oppers, Daniel .... HL 17.3, •HL 55.5, HL 55.6
Oppliger, Jens ..... FM 11.23
Opsomer, Eric .....DY 19.4, •DY 19.7
Orbons, Jerome ..... AKBP 14.2
Ordu, Mustafa .....CPP 46.62
Ordyna, Paweł ..AKBP 6.1, AKBP 6.2, •AKBP 6.3
Orel, Matic ..... DY 32.9, TT 45.9
Orenstein, G. ..... MA 4.4
Orfi, Alev .....DY 58.1, SOE 17.1
orio, hibiki .....O 82.3
Orlita, Milan ..... MA 23.2, TT 35.2
Orlob, Meret ..... TT 5.11
Orlov, German ..... O 56.3
Oros, Daniel ..... •BP 21.7
Oroszlány, László .MA 42.2, MA 58.3, MA 58.5, MA 58.10, •QI 2.8, AKPIK 5.12
ORTAÇ, Bülend . CPP 17.30, •FM 19.3, FM 19.6, MM 12.9, MM 16.4
Ortega-Arroyo, Jaime .....CPP 10.12, DY 16.12
Orth, Peter .....QI 14.13
Orth, Peter P. .... MA 52.15, TT 43.12
Ortix, Carmine .... HL 20.55, HL 23.1
Ortiz, David ..... •DY 48.3
Ortlepp, Thomas .....FM 7.1, HL 31.3
Ortmann, Frank CPP 15.6, CPP 17.23, CPP 25.3, CPP 40.1, CPP 40.3, CPP 53.4, CPP 57.6, •DS 18.8, DS 20.45, HL 23.7, HL 40.3
Ortuzar, Jon O 99.7, TT 50.6, TT 73.5
Örüm, Diana ..... BP 14.35
Osada, Alto ..... MA 59.4
Osat, Saeed .....•CPP 28.4, DY 27.6, •DY 29.4
Oschatz, Martin .....CPP 21.5
Oschinski, Hedda .....•MM 13.7
Oshchepkov, Alexandr ..... O 69.5
Osinski, Ben .....•DD 5.3
Osipov, Nikita .....•O 69.12
Oskar Liedke, Maciej ..... MM 11.2
Osmic, E. .....•TT 74.5
Osmolska, Weronika ..... O 80.3
Osmond, Israel .....TT 80.3
Ossenschmidt, Mika •MA 5.1, •TT 7.1
Ossinger, Sascha .....O 89.9
Ostanin, Sergey .....DS 11.8
Ostap, E. Michael .....BP 12.2
Ostatnicky, Tomas ..... O 96.5
Osterhage, Hermann .O 15.3, •O 89.7, O 99.9
Osterhoff, Jens AKBP 8.4, AKBP 12.4
Osterhoff, Markus CPP 27.4, DY 26.4
Osterloh, Niklas ..... MM 11.3
Ostheimer, David .....HL 26.41
Östlin, Andreas .....TT 81.2
Ostmeyer, Johann .... TT 17.3, QI 4.3
Ostrowicki, Andreas ..... •AIW 2.4, •AIW 2.5
Oswald, Luc ..... HL 13.7, HL 20.5
Oswald, Luc Frederik .....•HL 20.6
Oswald, Sascha .....UP 7.5
Otal, Eugenio .....FM 11.12, FM 11.20
Otero Fumega, Adolfo ..... DS 12.6, MA 17.5
Otschkowski, Daniel .....•CPP 46.44
Otsuki, Junya .....MA 11.2, TT 21.2
Ott, Jan Phillip .....CPP 37.6
Ott, Tatjana .....•MM 19.20
Otte, Sander ..... O 17.2
Otto, Felix ..... O 6.8, O 10.7, O 28.3, O 44.14, O 45.3, •O 45.8, O 45.11, O 83.2, TT 16.7
Otto, Florian ..... MA 6.2
Otto, Frederik ..... FM 19.5
Otto, Fynn .....•QI 12.7
Otto, Johannes .... O 40.13, TT 37.13
Otto, Oliver BP 7.34, BP 7.35, BP 7.36, BP 7.38, BP 7.40, BP 37.3
Ou, Lifeng .....•O 71.2, •TT 66.2
Ouazan-Reboul, Vincent ...•BP 10.10, •CPP 18.10, •DY 18.10
Ouisse, Thierry .... DS 14.4, MA 50.8
Ouitrakoon, Phuthiphong ...CPP 26.1
Ouladdiaf, Bachir .....TT 57.2
Oulton, Rupert .....O 96.10
Ouzan-Reboul, Vincent .... CPP 20.2, DY 23.2
Ovcharenko, Sergei .....•DS 20.37
Overby, Christian ... O 95.11, TT 96.11
Overchenko, Aleksei .....•O 13.9
Overwin, Tim .....•DD 30.10
Ovri, Henry ..... MM 3.2, MM 19.19
Oz, Yahya ..... CPP 39.3
Ozawa, Akihiro ...TT 44.11, •TT 44.12
ozawa, kenichi ..... O 95.7, O 95.9, TT 96.7, TT 96.9
Ozbey, Dogukan Hazar .....•HL 10.6, •TT 20.6
Ozdemir, Cagdas .....QI 12.5
Özden, Ayberk ..... MM 19.46
Ozen, Sercan .....HL 4.7
Özkara, A. .....TT 22.31
Ozkutlu Demirel, Merve ...•CPP 39.3
Ozturk, Zeynep Reyhan .....•DS 3.2, •O 2.7
Özyigit, Furkan .....•O 40.8, •TT 37.8
P. A. Santos, Júlio ..... •CPP 42.4
P. Fellows, Alexander ..... O 51.2
P, Lakshmi Madhuri ..... MA 49.9
P. Rugeramigabo, Eddy .....DS 20.21
P. Schmidt, Paul ..... O 44.12
P. T. Masilamani, Muthu .....•O 76.1
Paarmann, A. .....O 57.6
Paarmann, Alexandar O 95.5, TT 96.5
Paarmann, Alexander ..... MA 39.7, O 85.4, O 96.8
Pabi, Biswajit .....O 17.10
Pabshettiwar, Chinmay .... CPP 49.1
Paçal, Serkan ..... HL 16.4
Pachauri, Vivek .....O 96.3
Pacher, Korbinian ..... BP 14.90
Pacini, Bianca .....•BP 14.90
Padeken, Jan ..... CPP 17.4
Padhan, Nadia Bihari .....•CPP 10.8, •DY 16.8
Padhi, Anshuman .. O 84.9, •TT 22.2, TT 84.9
Padilla-González, Daniel ...•DY 43.10
Padniuk, Irena .....•TT 73.2
Padua, Agilio .....CPP 21.1
Padurariu, Ciprian ..TT 62.9, TT 82.5, TT 82.6, TT 85.4, •TT 89.4
Paech, Frederik ..... TT 23.18
Paeckel, Sebastian ..... TT 83.10
Paetzold, Ulrich W. .... HL 4.4, HL 4.5
Pagare, Kumudini ..... AKBP 10.4
Pagare, Kumudini Devendra •AKBP 11.1
Pagni, Vittorio .....QI 3.8, •QI 5.5
Pahujani, Sakshi .....•BP 21.5
Paiva, Carolina ....MA 25.3, MA 25.4
Pajanonot, Kristian .....BP 7.15
Pajanonot, Kristian Angeli . •BP 12.11
Pajusco, Nicolas .....HL 20.8
Pak, Seik .....MA 43.5
Pak, Taegyu ..... •AKBP 13.1
Paksoy, Aybike ..... •MA 52.31
Pal, Atindra Nath ..... TT 79.5
Pal, Ayan .....•TT 44.10
Pal, Banabir MA 7.13, O 84.9, TT 22.2, TT 84.9
Pal, Buddhadeb ..... TT 79.5
Pal, Mandira ..... HL 55.7, HL 56.5
Pal, Riju .....•TT 79.5
Pal, Shovon ..... TT 25.1
Pal, Sourav .....•DY 43.14
Palacios, Juan J. ..... O 15.1
Palacios, Juan José HL 30.7, TT 59.7
Palakkal, Jasnamol .....DS 16.10, MA 7.10
Palanakar, Raghvendra ..... MA 39.7
Palanichamy, Gayathri ....•MA 58.12
Palariya, Rakesh ...BP 10.1, CPP 18.1, DY 18.1
Palau, Anna .....•MA 44.4, •TT 76.4
Palazzo, Gabriele .....MM 19.47, •MM 35.2
Paleari, Fulvio .....HL 35.9
Palekar, Chirag ... HL 20.28, HL 54.6, •HL 54.7
Palekar, Chirag Chandrakant . HL 13.1
Pálffy, Adriana ..... TT 3.5
Palitza, Simon ... •HL 26.35, HL 38.7
Palkhivala, Shalom ..... •BP 9.5
Pallach, Roman ..... O 69.6
Palle, Grgur .....TT 57.11
Palm, Felix A. ..... •TT 83.10
Palmer, Guido ..... AKBP 11.2
Palmolahti, Lauri ..... •DS 9.2
Palomo Marcos, Miguel Angel •QI 14.5
Paloni, Matteo ..... BP 15.2
Palotás, Krisztián ..... •O 47.1
Paltiel, Yossi ..... MA 7.66, MA 29.2, TT 46.2
Palummo, Maurizia ..... O 58.3
Palyi, Andras . HL 38.6, QI 6.3, QI 6.4, QI 20.7
Pan, Feihao .....•MA 47.10
Pan, Gaopei .....•TT 90.3
Pan, Grace A. .....MA 27.7
Pan, Guangjiu .... CPP 4.6, CPP 12.4, CPP 16.2, CPP 44.3, CPP 44.5, CPP 46.17, CPP 48.2
Pan, Ming-Lun ..... O 9.11
Pan, Shihe .....DY 41.1
Pan, Weiyi .....•MA 7.45
Pan, Wun-Chang .....MM 11.3
Pan, Yiming .....•HL 46.5
Pan, Ying ..... O 23.1
Pan, Yong-He .....•MM 11.3
Pan, Yu .....•FM 22.1
Pan, Yue .....•CPP 46.61
Panaccione, Giancarlo ..... MA 47.2, O 38.2, O 98.7
Panagiotidis, Georgios ...•CPP 17.42
Panagiotopoulos, Andreas .•DY 41.15
Panagiotopoulos, Ioannis ...MA 57.3
Panda, Animesh ... DY 42.9, TT 63.9, TT 93.13
Panda, Anwesha .....SYBT 1.2
Panda, Arindam ... BP 10.1, CPP 18.1, DY 18.1
Pande, Shreerang .....BP 2.1
Pandey, Abhishek ..... •FM 11.14
Pandey, Esita ..MA 52.28, •MA 52.29
Pandey, Itu .....O 10.4, TT 16.4
Pandey, Shishir Kumar .....TT 25.1
Pandeya, Ram Prakash ..... O 10.11,

O 54.4, TT 16.11
Pandit, Atharva .....•CPP 49.2
Pandit, Vedhas ... DS 20.34, DS 21.4, •AKBP 6.5, AKBP 11.3
Pang, Chun Sum Brian ..... O 84.5, TT 84.5
Panhans, Michel .....•CPP 40.1, CPP 57.6, DS 20.45, HL 23.7
Pani, Ipsita .....•CPP 41.6
Panja, Soumendra Nath .... •TT 52.6
Pannullo, Laura ..... DD 39.1
Panosetti, Chiara .MM 9.9, MM 19.12, MM 22.1, MM 31.10, MM 41.7
Pant, Robert ..... •TT 22.26, QI 14.21
Panta, Uday ..... MM 37.3
Pantenburg, Isabel ..... CPP 16.1
Pantiri, Giulia .....•DD 31.1
Panwar, Sangeeta .....•TT 23.17
Panzera, Giacomo ..... O 67.10
Paolasini, Luigi ..... TT 49.1
Paoletti, Francesca .....•TT 6.4
Papadakis, Christine M. ... CPP 31.4, CPP 46.12, CPP 46.26, CPP 46.31, CPP 46.37, CPP 46.39, CPP 54.6
Papadimitriou, Nikolaos ..... •UP 5.2
Papageorgiou, Anthoula C. .... O 9.4, O 45.4, O 83.1
Papagiannoula, Andromachi •BP 20.7
Papapostolou, Antonia .....CPP 17.6
Papazoi, Thomais ..... UP 3.3
Pappa, Anna ... QI 3.7, QI 5.3, QI 18.5, QI 18.9
Pappalardi, Silvia . DY 59.11, TT 99.11
Pappenberger, Ronja ..... •HL 4.5
Paprotzki, Eva ..... TT 23.26
Paquet-Clouston, Masarah . •SOE 5.1
Paradiso, Nicola ... TT 73.7, •TT 97.2
Parak, Wolfgang ..... CPP 15.1
Parakh, Pranav D. ..... QI 6.10
Parala, Harish .....FM 11.24
Paralikis, Athanasios ..... HL 54.6
Parameswaran, Siddharth ... TT 86.6
Pardo, Victor .....•DS 12.6, MA 7.85
Pardo-Almanza, Markel ..... O 63.4, TT 55.4
Pare, Charles ..... MM 8.9, •O 23.4
Parida, Ciku .....MM 5.2
Parikh, Trupen .....AKBP 13.2
Paris, E. ..... MA 25.6
Parisen Toldin, Francesco .... TT 2.4
Park, Albert M. ..... MA 59.9
Park, Albert Min Gyu .....MA 52.12
Park, Byong-Guk .....MA 52.12
Park, Heonjoon ..... TT 44.4
Park, Je-Geun .....MA 43.5
Park, Junmo .....CPP 17.10
Park, Moon jip .....MA 43.5
Park, Pyeongjae .....MA 43.5
Park, Soyoung .. O 6.5, O 45.5, O 58.4
Park, Yongsup .....•O 82.2
Park, Youngwook ... •O 12.10, O 43.2
Parkb, JeongWon ..... O 65.2
Parkin, Stuart ..... DS 11.8, MA 7.13, MA 35.3, MA 35.4, •MA 44.1, O 42.1, O 63.4, TT 55.4, TT 60.3, TT 60.4, •TT 76.1
Parkin, Stuart S.P .. MA 30.2, O 84.9, TT 22.2, TT 41.2, TT 84.9
Parkinson, Gareth ..... O 94.3
Parkinson, Gareth S. .. O 5.6, •O 53.1, O 55.4
Parlak, Umut ..... FM 23.4, MA 30.9, O 64.4, •O 93.2
Parmar, Anshul D. S. ..... CPP 35.4, DY 37.4
Parmigiani, Fulvio ..... O 66.7
Parodi, Margherita .....•MA 4.6
Parra Lopez, Luis Enrique ... •O 22.1, O 43.4, O 43.10
Partovi-Azar, Pouya ..... •MM 12.3
Parui, Kaushick .... MA 7.2, MA 19.3, •MA 19.6, TT 31.3, •TT 31.6
Parui, Kaushick K. . MA 31.8, TT 47.8, TT 72.3
Parusa, Gian ..... MA 38.13
Parvangada, Appanna .....•HL 3.5
Parvini, Tahereh Sadat ..... TT 43.9
Paryab, Amirhosein ..... FM 11.32
Parzyck, C. .....TT 69.6
Paschke, Fabian .....O 3.2, O 9.12
Paschke-Bruehl, Franziska-Luise •AKBP 5.3
Paschke-Brühl, Franziska .. AKBP 5.4
Pascual, Jose Ignacio O 89.6, O 99.7, TT 73.5
Pascual, Nacho .....O 15.5
Pashaei Adl, H. ..... HL 54.12
Pashaei Adl, Hamid .....HL 54.9, •HL 54.10
Pashchenko, Mariia ..... DS 7.5
Pashkin, Alexej .... •HL 17.5, HL 23.1, HL 52.2, HL 52.3, MA 19.8, TT 31.8, TT 57.6
Pasko, Grigori ..... •O 68.1
Pasquier, Claude .....MM 40.5
Pasquier, Rémi .....•HL 24.8
Passig, Celina ..... •MM 30.4
Passon, Oliver .....•DD 40.2
Passos, Daniel ..... •MA 5.6, •TT 7.6
Pastewka, Lars ... CPP 8.2, CPP 10.7, DY 16.7
Pastor Luque, Laura Andrea •BP 14.47
Pastore, Mauro ....DY 58.9, SOE 17.9
Paszuk, Agnieszka .....HL 12.4, •HL 26.11, HL 48.3
Paszuk, Angieszka .....HL 26.13
Patel, Aavishkar A. ..... TT 56.8
Patel, Jimiben V. .....•O 13.1
Patel, Pawan .....•CPP 31.7
Patel, Riya .....•O 70.2, •TT 65.2
Patel, Sahaj .....HL 24.10
Patel, Sahil .....QI 11.8
Patel, Shubham .....•HL 24.12
Patel, Zeena .....•CPP 2.2, •SOE 3.2, •UP 1.2
Patera, Giuseppe .....QI 18.1
Patera, Laerte .. O 6.6, O 43.1, O 58.5
Pathak, Rohit ....MA 34.11, •MA 58.9
Pathak, Swapneel . MA 50.2, MA 58.1
Pathak, Swapneel Amit .....MA 34.4
Patra, Atanu .....HL 20.30
Patra, Chandan ... MA 11.5, TT 14.10, TT 21.5, TT 93.16
Patra, Manas .....MA 37.8
Patschinsky, Lilly .....MA 39.15
Pattloch, Sven .. •CPP 20.5, •DY 23.5
Paturej, Jarosław .....•CPP 39.2
Patwari, Jayita ..... O 16.2
Pätzold, Lara .... TT 23.13, •TT 23.18
Pätzold, Laura .....•O 86.4, O 86.5, O 95.8, TT 96.8
Patzschke, Felix Hermann ..•BP 33.8
Pauer, Christoph ..... BP 9.5
Paul, Diptabrata .....•DY 14.7
Paul, Dwaipayan ..... MM 31.9
Paul, Jonas .....•FM 11.22
Paul, Jonathan .....•O 23.10
Paul, Raja .....CPP 11.1, DY 17.1
Paul, Robin K. ..... MA 57.5
Paul, Sagar .....MA 42.6
Paul, Suvodeep .....MM 21.7
Paulin, Oliver ....•BP 29.2, •CPP 45.2
Paulin, Oliver W. .....DY 33.4
Paulsen, Michael .. TT 28.3, •TT 82.3
Paulus, Jonas .....•BP 14.74
Paulus, Michael .. BP 14.24, BP 14.72, BP 14.75, MM 19.30
Pauly, Fabian .....MM 31.1
Pausch, Richard ..... AKBP 5.4, AKBP 10.1, AKBP 10.2, AKBP 10.3, AKBP 12.5
Pauw, Fabian J. ..... TT 83.10
Pavan, Matilde .....CPP 4.4
Pavarini, Eva TT 3.4, TT 13.5, TT 56.7
Pavelec, Jiri ..... O 94.3
Pavelka, Martin .....MA 12.6
Pavin, Nenad .....BP 2.3, BP 32.11, DY 52.11
Pavlov, Andrei .....•TT 42.4, QI 17.5
Pavlova, Ketrin .....•DS 20.3
Pavlovskii, Nikolai •MA 19.3, •TT 31.3
Pavlovskii, Nikolai S. ..... MA 31.9, TT 47.9
Pavlů, Jana .....MM 8.10, MM 19.26, O 50.4
Pawbake, Amit .....DS 12.8
Pawlis, Alexander .. HL 12.1, HL 38.1, TT 73.6, QI 6.2, QI 14.26
Pawula, Florent ..... TT 49.4
Paz Corrales, Karla J. .....•DS 13.2
Paz, Karla .....DS 20.16
Pazniak, Hanna .... DS 14.4, MA 50.8
Pech, Lorenz .....•TT 23.3
Pécz, Béla .....DS 6.4
Pedaci, Francesco ..... BP 41.1
Peddibhotla, Phani Kumar .. MA 49.9
Peddinti, Raghavendra ..... DY 28.2
Peddinti, Raghavendra Dheeraj •QI 5.6
Peddis, Davide .....MA 44.7, TT 76.7
Pedersen, Jesper R. .....•MM 5.2
Pedrazzini, Pablo .....TT 5.7
Pedrini, Bill .....TT 62.6
Pedrini, Giancarlo ..... MA 7.80
Pees, Melina F. V. .....•HL 26.34
Peeters, Cole .....TT 15.1
Peeters, Wouter H.J. .....HL 17.1
Peets, Darren ..... MA 7.2, MA 19.3, MA 19.4, MA 19.6, TT 31.3, TT 31.4, TT 31.6
Peets, Darren C. . MA 31.8, •MA 31.9, TT 47.8, •TT 47.9, TT 72.3
Pei, Shujun .....•HL 26.17
Peil, Oleg ..... MM 21.4
Peil, Oleg E. ..... MM 41.6
Peinemann, Lukas ..... TT 23.29
Peinke, Joachim ... DY 8.4, •DY 15.11, DY 15.12, DY 41.5, DY 63.4
Peisert, Heiko ..... DS 20.44
Peixoto, Thiago R. F. .....O 42.9
Pekarek, Lukas ... BP 31.2, CPP 50.2
Peksa, P. .....HL 54.10
Pelcaru, Adrian .....•DY 48.1
Pellicer, Guillem .....•MM 40.6
Pelly, Max .....TT 29.5
Pelster, Axel ..... TT 44.8
pelster, jakob .....O 44.8
Pelz, Philipp .....•MM 29.1
Pemma, Swetha ..... MM 15.5
Peña, Diego .....O 9.10, O 83.5
Peña, Felipe ....AKBP 8.7, AKBP 12.4
Peña Román, R. J. .....•TT 24.7
Peña Román, Ricardo Javier .TT 92.2
Peña-Camargo, Francisco .... HL 4.8
Penc, Karlo ..... MA 8.9
Peneva, Petya ..... MA 7.27
Peng, Bo .....QI 13.5
Peng, Jun ..... DS 16.3, DS 20.10
Peng, Ruoming .... MA 43.6, TT 24.6, TT 92.5, QI 13.5, QI 20.3, QI 20.4
Peng, Wei-Tao ..... CPP 25.1
Peng, Xuan .....FM 6.11
Peng, Yu-Hsuan ..... CPP 54.4
Penkl, Maja ..... O 86.9
Penn, Aubrey .....HL 13.5
Penner, Alexander-Georg ... DY 32.2, TT 45.2
Penning, Jonas .....•BP 7.16
Pentcheva, R. ..... TT 69.3
Pentcheva, Rossitza ..... MA 20.3, MA 38.1, O 11.3, O 14.8, O 23.7, O 29.2, O 34.4, O 94.7
Perea-Causin, Raul ....HL 3.7, O 98.9
Pereira, Rui .....DS 1.2
Pereira, Tiago ..... DY 6.11
Pereira, Vanda M. ..... TT 25.2
Pereira-Alves, Felipe .....•DY 54.1
Pereiro, Manuel •MA 59.10, MA 59.11
Perekrestov, Vyacheslav .....MM 3.5
Peremadathil Pradeep, Reshma MA 44.2, TT 76.2
Perenon, Rémi .....AKPIK 6.6
Perepichka, Dmytro ..... O 33.2
Perera, Aurélien .....MM 19.30
Pereyra, Marc ..... BP 37.5
Perez, Daniel ..... MA 37.8
Perez Gonzalez, Beatriz ....•HL 31.2, MA 7.29
Perez, Nicolas .....•FM 22.5
Pérez Ortiz, Rodrigo ..... DY 45.5, SOE 14.5
Perez Penco, Ester .....•O 11.7
Perez Romero, Arturo .....•TT 23.30
Pérez, Rubén ... O 3.7, O 33.2, O 35.6
Perez-Acle, Tomas ..... BP 8.6
Pérez-Cervera, Alberto .....DY 63.1
Perez-Gonzalez, Beatriz .....HL 31.1
Perfeito, Lília ..... SYTP 1.4
Perlekar, Prasad ..... DY 62.9
Pernice, Wolfram .....•SYBT 1.3
Pernice, Wolfram H. P. .....MA 9.13, MA 52.14
Perronet, Karen ..... BP 9.2
Peruani, Fernando ..... DY 33.9
Perversi, Giuditta . MA 3.3, MA 52.35
Pervez, Waqas .....O 27.2, O 46.9
Pesch, P. .....HL 20.27
Pesch, Patricia ..... HL 47.1
Pesch, Raphael .....HL 4.4, HL 4.5
Peschanska, Oksana .....•MA 7.49
Peschel, Ulf .....HL 1.11, HL 35.6
Peschka, Dirk .....CPP 8.4
Peschke, Claudius .....AKBP 7.4
Peshcherenko, Nikolai .....DS 20.51, •TT 44.2
Pesquera, David ..... FM 18.2
Peter, Melina ..... HL 20.38
Peterlechner, Martin .....MM 3.5
Petermann, Eric .....•MA 7.51
Peters, Finn ..... MA 7.63
Peters, Iago .....•BP 14.91
Peters, Jannick A. .....•O 11.1, O 31.2
Peters, Leif .....•DY 44.13
Petersen, C. .....HL 46.6
Petersen, Christian .....•HL 24.1
Petersen, Clemens •HL 9.5, HL 26.40, HL 40.9
Petersen, Immo .....•UP 8.5
Petersen, Stefan ..... DD 37.1
Petersen, Torben .•O 71.21, •TT 66.21
Peterson, Jonas M. ..... TT 44.4
Petit-Watelot, Sébastien .... MA 48.1
Petiziol, Francesco •DY 59.7, •TT 99.7
Petkovic, Milena ..... FM 11.3
Petracic, O. ..... MA 3.8
Petracic, Oleg ..... MA 7.25
Petrescu, Alexandru .....QI 17.7
Petreska, Irina .. •DY 42.15, •TT 63.15
Petrocchi, Andrea .....•MA 34.4, MA 50.2, MA 58.1
Petrosyan, Davit .....MA 52.10
Petrov, Alexander ..... CPP 3.5
Petrovic, Cedomir ..... MA 30.4
Petrovic, Marin ..... O 72.1, TT 67.1
Petrunin, Alexander V. .....CPP 35.2, DY 37.2
Petry, Julian .....HL 4.5
Petry, Robin .....AKBP 2.3, AKBP 8.1
Petrychuk, Mykhaylo ..... BP 20.9
Petschke, Danny ..... FM 19.7
Pettinger, Nina ..... HL 8.4
Petzoldt, Philip ..... O 94.8, O 94.10
Pezzagna, Sebastien ..... •HL 11.3
Pezzè, Luca .....QI 15.3
Pfaff, Corentin ..... TT 14.12
Pfaffinger, Lea ..... TT 5.1, •TT 64.2
Pfahl, Michelle .....•HL 34.2
Pfalzgraf, Daniel .....•MM 39.8
Pfander, Isabel ..... TT 92.2
Pfanzelter, Julia ..... BP 3.9
Pfau, Bastian .....DS 6.1, MA 7.67
Pfeifer, Thomas ..... TT 71.5
Pfeifer, Veronika ..... BP 11.8
Pfeiffer, Florian .....•O 45.10
Pfeiffer, Mario ..... O 57.4
Pfeiffer, Martin .....CPP 17.9
Pfeiffer, Moritz ..... AKBP 8.6
Pfeiffer, Ramon .....•DS 20.40
Pfeiffer, Walter O 14.11, O 38.5, O 66.5
Pfenning, Andreas ..... QI 18.7
Pfeufer, Michael .....•HL 26.27
Pfister, Alison .....•HL 20.22
Pfister, Clara . O 86.4, •O 86.5, O 95.8, TT 96.8
Pfister, U. ..... HL 55.9
Pfister, Ulrich ....HL 20.37, HL 20.38, HL 20.42
Pflaum, Jens ..... CPP 22.2, HL 15.2, HL 26.15, O 96.1
Pfleiderer, Christian .....•CPP 36.1, MA 7.5, MA 7.33, MA 9.11, MA 37.7, MA 46.2, TT 23.3, TT 41.6, TT 61.6, TT 61.7, TT 62.1
Pfleiderer, Sina .....•DD 24.1
Pflug, Theo .....DS 21.9
Phadke, Parikshit ..... DS 20.13
Pham, An ..... TT 93.4
Pham, Le Viet Duc •MA 29.6, •TT 46.6
Pham, Phat Tan .....•CPP 46.32
Phan, Manh-Huong ..... MA 7.30
Phan, TL ..... MA 7.30
Phark, Soo-hyon ..... O 15.6, O 15.9, O 64.2
Phielepeit, Maximilian ..... •TT 61.6
Philipp, Julian .... BP 26.4, CPP 43.4
Philippaki, Eva ..... DD 12.3
Phillips, Jan .....•DS 1.3, DS 12.6
Phillips, Nicholas W .....MA 7.81
Phiw-Ondee, Satjawoot ..... •HL 9.1
Piamonteze, Cinthia .. O 10.2, TT 16.2
Piasecki, Tomasz ... HL 18.3, TT 32.3
Piasotski, Kiryl ..... TT 85.6
Piatek, Marcin .....CPP 24.4
Piazza, Francesco . DY 13.5, MA 7.29, TT 19.5, TT 44.5, TT 56.1, TT 91.2
Piazza, Luca ..... FM 15.1
Picatoste, Irene Ada .....•QI 7.6
Piccinini, Giulia ..... HL 10.1, TT 20.1
Pichard, Alan ..... BP 20.2
Pichler, Hannes ..... QI 3.10
Pichler, Julian .....•O 30.3
Pickard, Chris .....•TT 80.1
Picker, Julian .....HL 20.14, O 10.6,

•O 10.7, O 54.7, O 70.1, O 72.4, O 95.12, TT 16.6, •TT 16.7, TT 65.1, TT 67.4, TT 96.12
Piehler, Sebastian ..... HL 54.1
Piel, Pierre-Maurice HL 25.2, HL 39.3, HL 39.4, •HL 39.6
Pielić, Borna ..... O 71.8, TT 66.8
Pierantozzi, Gian Marco ..... O 38.2, O 98.7
Pierz, Klaus ..... HL 20.54, HL 25.1, O 73.3, O 95.1, TT 96.1
Pies, Leo ..... MM 19.42
Pietanesi, Laura ..... TT 74.12
Pietralla, N. ..... AKBP 1.1
Pietralla, Norbert ..... AKBP 4.4, AKBP 9.3, AKBP 9.4, AKBP 14.1
Pietrantuono, Patrick ..... HL 20.37
Pietsch, Frithjof ..... DS 16.5
Pietz, Anthony ..... •DS 20.6
Pietzonka, Patrick .. DY 21.8, DY 34.7
Pignedoli, Alessandro ..... •DY 61.4, MA 7.72, TT 6.6
Pignedoli, Carlo Antonio ..... MA 5.9, TT 7.9
Pikovsky, Arkady ..... •DY 8.1
Pilch, Patrick ..... MA 12.4, •TT 41.2
Pilch, Patrik ..... MA 7.46
Pile, Santa ..... MA 34.4, MA 50.2, MA 58.1
Piliai, Lesia ..... O 65.12
Pillai, Sumesh ..... UP 8.1
Pilorz, Krzysztof ..... DY 54.2
Piltz, Ross ..... MA 19.3, TT 31.3
Pilz, Wolfgang ..... HL 56.2
Pimenov, Andrei .... HL 10.5, MA 4.5, MA 17.11, TT 20.5
Pimenov, Anna ..... MA 4.5
Pimlott, Luke .... HL 24.12, •MM 15.1
Pimon, Martin ..... •MA 39.25
Pinar Solé, Andrés .. •O 15.11, O 77.6, O 99.11
Pincelli, Tommaso .. MA 7.18, O 38.4, O 38.7, O 40.11, O 71.10, •O 98.7, TT 37.11, TT 66.10
Pineda, Eufemio Moreno ..... O 99.2
Pinheiro, Diana ..... BP 3.10
Pinheiro, Fernanda ..... •BP 21.1
Pini, Anna ..... •CPP 35.5, •DY 37.5
Pini, Michele ..... TT 44.5, •TT 56.1
Pino, Manuel ..... TT 43.6
Pinto, Adrian John ..... •BP 2.4
Pinto Barros, Joao C. ..... QI 3.4
Pinto, Dinesh ..... TT 92.2
Pinto Pino, Agatha Belén ... BP 14.32
Pinto-Pino, Agatha Belén .. •BP 14.36
Pinto-Ramos, David ..... •DY 22.8
Pioda, Alessandro ..... •O 44.15
Piovano, Andrea ..... TT 95.7
Pipim, Lucas ..... TT 92.5
Pippan, Reinhard ..... MM 7.9
Pirker-Diaz, Paula •SOE 4.2, SOE 12.1
Píro, Michael ..... •MM 19.7
Piroird, Keyvan ..... CPP 58.4
Piroli, Lorenzo ..... QI 3.10
Piros, Eszter ..... TT 42.6
Pirro, Philipp ..... MA 9.3, MA 9.5, MA 9.10, MA 9.12, MA 39.14, MA 45.5, MA 48.1, MA 48.3, MA 48.4, MA 48.9, MA 52.19, MA 59.9
Pisoni, Stefano ..... •DY 28.2, QI 5.6
Pispas, Stergios ..... CPP 46.26
Pistidda, Claudio . MM 13.8, MM 34.7
Pisula, Wojciech ..... FM 10.4
Pivovarova, Anastasiia .. •CPP 46.59
Piwowar, Justyna .... O 77.5, •O 93.3
Pizzi, Giovanni .. MM 13.9, AKPIK 6.7
Plana-Ruiz, Sergi ..... TT 81.1
Plane, John . PSV I, •SYSC 1.5, UP 6.6
Planelles Prensa, Pablo ..... •O 44.4
Planer, Jakub .... O 6.1, •O 6.3, O 8.2, O 69.1
Plastovets, Vadim ..... •TT 91.2
Plate, Franz ... O 6.5, O 45.5, •O 58.4
Platena, Magnus J. R. ..... •QI 14.10
Platero, Gloria ..... DY 46.5, HL 38.4, TT 75.5
Plati, Andrea ..... DY 62.7
Platonov, Daniil ..... •TT 23.28
Platte, T. . MA 18.1, MA 52.24, TT 30.1
Platten, Florian ... BP 39.4, CPP 55.4
Plattner, Paul ..... •AKBP 9.5
Plautz, Markus ..... •HL 20.53
Plávala, Martin ..... •QI 12.2, QI 16.8
Plentz, Jonathan ..... O 73.2
Pless, Ole ..... BP 26.8, CPP 43.8
Pliushchai, Anna ..... MM 19.34
Plo, Juliette ..... O 95.6, TT 96.6
Plochocka, P. ..... HL 54.10
Plochocka, Paulina ..... HL 54.9
Płodzień, Marcin ... DY 53.5, TT 87.5
Plokhikh, Igor ..... •MA 3.12
Plotkin-Swing, Ben ..... FM 15.1
Plucinski, Lukasz .... •MA 5.8, O 2.2, •TT 7.8
Plyushchay, Inna . MM 3.9, MM 19.33, MM 19.34
Poboiko, Ihor ..... •QI 21.6
Poccia, Nicola ..... TT 4.11, TT 49.2, TT 73.11
Poder, Kristijan ..... AKBP 13.1
Poderini, Davide ..... QI 12.6
Podhaisky, Georg ..... •DY 63.1
Podhorsky, Martin ..... HL 13.1
Pogge von Strandmann, Philip •O 5.1
Poggio, Martino ... MA 49.2, QI 14.25
Pogio, Martino ..... MA 49.3
Pogorelov, Ivan ..... QI 16.1
Pohl, Darius DS 4.1, FM 19.1, FM 19.4, FM 19.9, HL 22.6, MA 3.11, MA 7.65, MA 30.6
Pohl, K. Linus H. ..... O 58.1
Pohl, Linus ..... O 69.7
Pöhler, Paul ..... DS 20.28
Pohlitz, Michael ..... FM 19.9
Pöhlker, Mira ..... UP 3.5
Pöhls, Jonas ..... O 40.21, TT 37.21
Pokart, Tim ..... •DY 46.8, •TT 75.8
Pokharel, Ganesh ..... TT 57.12
Pokorný, Vladislav ..... •TT 85.3
Pokusinskyi, Anton TT 14.12, •TT 97.7
Polák, Marcel ..... •TT 22.5
Polesya, Svitlana ... MA 14.3, MA 17.1
Poletto, Luca ..... O 14.10, O 40.19, TT 37.19
Polfus, Jonathan ..... FM 10.2
Pollack, Lois ..... BP 20.6
Pollack, Yoav G. .... BP 7.54, DD 24.4
Pollenske, Tobias DS 20.15, DS 20.27, O 28.4, •O 28.6, O 28.7
Polley, Craig .. O 74.5, O 76.7, TT 68.5
Polling, Lotte ..... •HL 26.53
Pollmann, Frank .... DY 13.8, DY 13.9, MA 19.11, TT 19.8, TT 19.9, TT 31.11, TT 33.5, TT 51.7, TT 51.8, TT 51.9, TT 72.1, TT 86.2, QI 1.9, QI 15.6
Pollock, Jonathan ..... BP 14.7
Polo-Filisan, Sara ..... FM 23.6
Polonskiy, Igor ..... •AKPIK 5.2
Polovnikov, Kirill . BP 36.10, BP 36.11, DY 57.10, DY 57.11
Pols, Mike ..... •MA 25.7
Poltavskyi, Igor ..... DY 14.11
Polyakov, Dmitry ..... SYBS 1.2
Polyansky, Anton ..... BP 14.76
Pomjakushin, Vladimir ..... MA 3.7
Pomjakushina, Ekaterina .... MA 17.2
pongo, tivadar ..... DY 19.3
Pongsangangan, Kitinan ... MM 26.5, O 62.10, TT 54.10
Ponomaryov, Alexey ..... MA 7.46, MA 12.4, MA 25.8
Pontanel, Jacques G ..... TT 52.6
Pontius, N. ..... MA 27.8
Pontius, Niko ..... MA 7.16, MA 27.2, MA 38.2, MA 38.6
Poolamanna, Ashwathi ..... BP 2.5
Poon, Wilson ..... DY 21.7
Pop, Ioan TT 14.2, TT 22.12, •TT 50.2, QI 8.1, QI 11.2, QI 11.4
Pop, Ioan M. ..... TT 43.6, QI 11.5
Pope, Michael A. ..... HL 20.12
Popkov, Nikita ... •DY 41.13, MA 7.23, MA 52.40
Popov, Alexey .... MA 36.12, TT 40.3
Popović, Marko ..... BP 3.2, BP 3.4, BP 7.47
Popp, Andreas ..... DS 9.5
Popp, Ulrich ..... AKBP 7.4
Poppinga, Simon ..... •BP 37.6
Porcar, Lionel ..... BP 16.11
Porer, Michael ..... HL 8.10
Portalupi, S. ..... HL 55.9
Portalupi, Simone L. ..... HL 20.37, HL 20.42, HL 34.2
Portalupi, Simone Luca .... HL 20.38, HL 31.4, HL 34.1, HL 34.4, QI 18.6
Portillo, Joaquim ..... TT 81.1
Pöschl, Franz .... •MA 23.1, •TT 35.1, QI 14.5
Pöschl, Lukas ..... BP 8.5, •BP 14.61
Poschmann, Michael ..... CPP 4.3
Pospiech, Gesche .... DD 3.1, DD 3.2, •DD 3.3, DD 14.1, DD 30.2
Pospisil, J. ..... MA 47.7
Pospíšil, Jiří ..... TT 23.3
Posske, Thore ..... MA 39.5
Post, Matthias ..... •BP 15.11
Postnikov, Andrei ..... MM 14.2
Potenza, Marco ..... CPP 46.6
Pothier, Hugues ..... •TT 50.6
Poths, Patricia ..... •O 55.5, O 88.3
Potoyan, Davit A ..... BP 15.1
Potthoff, Michael . MA 45.6, TT 61.10, TT 90.2
Potts, Mark ..... •TT 86.6
Pou, Pablo ..... O 3.7, O 33.2
Poul, Marvin ..... MM 13.4
Pouliquen, Olivier .. •DY 19.1, DY 19.2
Poulsen, Victor Møller ..... SOE 2.8
Pourdahrany, Shaghayegh .. HL 20.12
Pournaki, Armin ..... •SOE 11.5
Pourovskii, Leonid MA 19.2, MA 51.7, •TT 26.3, TT 31.2, TT 88.7
Povarov, Kirill ..... TT 94.6, •TT 98.1
Povolotskiy, Maksim ..... •MA 7.34, MA 33.4
Powell, Annie ..... MA 7.75
Powell, Annie K. ..... MA 36.13
Power, Stephen R. ... O 62.9, TT 54.9
Požar, Martina ..... MM 19.30
Pozsar, Daniel ..... MA 58.10
Pozzi, Marcello ..... •O 96.12
Prabhakar, J. Manoj ..... MM 39.6
Prabhakar, Manoj ..... FM 2.1
Prabhakar, Prabhakar ..... •MA 34.12
Prabhakaran, Dharmalingam . MA 4.3
Prabhu B N, Balakrishna .... •SOE 2.9
Prachurja, Protyasha ..... •MA 52.23
Prada, Benjamin ..... •SOE 4.3
Prada, Marta ..... HL 13.6
Pradenas, Bastian .•MA 19.1, •TT 31.1
Pradhan, M. ..... O 57.6
Praest, Katarina Ogliara ..... O 85.3
Prager, Lukas ..... FM 11.24, HL 56.2, •QI 2.9
Prager, Michael ..... TT 73.7
Prajapati, Gulloo .. MA 7.46, MA 12.4
Prakash, Manu ..... SOE 4.1
Prakash Singh, Ravi ..... TT 14.10
Prampolini, Giacomo ..... MM 31.2
Pranav, Manasi ..... •CPP 40.2
Prange, Christian .. MA 33.4, TT 12.6, TT 14.1
Pranger, Stefan ..... O 8.4
Prasanna, Sreelakshmi ..... •DS 11.6
Praßelsperger, Alexander AKBP 10.4, AKBP 11.1
Prasse, Fabian ..... DS 18.7
Pratama, Fenda Rizky ..... HL 3.12
Prati, Enrico ..... DY 14.12
Pratsch, Christoph ..... CPP 16.4
pratzer, marco ..... O 44.8
Prehl, Janett ..... •DY 47.5
Preißler, Dustin-Philipp ..... DD 20.4
Preißler, Hannes ..... TT 28.9
Preiss, Helen ..... •MA 36.7
Preissler, Dustin-Philipp ..... •DD 7.3, DD 17.2
Prelovšek, Peter ..... TT 23.2
Prem, Sarath ..... TT 15.2
Preston, Riley ..... •TT 42.9, TT 42.10
Preti, Francesco ..... QI 16.5
Preuß, Antonia ..... BP 14.74
Preuß, Ekhardt ..... •DD 5.1
Preuß, Oliver .... •MM 23.5, MM 27.3
Prévost, Sylvain . CPP 30.5, CPP 42.2
Preziosi, D. ..... TT 69.3
Pribram-Jones, Aurora ..... MM 41.4
Pribytova, Ekaterina ..... •TT 97.9
Priessnitz, Jan ..... MA 8.5, MA 29.7, •MA 33.13, MA 54.6, TT 46.7
Prieto, Gerardo ..... CPP 7.4
Prieto, Mauricio ..... O 65.5
Prieto-Curiel, Rafael ..... SOE 6.3
Printschler, Axel .. DS 14.9, •HL 20.14, O 10.6, TT 16.6
Prinz, G. ..... HL 20.27
Prinz, Günther ..... HL 20.12, HL 47.1
Prisle, Nønne .... •CPP 19.1, •DY 20.1
Pritzl, Stefanie D. ..... BP 14.80
Priyadarshi, Debankit ..... MA 24.2, MA 45.2, TT 25.3, •TT 33.3, TT 36.2
Pröbster, Tamara .. SYFC 1.5, •O 74.1, •TT 68.1
Procházka, Pavel . O 6.1, O 6.3, O 69.1
Prodan, Lilian ..... MA 7.35, MA 7.50, MA 8.9, MA 17.6, •MA 23.4, MA 54.2, O 42.2, •TT 35.4, TT 57.6
Profe, Jonas ..... •TT 51.1
Profe, Jonas B. ..... TT 98.3
Profeta, Gianni .... HL 36.2, MA 17.5, O 63.8, TT 55.8
Proft, Dennis .... AKBP 1.2, AKBP 1.3, AKBP 2.4, AKBP 3.5, AKBP 7.2, AKBP 7.6, AKBP 14.2
Prokhnenko, O. .... MA 23.5, TT 35.5
Prokisch, Leonard ..... TT 92.10
Proksch, Roger ..... FM 4.6
Pronin, Artem ..... MA 33.4
Proschek, Petr ..... MA 17.3
Prosen, Tomaz ... DY 46.10, TT 75.10, QI 9.4
Prost, Tobias ..... O 19.5
Protik, Nakib H. ... HL 23.2, MM 31.3, MM 31.8, •MM 31.9
Prots, Yu. ..... TT 5.9
Prots, Yurii .. MA 2.6, TT 5.8, TT 94.3
Pruchnik, Bartosz ... HL 18.3, TT 32.3
Prucnal, Slawomir .. HL 17.5, HL 17.9, HL 20.46, AKBP 3.6
Pruessner, Gunnar ..... DY 62.6
Prus, Bernadeta ..... O 24.4, O 24.5, O 24.6
Prusakov, Maksim ..... •SOE 2.6
Prusik, Paulina J. ..... •MA 30.8
Pruy, V. ..... AKBP 1.1
Pruy, Vincent ..... •AKBP 14.1
Pryds, Nini ..... FM 18.2
Prytz, Øystein ..... FM 10.2
Przibylla, Niclas ..... •O 19.9
Przychodnia, Marta . O 40.14, O 71.22, O 71.23, TT 37.14, TT 66.22, TT 66.23
Psaroudaki, Christina ..... DY 53.5, TT 87.5
Psoma, Vasiliki ..... DD 38.2
Ptaszyński, Krzysztof ..... •DY 9.1, DY 27.5
Puchert, Anna ..... AKBP 8.4
Puddu, Alessandro HL 17.9, HL 20.46, HL 20.56, •HL 56.1
Pudell, Jan-Etienne . •O 40.15, O 98.3, •TT 37.15
Puebla Hellmann, G. ..... MA 3.8
Puebla Hellmann, Gabriel ..... DD 7.2
Puebla-Hellmann, Gabriel ... MA 6.2, MA 6.9
Puel, Tharnier ..... MA 48.10
Puerta, Adrián ..... •BP 33.3
Pugini, Michele . •CPP 23.4, •DY 24.4
Pugliese, Leo ..... HL 29.2, TT 58.2
Puidokas, Giedrius ..... HL 15.9
Puig, Joaquin ..... TT 11.4
Pukenas, Aurimas ..... MM 7.9
Pukhareva, Natalia •FM 6.10, MM 11.3
Puleri, Anusree V. .. MA 24.2, TT 36.2
Puleva, Mirela ..... •BP 2.10
Pulgarin Mosquera, Juan Felipe •MA 11.8, •TT 21.8
Pulikkal Hamza, Hanna Shirin •MA 39.22, O 70.4, O 70.5, TT 65.4, TT 65.5
Pulkkinen, Aki O 21.2, •O 67.6, O 76.2, O 76.3, O 93.6, TT 52.5
Pumera, Martin ..... FM 5.9
Pundt, Astrid ..... MM 3.6, MM 19.18, MM 19.47, MM 30.2, MM 30.3, MM 34.1, MM 35.2, MM 39.3
Punt, Astrid ..... MM 34.2
Puphal, Pascal ..... O 93.5, TT 39.6, TT 39.7
Pupim, Lucas ..... TT 24.6
Pürling, Thorben ..... •MA 40.2
Pusch, Alexander ..... DD 6.3
Puschnig, Peter . O 6.8, O 9.1, O 45.9, O 61.1, O 61.7, O 66.9, O 69.2, •O 83.2, O 83.6
Pusskeiler, Jan ..... TT 14.1, •TT 14.2
Puster, Felix ..... TT 83.9
Puthirath Balan, Aravind .... MA 39.2
Putz, Bernhard ..... TT 92.4
Pütz, Frederik ..... O 61.7
Pütz, Lars ..... •O 17.5
Putzke, Carsten .... TT 17.2, TT 57.7, TT 97.5, QI 4.2
Puy, J. ..... MA 52.22
Puy, Johannes .... MA 13.4, •MA 13.7
Puzyrev, Dmitry ... DY 25.3, •DY 25.4, DY 25.5
Pyanzina, Elena ..... DY 44.11
Pylypovskyi, Oleksandr ..... MA 44.6, MA 49.5, TT 76.6
Pylypovskyi, Oleksandr V. .. MA 7.20, MA 30.8, •MA 44.7, •TT 76.7
Pyrialakos, Georgios G. ..... DY 48.6

Pyrpassopoulos, Serapion . . •BP 12.2
Qahosh, Mohammed . . . . . O 2.2
Qaisrani, Muhammad Nawaz CPP 48.3
Qaisrani, Nawaz . . . . . CPP 9.6
Qaiumzadeh, Alireza . . . . . MA 51.5, TT 88.5
Qamar, Rabia . . . . . CPP 19.4, DY 20.4
Qazi, Saib . . . . . CPP 57.4
Qazi, Saib Jahan . . . . . •CPP 17.22
Qazvini, Hamed . . . . . BP 16.9
Qi, Jing . . . . . O 31.6
Qi, Ruoxuan . . CPP 17.26, •CPP 17.32
Qi, Siyuan . . . . . •AKPIK 6.1
Qi, Yanpeng . . . . . MA 7.34
Qian, Chen . •MM 9.4, O 62.4, TT 54.4
Qiang, Yicheng . . . . . BP 7.6, CPP 10.4, DY 16.4, DY 33.4, •DY 49.2
Qiao, Junfeng . . . . . MM 17.4
Qiao, Le . . . . . •BP 29.4, •CPP 45.4
Qiao, Yulong . . . . . •DY 9.9
Qiu, Caihao . . . . . MM 30.1
Qiu, Jonny . . . . . •HL 18.1, MA 59.5, •TT 32.1
Qiu, Yan Yan Grisan . . . . . O 83.4
Qiu, Zheru . . . . . DS 20.33, QI 2.6
Qu, Bin . . . . . BP 40.2
Qu, Jinping . . . . . CPP 28.1, DY 29.1
Qu, Shitao . . . . . •TT 23.15
Quail, Thomas . . . . . BP 12.10
Quan, Haoyuan . . . . . •DY 54.4, O 25.2
Quan, Jingkai . . . . . •O 79.3
Quas, Annemarie . . . . . •BP 14.59
Quasebarth, Gwendolyn . . . . SOE 16.1
Queisser, Friedemann O 59.5, •O 62.1, O 71.1, O 71.18, TT 2.5, TT 23.35, TT 48.5, •TT 54.1, TT 66.1, TT 66.18
Quek, Su Y. . . . . DS 21.5
Quek, Su Ying . . . . . HL 20.11
Quensen, Martin . . . . . QI 15.3
Quenter, Ruwen . . . . . •O 42.8, O 93.4
Querci, Lapo . . . . . O 42.4
Querlioz, Damien . . . . . •SYBT 1.5
Quesada Pérez, Carlos . . . . . •O 17.6
Quidant, Romain CPP 10.12, DY 16.12
Quin, Michael . . . . . •AKBP 4.5
Quintern, Matthias . . . . . •HL 1.1
Quitmann, Christoph . . . . . •AKBP 8.6, •AIW 2.2, •AIW 2.5
Quoika, Patrick K. . . . . BP 18.2
Qvarfort, Sofia . . . . . QI 17.3
R. B. Thomassen, Patrick . . . MA 6.11
R. Nagy, Péter . . . . . BP 2.10
R. Puente-Uriona, Álvaro . . . . . TT 71.7
R.T. Zahn, Dietrich . . . . . O 79.6
Raab, Klaus . . . . . MA 21.1, MA 55.3
Raabe, Dierk . . . . . FM 5.8, MM 9.1, MM 15.4, MM 34.5, MM 39.6
Raabe, Jörg . . . . . DS 6.1, •MA 7.81, MA 46.4
Raabgrund, Andreas . O 72.5, TT 67.5
Rabe, Anna . . . . . MA 36.1
Rabe, Thorid . . . . . DD 39.1, DD 39.3
Rabia, Rabia . . . . . •CPP 46.4
Rabkin, Eugen . . . . . MM 21.2
Rabl, Peter . . . . . MA 23.1, TT 23.28, TT 35.1, TT 43.11, QI 14.5, QI 18.3
Raboni Ferreira, Marina . . . . . MA 6.4
Raboni-Ferreira, Marina . . . . •MA 6.10
Rachel, Stephan . . . . . O 15.8, •TT 15.1, TT 29.7, TT 56.12
Rachow, Fabian . . . . . O 23.3
Räcker, Günther . . . . . BP 11.1
Radaelli, Paolo . . . . . MA 4.3
Radhakrishnan, Harini . . . . . TT 64.1
Radice, Emma . . . . . •DS 14.5
Radke, Lucas . . . . . TT 43.4
Rädler, Joachim . . . BP 7.42, BP 26.3, BP 26.4, BP 37.4, CPP 43.3, CPP 43.4
Radoslaw Piatek, Marcin . . CPP 29.5
Radova, Mariia . . . . . O 4.1
Radovic, M. . . . . MA 25.6
Radtke, Guillaume . FM 15.1, MM 41.9
Radu, F . . . . . MA 19.7, TT 31.7
Radu, Florin . . . . . DS 12.9, MA 7.47, MA 16.4, MA 30.8
Radulov, Iliya . . . MA 52.31, MA 52.32
Raeliarijaona, Aldo . . . . . •FM 4.3
Rafaja, David . . . . . MM 13.3
Rafiezadeh, Shohreh . . . . . O 23.7
Rahat, Md. Zobaer Ahmed CPP 17.22
Rahause, Crina . . . . . •CPP 46.8
Rahe, Philipp . . . O 5.5, O 36.2, O 44.5
Rahimi, Ahmad . . . . HL 55.7, HL 56.4, HL 56.5
Rahimi-Iman, Arash . . . . . •TUT 3.1, •AKPIK 1.1, •AKPIK 3.5, AKPIK 5.10
Rahimkhani, Masoumeh . . . . •TT 23.9
Rahimzadeh, Amin . . . . . •CPP 30.4, CPP 46.13
Rahm, Marco . . . . . •AKPIK 4.2
Rahman, Mohammad Mostafizar •CPP 16.3
Rahman, Mostafizar . . . . . CPP 17.39
Rahmel, Rebecca . . . . . •O 57.5
Rahn, Marein . . . . . MA 11.3, •MA 16.1, TT 21.3, TT 81.6
Rai, Venus . . . . . •MA 46.1
Rai, Vibhuti . . . . . O 12.1, O 43.9
Rai, Vibhuti N. . . . . O 43.6, •O 80.4
Raif, Patrick . . . . . •QI 14.25
Raimondi, Roberto . . . . . MA 33.9
Rainò, Gabriele . . . . . HL 20.49
Raissi, Zahra . . . . . •QI 21.2
Raith, Liesa . . . . . HL 56.4, HL 56.5
Raja, Arslan Sajid . . . . . QI 2.6
Rajabpour, Siavash . . . . . HL 20.11
Rajak, Soumyajit . . . . . O 55.4
Rajapitamahuni, Anil . . . . . HL 24.10
Rajaraman, Gopalan . . . . . MA 42.6
Raji, A. . . . . TT 69.3
Raji, Aravind . . . . . TT 69.4
Rakovszky, Tibor . . . . . QI 21.9
Rakow, Tom . . . . . HL 55.10
Ralf, Bechstein . . . . . O 5.2
Ráliš, Vojtěch . . . . . •MA 34.5
Ralko, Arnaud . . . . . TT 4.2
Ramakrishna, Kushal . . . . . •MM 22.7
Raman, Shreyas . . . . . DY 2.2, TT 1.2
Ramasamy, Parthiban . . . . . MM 35.1
Ramasubramaniam, Ashwin HL 39.10
Ramchandani, Sagar . . . . . •TT 33.4
Ramermann, Daniela . . . . . •CPP 4.3
Ramirez Amado, Johan Sebastian MA 9.3
Ramírez-Atencia, Cristian . . . . . O 47.4
Rampp, Michael A. . DY 32.5, TT 45.5
Ramsauer, Bernhard . . . . . •O 8.4
Ramsauer, Sebastian . . . . . TT 73.7
Ramsey, Michael G. . . . O 61.1, O 83.2
Ramsperger, Anja F. R. M. . . CPP 41.7
Ramzan, Muhammad Sufyan CPP 26.2, HL 20.14, HL 54.1, O 10.6, TT 16.6
Ran, Yan . . . . . •CPP 4.5
Rana, Mohammad Jony . . . . CPP 16.3
Rana, Navdeep . . . . . DY 62.9
Rana, Sravendra . . . . . CPP 41.4
Rana, Vidisha . . •AKBP 5.4, AKBP 6.5
Randall Heinrich, Sierra . . . •FM 11.33
Ranecki, Robert O 17.4, O 77.5, O 77.6, •O 83.10
Ranft, Jonas . . . . . DY 49.3
Ranftl, Demian . . . . . •TT 42.6
Rangel Hernandez, Rodolfo A. TT 57.5, •TT 94.6
Rani, Pooja . . . . . •FM 23.3
Rani Sahoo, Krishna . . . . . MA 12.1
Ranitzsch, Philipp . . . . . TT 82.3
Ranjan, Nisha . . . . . •O 19.1
Ranna, A. . . . . •TT 69.6
Ranoo, Surojit . . . . . CPP 49.1
Rapaka, Narsimha . . . . . QI 5.6
Rapf, Dominic . . . . . HL 9.4, HL 12.5
Rapp, Julian . . . . . QI 2.2
Rappe, Andrew . . . . . •MA 4.1
Rappich, Jörg . . . . . O 13.11
Rappold, Mechthild BP 1.10, CPP 1.10, DY 4.10
Rasabathina, Lokesh DS 18.1, DS 18.3
Raschke, Markus . . . . . HL 46.1
Raschke, Paul . . . . . DY 40.3
Rasheed, Ahmed . . . . . MA 52.34, MA 52.36
Raskhodchikov, Dimitri . . . . . MA 52.5, MA 52.14
Raskhodchikov, Dmitrii . . . . . MA 9.13
Rasouli, Hamid Reza . . . . . BP 26.11, CPP 43.11, •DS 14.9
Raspagni, Valentina . . . . . CPP 46.6
Rass, J. . . . . HL 37.6
Rastelli, Armando . . . . . HL 20.38
Rastogi, Shivani . . . . . MA 13.6
Rasulyar, M. . . . . •HL 20.39
Rata, Aurora Diana . . . . . MA 30.12
Rata, Diana . . . . . •MA 39.15
Räth, Christoph . . . . . •DY 6.8
Rath, Gabriel . . . . . QI 17.1
Rathod, Shivam . . . . . TT 61.4
Ratschmeier, Björn . . . . . •O 25.1
Ratzke, Markus . . . . . O 96.6
Ratzker, Barak . . . . . FM 2.1, MM 15.4
Rau, Jeffrey G. . . . . MA 31.1, TT 47.1
Rauh, Manfred . . . . . BP 7.44
Rauhut, Guntram . . . . . O 88.6
Rauls, Simon . . . . . FM 11.31
Raum, Yorick . . . . . QI 18.7
Rauschenbach, Stephan . . . BP 14.77, •O 19.3, O 19.9, O 35.7, O 69.13
Raußendorf, Robert . . . . . QI 16.3
Raussendorf, Robert . . TT 17.6, QI 4.6
Rave, Lucas . . . . . •DS 16.3, DS 20.10
Ravesteyn, Thomas W. van . BP 32.11, DY 52.11
Ravichandir, Shashank . . . . . •DY 55.4
Ravishankar, Rachappa . . . . . MA 6.3
Ravoo, Bart Jan . . . . . BP 7.27
Rawat, Nidhi . . . . . •O 48.4
Ray, Avijeet . . . . . •MA 2.1
Ray, Debes . . . . . BP 39.4, CPP 55.4
Ray, Nathan . . . . . AKBP 8.3
Raya-Moreno, Martí . . . . . HL 23.2, AKjDPG 1.4
Raza, Syed A. . . AKBP 5.2, •AKBP 8.5
Razavi, Atieh . . . . . CPP 46.13
Razavi, Sepideh . . . . . BP 5.2
Razpopov, Aleksandar . . . . . MA 33.10
Razumovskiy, Vsevolod . . . . MM 21.4
Razumovskiy, Vsevolod I. . . MM 41.6
Razzoli, E. . . . . MA 25.6
Razzoli, Elia . . . . . MA 38.13
Reale, Stefano . . . . . O 15.6, O 15.9
Reascos, Leander . . . •HL 38.8, QI 3.5
Rebl, Henrike . . . . . BP 33.9
Recher, Patrik . . . . . TT 15.10
Reck, Kristian . . CPP 17.15, CPP 17.42
Reddy, Vibha . O 33.3, •O 62.6, O 66.8, •TT 54.6
Redi, Laxman Nagi . . . . . O 93.6
Reecht, Gaël . . . . O 9.9, O 17.8, O 44.1, •O 59.5, O 71.1, O 71.18, •TT 48.5, TT 66.1, TT 66.18
Reehuis, Manfred . . . . . TT 57.2
Reents, Timo . . . . . •MM 13.9
Reese, Greta S. . . . . •TT 56.2
Regmi, Resham B. MA 33.11, MA 54.8
Rehberg, Ingo . . . •MA 46.3, MA 52.30
Rehfeldt, Florian . . . . . BP 27.9
Rehfeldt, Tom . . . . . •MA 36.3
Rehm, Jana . . . . . DS 9.5
Rehm, O. . . . . •DS 3.4
Rehm, Oliver FM 4.2, FM 23.4, O 19.2, O 93.2
Rehwald, Martin AKBP 6.1, AKBP 6.2, AKBP 6.5, AKBP 8.8
Reich, Adrian . . . . . •TT 85.6
Reich, Johanna . . . . . O 23.9
Reichelt, Matthias . . . . . •HL 1.3
Reichelt, Stephan . . . . . MA 7.80
Reichert, Joachim . . . . . O 9.4, O 45.4, O 83.1
Reichl, Christian . . . HL 10.5, HL 29.4, HL 38.2, TT 20.5, TT 58.4
Reichling, Michael . . . . . O 39.2
Reichlova, H. . . . . MA 47.7
Reichlová, Helena . . MA 7.52, MA 8.3
Reichman, David R. . . . . HL 23.7
Reichmann, Klaus . . . . . MM 4.4
Reif, Miriam . . . . . TT 22.36
Reifenberg, Andreas . . . . . TT 82.2
Reifenberger, A. . . . . TT 22.31
Reifenberger, Andreas . . . . . TT 22.20, TT 22.21, TT 22.22, TT 22.27, TT 22.28, TT 22.29, TT 22.30, TT 28.2
Reiker, Tobias . . . . CPP 17.11, DS 20.7
Reim, Luca B. . . . . •HL 45.2
Reimann, Andre . . . . . O 84.6, TT 84.6
Reimann, Jonas . . . . . •TT 44.4
Reimer, Maike . . . . . •AKC 1.2
Rein, Kevin . . . . . MM 16.3
Reina-Galvez, Jose . . . . O 15.2, O 17.9, O 99.4
Reinauer, Alexander . . . . . •DY 44.16
Reineke, Sebastian . . . . . CPP 17.12, CPP 17.13, CPP 29.1, CPP 29.3, CPP 37.3, HL 26.16
Reiner, Jan . . . . . QI 14.4
Reiner, Jan-Michael . . . . . MA 6.8
Reinert, Friedrich . . . MA 47.5, O 42.7, O 48.5, O 76.1, O 80.5, TT 25.11
Reingruber, Adrien . . . . . MM 26.5, •O 62.10, •TT 54.10, TT 92.13
Reinhard, Marco . . . DS 14.9, FM 11.31
Reinhard, Richter . . . DY 19.9, DY 25.2, •DY 41.2
Reinhardt, Dominic . . . . . HL 26.32
Reinhardt, Simon . . . . . •TT 43.8
Reinhart, Max . . . . . •TT 5.1
Reinheimer, Sonja •O 71.17, •TT 66.17
Reinhold, Tom . . . . . DS 14.9
Reining, Lucia . . . . . MM 37.1, O 59.6, TT 48.6
Reinken, Henning . . . . . •CPP 20.8, •DY 23.8
Reinold, Anneke . . . MA 7.46, MA 12.4
Reis, Fabio . . . . . DS 1.1
Reischl, Bernhard . . . . . O 5.3
Reiser, Andreas . . TT 22.18, TT 22.19
Reiser, Pablo . . . . . •DY 42.8, •TT 63.8
Reiser, Patrick . . . . . MA 43.4
Reiserer, Andreas . . . . . •QI 6.1
Reißig, Luca . . . . . UP 6.2
Reiss, Günter . . . . . CPP 3.4, MA 7.54, MA 7.62, MA 7.63, MA 47.8, MA 54.11
Reiter, Florentin . . . . . QI 13.3, QI 16.7
Reiter, Günter . . . . . CPP 17.43
Reith, Heiko . . . . . DS 20.51, MA 13.3
Reitner, Matthias . . . . . TT 13.7
Reitzenstein, Stephan . . . . . HL 13.1, HL 20.28, HL 54.6, HL 54.7, HL 55.1, AKPIK 3.4
Rejman, Sebastian . . . . . •AKPIK 3.2
Rejnhardt, P. . . . . CPP 32.3, DY 35.3
Rellinghaus, Bernd . . DS 4.1, FM 19.1, FM 19.4, HL 22.6, MA 3.11, MA 7.65, MA 7.82
Remalli, Nagarjuna . . . . . •MM 21.1, MM 21.9
Rembold, Phila . . . . . QI 13.8
Remini, Khalil . . . . . •CPP 8.4
Remy, Quentin . . . . . MA 7.8, •MA 27.1
Ren, Wei . . . . . MA 8.7
Ren, Xinguo . . . . . O 12.3
Renard, Vincent . . . . . O 74.6, TT 68.6
Renard, Vincent S . . . . O 62.3, TT 54.3
Renard, Vincent T. . . . . O 62.2, O 62.3, TT 54.2, TT 54.3
Renck, Louis . . . . . •DY 42.4, •TT 63.4
Rende, Eric . . . . . CPP 46.37
Rene, Alexandre . . . DY 58.7, SOE 17.7
Renger, Jan . . . . . BP 33.4
Renger, Markus . . . . . TT 22.22
Renn, Lukas . . . . . DS 20.50
Rentschler, Eva . . . . . MA 36.9, O 61.7, O 83.10
Rentzsch, Anne . . . . . •AKPIK 6.6
Renz, Luise . . . O 15.4, O 17.7, •O 17.11, O 89.3, O 99.10
Renz, Wolfgang . . . . . SOE 10.1
Řepa, Rostislav . . . . . •O 27.1, O 96.7
Repček, Dalibor . . . . . MA 25.8
Repke, Jens-Uwe . . . . . DY 41.15
Repp, Jascha . . O 9.10, O 9.12, O 12.8, O 83.5
Resch, Christoph . . . . . MA 9.11
Resch, Lucas . . . . . •QI 21.8
Resch, Miriam . . . . . QI 20.2
Residori, Mirko . . . . . BP 1.2, •BP 1.5, CPP 1.2, •CPP 1.5, DY 4.2, •DY 4.5
Resmann, Emma . . . . . TT 24.3
Ressouche, Eric . . . . . MA 47.10
Rethfeld, Baerbel . . . . . O 40.1, O 40.2, O 40.3, O 40.4, O 40.5, O 40.6, O 98.6, TT 37.1, TT 37.2, TT 37.3, TT 37.4, TT 37.5, TT 37.6
Reticcioli, Michele . . . . . O 93.8
Rettenberger-Zweck, Julian •QI 12.10
Rettig, L. . . . . •MA 27.8
Rettig, Laurenz . . . . MA 7.16, MA 7.18, MA 27.2, O 27.5, O 38.4, O 38.7, O 40.11, O 98.4, O 98.7, TT 37.11
Reuer, Kevin . . . . . QI 16.10
reul, michiel . . . . . O 44.8
Reupert, Aaron . . . . . DS 13.2
Reustlen, Denise . . . MA 29.8, TT 46.8
Reuter, Danny . . . . . TT 43.4
Reuter, Dirk . . . . . HL 48.7
Reuter, K. . . . . O 57.6, O 88.11
Reuter, Karsten CPP 15.7, CPP 46.66, DS 14.1, DY 6.12, DY 14.5, DY 41.12, DY 43.4, DY 43.7, FM 5.7, FM 11.13, MM 5.4, MM 8.9, MM 9.9, MM 12.5, MM 13.5, MM 13.7, MM 19.8, MM 19.11, MM 19.12, MM 19.14, MM 22.1, MM 22.9, MM 31.10, MM 37.2, MM 41.7, O 13.1, O 13.2, O 13.8, O 18.5, O 23.4, O 23.5, O 24.3, O 34.1, O 55.5, O 65.3, O 65.8, O 65.11, O 81.3, O 81.7, O 85.6, O 86.10, O 88.3, O 96.8, O 97.7, O 97.10, O 97.11
Reuter, Ricarda . . . . . •MA 7.77
Reutter, Andreas . . . . . O 43.14

Reutzel, Marcel ..... •PRV V, O 14.10, O 40.18, O 40.19, O 40.20, O 40.21, O 66.9, O 98.10, TT 37.18, TT 37.19, TT 37.20, TT 37.21, TT 44.9
Reventlow, Bertram ..... •UP 7.3
Reyher, Thomas ..... MA 7.33
Reynaerts, Robby ..... •O 69.11
Reznik, Dmitry .... MA 39.18, TT 95.2
Rheinlaender, Johannes .... •BP 27.6
Rhensius, Jan ..... MA 6.2
Rhode, Christian ..... FM 11.21
Rhodes, Luke ..... O 93.7
Rhodes, Luke C. ..... O 93.5, TT 5.10, TT 29.2
Rhouma, Taher ..... O 74.6, •TT 4.3, TT 68.6
Riabov, Maksim ..... DS 14.4
Riahi, Mohamed K. ..... QI 5.6
Rial, Javier ..... MA 7.52
Riazanova, A.V. ..... MA 7.21
Ribechini, Asier ..... •TT 71.7
Ribeiro de Assis, Ismael ... •MA 55.1
Ribeiro, Pedro ..... QI 9.4
Ricci, Emanuele ..... •TT 23.19
Ricci, Pier Carlo ..... CPP 12.4
Riccius, Felix .... MM 19.12, •O 86.10
Richard, C ..... BP 27.8, BP 37.2
Richard, Christopher J. .... AKBP 3.4
Richard, Léa TT 22.25, QI 8.3, QI 11.6, QI 11.9
Richter, Andreas ..... UP 6.2
Richter, Carsten ..... FM 23.6
Richter, Christine ..... O 14.1, O 93.6
Richter, Clemens CPP 19.5, CPP 27.3, DY 20.5, DY 26.3
Richter, Jona ..... HL 18.5, •HL 26.1, TT 32.5
Richter, Julia ..... •FM 7.5
Richter, Justus ... •O 40.10, •TT 37.10
Richter, Klaus ..... DS 8.3, DY 42.13, DY 59.5, TT 63.13, TT 74.12, TT 97.2, TT 99.5
Richter, Lea ..... O 76.7
Richter, Marten ..... HL 20.2
Richter, Martin ..... •O 46.3
Richter, Peter ..... •O 31.1, O 93.1
Richter, Ralf ..... CPP 26.5, CPP 31.6
Richter, Stefan ..... •QI 14.1
Rickert, Lucas ..... QI 18.7
Rickert, Simon Christian ..... O 77.4
Rickhoff, Clara ..... •BP 14.20
Rico, Albert ..... •QI 15.5, QI 15.8
Rico, Enrique ..... QI 3.1
Riddiford, Lauren J. ..... FM 23.5
Ridgen, Jennifer ..... O 66.8
Ridier, Karl ..... O 17.8, O 83.3
Ridley, Ch. ..... CPP 32.3, DY 35.3
Rieche, Antonia •MA 30.12, MA 39.15, O 38.3
Riedel, Björn ..... •O 88.10
Riedel, Moritz ..... DY 15.2
Riedel, Saskia ..... •DD 16.1
Riedel, Tim .... O 7.5, O 70.3, O 71.16, O 71.19, O 71.21, TT 9.5, TT 65.3, TT 66.16, TT 66.19, TT 66.21
Riedel, Uwe ..... PSV I, •SYSC 1.4
Rieger, Dennis TT 14.2, QI 11.4, QI 11.5
Rieger, Hanna ..... CPP 14.7
Rieger, Heiko .... CPP 11.1, CPP 11.11, CPP 11.12, DY 17.1, DY 17.11, DY 17.12, DY 21.3, DY 44.9, DY 44.10
Rieger, Philipp .... •MA 7.11, MA 14.3, MA 40.10
Riegler, Peter ..... TUT 2.1, DD 1.1
Riemer, F. ..... BP 27.8, BP 37.2
Rienitz, Olaf ..... FM 5.11
rienks, emile ..... TT 25.11
Riepl, Josef ..... HL 39.8, MA 12.2
Riese, Daniel ..... MA 12.2
Riesterer, Felix ..... •DY 54.9
Rieth, Tim ..... HL 12.7, O 97.8
Rigamonti, Santiago ..... MM 9.6
Rigden, Jenny ..... O 76.5
Righi, Maria Clelia ..... DS 13.4
Rignanese, Gian-Marco ... AKPIK 6.7
Rigo, Jonas ..... DY 14.13, DY 53.6, •MA 34.10, TT 87.6
Rigvedi, Prajwal .. MA 7.13, •MA 30.2, O 84.9, TT 84.9
Rilloraza, Paco ..... TT 51.12
Rimek, F. ..... HL 17.7, HL 20.39
Rimek, Fabio ..... HL 55.5, HL 55.6
Rinaldi, Matteo ..... MM 12.5
Ringbauer, Martin ..... QI 15.2
Ringel, Zohar ..... DY 58.8, SOE 17.8
Ringleb, Andreas ..... •JOB 1.2
Ringling, Julian ... CPP 20.3, DY 23.3
Rinke, Patrick ..... CPP 38.2, HL 4.6, MM 9.5, MM 19.9, AKPIK 2.1
Ripoll, Marisol .... BP 14.12, •DY 34.1
Rishi, Chaurasia ..... CPP 8.5
Ritcher, Christine ..... O 76.3
Ritschel, Christian ..... BP 9.5
Rittaud, Antoine ..... BP 12.2
Ritter, Christian ..... TT 22.29
Ritterhoff, Christian L. ..... MM 19.6, •MM 19.10
Ritzinger, P. ..... MA 47.7
Ritz-Zwilling, Anna ..... •TT 74.9
Riva, Michele ..... O 94.5
Riva, Simone ..... •CPP 21.2
Rivas, Daniel E. ..... AKBP 8.7
Rivera Hernandez, Sergio ... •DD 41.1
Rivero, Pedro ..... QI 3.1
Riwar, Roman-Pascal ..... TT 43.1, •TT 53.7, TT 83.8
Rizzi, Matteo ..... DY 32.1, TT 45.1, TT 73.12
Robertson, Hayden ..... CPP 29.4, CPP 39.5
Robillard, Alexander N. ... •MM 19.39
Robinson, Jeremy ..... DS 12.3
Robinson, Joshua ..... DY 43.11
Robinson, Joshua A. ..... DS 21.5, HL 20.11, O 33.3, O 66.4
Robles, Roberto ..... O 35.1, O 35.2, O 35.3, O 77.1
Robnik, Marko ..... DY 32.9, TT 45.9
Robson, Drew N. ..... BP 14.68
Rocco, Maria Luiza Miranda CPP 37.5
Roch, Nicolas ..... •TT 50.3
Rockinger, Tobias .. HL 30.2, TT 59.2
Rockstuhl, Carsten ... DS 21.2, O 12.1, O 46.3
Rödel, Max ..... O 96.1
Rödel, Maximilian .. HL 15.2, •O 43.17
Rodemund, Tom Simon ..... DY 59.3, TT 99.3
Roden, Stephanie .. •O 40.6, •TT 37.6
Rodenbücher, Christian .... •MM 27.4
Röder, Falk ..... FM 19.9, MA 57.6
Rodgers, Andrew ..... FM 12.6
Rodier, Clement ..... BP 37.12
Rodin, Aleksandr ..... O 9.5
Rodney, David ..... •MM 6.1
Rodrigues, Davi R. ..... MA 55.2
Rodriguez, A. ..... HL 20.27
Rodríguez Agudo, José Alberto CPP 15.2
Rodriguez, Alberto ..... HL 47.1
Rodriguez, Anne ..... HL 3.9
Rodriguez, Constanza ..... CPP 33.4
Rodriguez Diaz, Fernando . CPP 23.1, DY 24.1
Rodríguez Fernández, Sergio •MA 7.55
Rodríguez Gómez, Laura ... •DD 16.3
Rodriguez, Jean-Baptiste ... HL 29.5, TT 58.5
Rodriguez, Victor CPP 17.7, CPP 22.6
Rodriguez-Barea, Borja ..... FM 11.36
Rodriguez-Fernandez, Angel O 40.15, O 98.3, TT 37.15
Roelcke, Carmen ..... O 12.8
Roeper, Matthias .. FM 12.2, FM 14.2, •FM 18.3
Roesch, Diego ..... •BP 14.18
Roffay, Chloé ..... BP 3.10
Rog, Matthijs ..... •TT 28.4, TT 57.9, QI 20.8
Rogal, Jutta ..... DY 14.2, O 86.10
Rogalev, Andrei ..... MA 51.1, TT 88.1
Rogalev, Victor ..... O 8.5
Rogalla, Pascal S. •BP 32.4, •DY 52.4
Rogero, Celia ..... O 10.2, TT 16.2
Rogers, Andrew ..... FM 12.5
Rogge, Uwe ..... TT 14.1
Rohde, Lisa ..... •DY 62.4
Rohlfing, Michael ... HL 3.2, HL 25.2, MA 52.1, O 7.3, O 61.2, TT 9.3
Röhlsberger, Ralf ..... DS 13.2
Rohrbach, Alexander ..... BP 14.82, BP 33.2, BP 40.4
Rohringer, Georg ..... •TT 10.3
Röhrl, Michael .... CPP 27.2, DY 26.2
Rohrmüller, Korbinian ..... DS 8.3
Rohshap, Stefan ..... TT 23.23
Roichman, Yael ..... DY 21.9
Rojas, Susana ..... BP 5.3
Rojas-Castillo, Julián D. ..... O 15.3
Rolapp, Alexander .. DS 14.9, HL 31.3
Roldan Cuenya, Beatriz ..... O 65.5
Roling, Bernhard ..... •CPP 16.1
Röll, David ..... •TT 23.1
Rölleke, Ulrike ..... BP 7.14, BP 14.30, BP 40.1
Rolli, Rolf ..... MM 34.2
Rollinde, Emmanuel ..... DD 22.2
Roma, Riccardo ..... •QI 3.9
Romaguera, Arnau C. ..... MA 38.13
Roman, Kuzian ..... TT 94.4
Román, Ricardo Javier Peña . TT 92.1
Roman, Sabin ..... •UP 5.5
Romanczuk, Pawel ..... BP 14.90, BP 36.8, BP 36.9, CPP 11.7, DY 17.7, DY 57.8, DY 57.9, SOE 4.4, •SOE 5.2
Romanin, Davide ..... MA 33.12
Romeiro, João ..... QI 8.3
Romeis, Dirk .... CPP 31.7, •CPP 42.3
Romen, Anton ..... •TT 2.3
Romeo, Michelangelo ..... O 12.4
Romero, Camila .... BP 36.7, DY 57.7
Romero-Lara, Francisco ..... •O 99.7
Romero-Muniz, Carlos ..... FM 11.24
Romhányi, Judit ..... QI 2.8
Römling, Ute ..... BP 7.9
Romodin, Mikhail ..... CPP 12.5
Ron, Alon ..... MA 11.2, TT 21.2
Ronceray, Pierre .. CPP 20.2, DY 23.2
Rončević, Igor ..... O 3.2, O 9.12
Rondoni, Lamberto ..... DY 47.1
Rong, Alena ..... MA 39.7
Ronning, Carsten ... DS 13.2, DS 16.7, DS 16.8, DS 20.8, DS 20.16, DS 20.33, HL 16.7, HL 20.21, HL 26.47, HL 35.4, HL 35.5, HL 56.3
Rønnow, Henrik M. ..... TT 22.33
Rontani, Massimo ..... TT 10.6
Röntgen, Malte ..... DY 59.4, TT 99.4
Roosz, Gergo ..... •TT 10.1
Root, Maxim ..... •DY 49.9
Ropers, Claus ..... FM 11.33, HL 8.5, MA 27.3, MA 55.6, O 22.2, O 22.3, O 40.13, O 49.3, O 79.7, O 86.2, O 86.7, TT 37.13, QI 2.6, AKBP 4.3, AKBP 9.6
Ropert, Samuel ..... •BP 8.6
Roque dos Santos, Edmilson •DY 6.11
Rosa, Bárbara ..... HL 54.7
Rosa, Priscila ..... MA 11.3, TT 21.3, TT 62.3
Rosa, Priscila F. S. ..... TT 52.3
Rosati, Francesco ..... QI 17.1
Roßbach, Jon ..... AKBP 7.4
Rosch, Achim ..... DY 63.5, MA 7.69, MA 23.6, O 89.8, TT 35.6, TT 61.2, TT 61.11, TT 98.8
Rösch, Niels ..... •DS 20.42
Rose, Hendrik ..... HL 1.5, QI 14.22
Rose, Jonas ..... •HL 24.6, HL 35.1
Rose, Marc-Andre ..... O 79.4
Roseker, Wojciech ..... HL 4.1
Rosén, S. ..... TT 22.31
Rosenauer, Andreas HL 9.1, HL 20.66, HL 24.1
Rosenberg, Margaret ..... •CPP 30.2, DY 49.11
Rosenow, Bernd ... DY 58.3, DY 58.4, SOE 17.3, SOE 17.4, TT 64.1, TT 83.9, QI 17.5
Rosenzweig, Philipp .. O 62.6, O 74.5, TT 54.6, TT 68.5
Rosfelter, Anne ..... BP 3.5
Roshap, Jheng-Wei ..... TT 23.23
Roskamp, Thijs ..... •TT 28.5
Rosławska, Anna ..... •PRV III, O 9.8, O 12.6, O 95.6, TT 96.6
Rößler, Annegret ..... •PSV VI
Rößler, Clemens ..... •HL 22.1
Rößler, Sahana ..... •MA 2.6, TT 98.1
Rößler, Ulrich K. ..... MA 2.6, TT 57.2
Rösner, Benedikt ..... MA 46.4
Rosner, H. ..... TT 62.5
Rösner, Harald ..... MM 3.5, MM 18.1
Rosner, Helge ..... MA 2.6, MA 34.2, TT 61.3, •TT 94.3
Rösner, Malte ..... MA 34.9, O 76.4, TT 12.7, TT 27.4, TT 51.1, TT 92.18
Rosnes, Andreas ... •FM 10.2, HL 9.5
Rosowski, Frank ..... O 23.4, O 81.7
Ross, Caroline A. ..... MA 37.2
Ross, Frances M. ..... HL 13.5
Ross, Jackson ..... MA 43.6
Ross, Ulrich ..... DS 16.10
Rossetti, Andrea ..... •O 43.4, O 43.8
Rossetti, Leone ..... BP 27.2
Rossetto, Riccardo ..... •BP 14.95, BP 32.1, DY 52.1
Rossi, Antonella ... MA 29.3, TT 46.3
Rossi, Giorgio ..... O 38.2
Rossi, Mariana ..... DY 14.8, DY 14.9, O 9.2, O 11.6, O 14.7, O 59.8, O 61.5, O 72.6, O 86.5, TT 48.8, TT 67.6
Rossi, T. C. ..... HL 46.6
Rossi, Thomas C. ..... •HL 8.10
Rössiger, Carina ..... CPP 17.8
Rossini, Mirko ..... •DY 40.3, QI 20.2
Rössle, M. ..... HL 46.6
Rössle, Matthias ..... HL 26.52
Rossnagel, K. O 19.10, O 59.2, TT 48.2
Rossnagel, Kai .... HL 39.2, MA 24.3, O 7.5, O 14.4, O 59.5, O 66.4, O 70.3, O 71.1, O 71.16, O 71.17, O 71.18, O 71.19, O 71.20, O 71.21, TT 9.5, TT 14.4, TT 25.11, TT 36.3, TT 48.5, TT 65.3, TT 66.1, TT 66.16, TT 66.17, TT 66.18, TT 66.19, TT 66.20, TT 66.21
Rosso, Kevin ..... O 97.2
Rost, Andreas W. ..... TT 29.5
Rost, Marcel J. ..... •O 97.9
Rostami, Habib ... DY 42.8, HL 24.12, •MA 8.2, MM 15.1, TT 63.8
Röstek, Anita ..... FM 5.11
Roszak, Katarzyna . DY 53.5, TT 87.5, QI 9.2, QI 14.2
Rotenberg, Eli ..... MA 5.8, TT 7.8
Roth, Christopher .. DY 58.1, SOE 17.1
Roth, Heinrich T. ..... •CPP 24.2
Roth, Jakob ..... O 46.2, •O 46.4
Roth, Johannes ... MM 19.38, O 29.1, O 29.3, •O 94.11
Roth, S. ..... O 19.10
Roth, Siegmar ..... TT 14.4
Roth, Stephan V. CPP 15.1, CPP 17.15, CPP 17.42, CPP 25.4, CPP 32.4, •CPP 38.4, CPP 44.3, CPP 46.24, CPP 46.45, CPP 46.51, DY 35.4
Roth, Tobias Alexander ..... •DY 41.8
Rothe, Carsten ..... HL 26.16
Rothe, Karl ..... O 74.7, TT 68.7
Rothfuchs-Engels, Charlotte HL 20.35
Rothhardt, Daniel .... •O 9.11, O 44.12
Rothmund, Benedict ..... TT 43.4
Rothörl, Jan ..... MA 21.1, AKPIK 5.6
Rott, Karsten ... CPP 46.14, MA 7.54, MA 7.62, MA 7.63, MA 47.8
Rott, Kathrin ..... •BP 14.40
Rotter, Martin ..... MA 55.11
Röttger, Arne ..... MM 19.48
Rotthardt, Daniel ... MA 44.2, TT 76.2
Rottstaedt, Yves ..... •QI 17.5
Rotzinger, Hannes .. O 19.7, TT 22.11, TT 22.14, TT 22.15, TT 22.16, TT 43.2, TT 43.3, TT 43.4, TT 43.7
Rouches, Mason ... BP 32.5, DY 52.5
Rouco, Victor ..... MA 3.1
Roulleau, Preden ... HL 29.2, TT 58.2
Rousseau, Roger ..... O 65.10
Rout, Jyotiranjan ..... •MA 17.4
Rout, Minushree ..... •HL 3.7
Rouxel, Malo ..... TT 26.1
Rouzegar, Reza ..... MA 7.8, MA 27.1
Roy, Arnab BP 10.2, CPP 18.2, DY 18.2
Roy, Debojyoti ..... •O 51.2
Roy, Nicolas ..... AKPIK 5.10
Roy, Niloyendu .•CPP 10.11, •DY 16.11, DY 54.3
Roy, Renjith Mathew ..... TT 12.6
Roy, Saswata ..... TT 43.8
Roy, Subhojit ..... •TT 29.9
Roy, Tanay ..... QI 14.13
Roy-Chowdhury, Mouli ..... MA 39.18
Roychowdhury, Subhajit .... MM 40.3
Rozov, Pavel ..... •MM 19.13
Rózsa, Levente ... MA 7.68, MA 12.3, MA 55.7, •MA 58.4, TT 15.12, TT 15.13
Ruan, Zilin ... •O 61.4, O 69.5, O 69.7, O 77.3
Ruban, Andrei ..... MM 21.4
Ruban, Andrei V. ..... MM 41.6
Rubeck, Jan ..... BP 7.9, •CPP 46.64
Ruben, Mario ..... O 9.4, O 99.2
Rubenstein, Daniel ..... SOE 9.5
Rubin, Noa ..... DY 58.8, SOE 17.8
Rubin, Tom ..... •O 85.1
Rubinstein, Michael ..... •BP 35.1, •CPP 51.1
Rubio, Angel ....•SYFC 1.2, DS 20.52, HL 8.10, HL 35.2, O 49.1, O 49.4, O 49.5, O 61.1, O 66.3, O 79.1, O 79.3
Rübling, Moritz ..... TT 92.10

Ruchka, Pavel . . . . . HL 55.7
Ruck, Michael . . . . . FM 22.5, MA 24.1, TT 36.1, TT 74.6
Rückriegel, Andreas . . . . . •TT 13.12, TT 13.13
Rudack, Till . . . . . BP 14.73
Rudengren, Isabella . . . . . MA 34.11
Rudge, Samuel . . . . TT 42.9, TT 42.10, TT 53.4
Rudge, Samuel L. . DY 46.12, TT 75.12
Rüdiger, Klingeler . . . . . TT 94.4
Rudno-Rudziński, Wojciech HL 20.34
Rudolf, Petra . . . . . HL 48.5
Rudorf, Sophia . . . . . BP 7.19, BP 15.10
Rudzinski, J.F. . . . . •AKPIK 6.5
Rudzinski, Joseph F. . FM 6.4, FM 6.5, MM 22.3, AKPIK 6.3
Rudzinski, Witold . . . . . HL 4.1
Ruellou, Julie . . . . . CPP 26.1
Ruet, Simon . . . . . TT 29.5
Ruf, Leon . . . . . TT 28.1, •TT 28.12
Ruffieux, Pascal . . . . . MA 5.9, TT 7.9
Ruffine, Valentin . . . . . BP 27.11
Ruffing, Elke Neu . . . . . MA 52.39
Ruffino, Martina . . . . . •MM 15.4
Rugeramigabo, Eddy . . . . . HL 20.49
Rugeramigabo, Eddy P. . . . . HL 20.45, HL 55.10
Rugeramigabo, Eddy. Patrick HL 31.4
Rugeramigabo, Eddy Patrik HL 20.50
Ruggenthaler, Michael . . . . . O 49.4
Ruini, Alice . . . . . HL 35.9
Ruiz Alvarado, Isaac Azahel . •O 36.2
Ruiz-Clavijo, Alejandra . . . . . HL 20.23, HL 20.24
Ruiz-García, Miguel . . . . . DY 62.8
Ruiz-Gómez, Sandra . . . . . MA 6.10, •MA 44.5, •TT 76.5
Ruiz-Rena, Emilio CPP 10.12, DY 16.12
Ruland, Holger . . . . . CPP 4.3
Rulands, Steffen BP 10.12, CPP 18.12, DY 18.12
Rule, Kirrily . . . . . MA 7.3, TT 23.1
Rule, Kirrily C. . . . . TT 57.2, TT 57.3
Rumiantsev, Egor . . . . . MM 9.2
Runeson, Johan E. . . . . CPP 53.5
Runge, C. . . . . •MA 52.8, MA 59.8
Runge, Daniel . . . . . O 81.7
Runge, Erich TUT 3.2, DY 43.2, HL 1.2, MM 17.2, MM 17.6, MM 26.2, AKPIK 1.2
Runge, Jonas . •CPP 31.2, CPP 46.33, CPP 46.38
Runge, Milena . . . . . BP 14.74
Rupp, Jennifer L.M. . . . . FM 10.3
Rupp, Matthias . . . . . HL 11.6
Rupprecht, Lea . . . . . •BP 7.28
Rupprecht, Patrick . . . . . TT 71.5
Ruskaup, Nico . . . . . •DS 20.4
Russell, Danny R. . . . . MM 7.7
Russell, Thomas . . . . . CPP 17.42
Russina, Margarita . . . . . •CPP 34.4, •DY 36.4
Russo, Matteo . . . . . HL 3.10, •HL 8.12
Rustamov, Jeyhun . . . . . •DS 20.34, DS 21.4, AKBP 6.5
Rusu, Marin . . . . . DS 20.36
Rusz, Ján . . . . . MA 3.11, MA 30.6
Rüther, Frederik . . . . . O 23.4
Rutschmann, Adrian . . . . . TT 62.6
Rütten, Lisa M. . . . . O 71.4, O 99.5, TT 66.4
Ruvalcaba Briones, Ricardo . . . O 58.5
Ruz, Benjamin . . . . . BP 5.3
Ryabov, Artem . . . . DY 43.20, DY 61.5
Rybakov, Filipp N. . MA 16.9, MA 44.7, TT 76.7
Rybicki, Marcin . . . . . MM 32.5
Rybski, Diego . . . . . SOE 6.1, •SOE 6.2
Rydberg, Anders . . . . . MA 12.6
Ryee, Siheon . . . . . O 84.2, •TT 69.8, TT 84.2
Ryndyk, Dmitry . . . . . •CPP 14.6
Ryndyk, Dmitry A. . . CPP 31.3, O 58.4
Rysak, Andrzej . . . . . DY 8.6
Rytz, Daniel . . . . . TT 79.4
Ryu, Jung-Wan . . . . . DY 59.3, TT 99.3
Ryzhkov, Maksim . . . . . •MA 4.5
Ryzhov, Anton . . AKBP 2.2, AKBP 2.5
S. Cheng, Tin . . . . . O 95.6, TT 96.6
S. Foster, Adam . . . . . O 35.6
S. Hofmann, Johannes . . . . . TT 44.7
S. Jestilä, Joakim . . . . . O 35.6
S. Nair, Akhil . . . . . •MM 5.3
S. Pillai, Hemanth . . . . . •O 65.11
S. Schwarz, Ulrich . . . . . •BP 15.5
S. Uhrig, Götz . . . . . TT 71.2
Saak, Clara M. . . •CPP 19.2, •DY 20.2
Saalfrank, Peter . . . . . DY 43.3
Saalwächter, Kay . . . . . •CPP 54.1
Saavedra, Daniel . . . . . •BP 5.3
Saavedra Garfias, Pablo . . . . . UP 3.5
Saavedra-Fredes, María . . . CPP 41.3, •O 56.7
Sabass, Benedikt . . . BP 7.24, BP 11.5, •BP 41.4, DY 43.16, DY 43.17
Sabater, Carlos . . . HL 30.7, MM 40.6, •MM 40.8, TT 59.7
Sabath, Franziska . CPP 5.1, •CPP 8.1, CPP 8.3
Sabharwal, Snigdh . . . . . MA 19.10, TT 31.10
Sabitova, Aizhan . . . . . O 9.5
Sach, Michael . . . . . •UP 2.4
Sachdev, Subir . . . . . TT 56.8
Sachdeva, Parrydeep Kaur •HL 40.10
Sack, Freddy . . . . . •HL 20.10
Sackey, Ailu . . . . . •FM 11.34
Sadashivaiah, Sakshath . . . . MM 21.8
Sadeddin, Iyad . . . . . O 65.2
Sadeghi Bogar, Mohsen . . . . . FM 19.4
Sadeqi-Moqadam, Mohsen . . FM 18.8
Saeed, Umair . . . . . •FM 18.2
Saeedi, Meysam . . . •HL 11.7, HL 55.2
Sáez-Toro, Guidobeth . . . . . •MA 20.5
Saf, Robert . . . . . CPP 6.4
Safarifard, Vahid . . . . . CPP 46.40, CPP 46.41
Safeer, Affan . . O 10.1, O 10.5, O 10.8, O 15.4, O 17.7, O 17.12, •O 59.1, O 62.8, O 89.8, O 99.10, TT 16.1, TT 16.5, TT 16.8, •TT 48.1, TT 54.8
Saggar, Siddhartha . . HL 2.5, HL 15.9, HL 22.6, HL 26.18
Saggau, Christian Niclaas . . FM 22.5
Sagnimorte, Aude CPP 20.4, DY 23.4
Saha, Debasish . . . . . •BP 15.9
Saha, Kush . . . . . TT 86.5
Saha, Parbati . . . . . DY 15.6
Saha, Rupayan . . CPP 10.11, DY 16.11, •DY 54.3
Saha, Sandip . . . . . •TT 22.7
Saha, Surajit . . . . . MA 3.9, MA 19.9, MM 21.7, TT 31.9
Saha, Suropriya . . . . . •DY 49.1
Sahel-Schackis, Samuel . . . MA 33.11
Sahinovic, Armin . . . . . •O 34.4
Sahoo, Bhabani . . . . . HL 20.28
Sahoo, Bhabani Sankar . . . . . •HL 13.1
Sahoo, Bibhut . . . . . •DY 43.15
Sahoo, Chakradar . . O 95.11, TT 96.11
Sahoo, Chakradhar . . . . . O 66.8
Sahoo, Krishna Rani . . . . . •MA 7.7
Sahoo, Manaswini MA 39.19, •TT 11.1, TT 93.5
Sahoo, Priyatosh •MA 50.5, MA 52.32
Sahoo, Sophia . . . . . DS 20.13
Sahoo, Subhamoy . . . . . HL 20.30
Sahu, Himanshu . . . . . QI 21.2
Sai, Pavlo . . . . . HL 52.2, HL 52.3
Sai, Trisha . . . . O 15.5, •O 89.6, O 99.7
Said, Ayman . . . . . TT 95.2
Said, Tarek Al . . . . . MA 36.10
Saigal, Nihit . . . . . HL 3.6
Saika, Bruno . . . . . O 76.7
Sailer, Elias . . . . . AKBP 8.3
Sailler, Sebastian . HL 18.1, •MA 29.8, MA 59.5, TT 32.1, •TT 46.8
Saini, Vishu . . . . . •BP 14.12
Saiseau, Raphael . •CPP 5.2, CPP 5.4
Saiti, Arbesa . . . . . BP 20.7
Saito, Keiji . . . . . DY 21.1
Saitoh, Eiji . . . . . MA 29.10, TT 46.10
Sajan, Sandra . . . . . O 86.4, •TT 14.10, TT 74.1
Sajjad, Arooj . . . . . BP 37.6
Sajjan, Mohammad . . . MA 5.4, TT 7.4
Sakai, Hideaki . . . . . TT 41.5
Sakamoto, Kazuyuki . . O 60.4, O 64.5, O 67.5
Sakamoto, Shoya . . . . . MA 30.1
Sakar, Baha . . . . . MA 7.78
Sakevarashvili, Archili . . . . . SOE 5.2
Šako, Marin . . . . . CPP 27.1, DY 26.1
Sakradzija, Mirjana . . . . . •UP 5.1
Saksena, Aparna . . . . . MM 39.6
Sala, Alessandro . . . . . O 83.6
Sala, Giacomo . . . . . MA 29.3, TT 46.3
Sala, Pablo . . . . . DY 13.8, TT 19.8
Salah Soliman Asser, Mohamed FM 2.5, •FM 2.5
Salamon, Soma . . MA 36.1, MA 52.26
Salarinasab, Milad . . . . . •O 94.9
Salas-Llabrés, Joan . . . . . •DY 54.10
Salazar, Raphaël . . . . . O 76.3
Salazar-Meija, C. . . . . MA 52.24
Salazar-Mejia, Catalina . . . . •MA 18.5, •TT 30.5
Saldarelli, Umberto . . . . . •O 96.4
Saldatov, Ivan . . . . . DS 18.3
Salditt, Tim . . . . . CPP 27.4, DY 26.4
Saleem, Sumiya . . . . . MA 39.10
Saleh, Muhammad . . . . . O 36.1
Salehi, Mohammad . . . . . •O 83.1
Salehi, Nastaran MA 59.10, •MA 59.11
Salgado-Linares, Ignacio . . . . •TT 79.1
Saliba, Michael . . . . . •CPP 44.1
Salikhov, Ruslan . . MA 7.46, MA 12.4, MA 35.6, TT 60.6
Salje, Ekhard . . . . . FM 12.10
Salmeron, Noe . . . . . •TT 51.2
Salusti, Francesco . . . . . HL 55.4
Salvalaglio, Marco DS 14.5, •MM 30.1
Salvan, Georgeta . . . . DS 18.1, DS 18.3
Salvatore, Robin . . . . . TT 49.4
Samad, F. . . . . TT 24.7
Samadi, Mohsen . . . . . HL 1.9
Samal, Pankaj Kumar . . . . . O 13.12
Samaner, Çağlar . . . . . HL 16.4
Samanta, Amit K. . . . . BP 33.10
Samanta, Atanu . . . . . MA 4.1
Samanta, Dibyendu . . . . . •TT 97.4
Sambale, Anna Katharina . •CPP 59.1
Samir, Mohamed . . . . . •AKBP 11.4
Sammalkorpi, Maria . . . . . BP 26.5, CPP 43.5, DY 41.11
Sammartino, Francesco . . . . . •O 66.7
Sampathkumar, Arunodhayan •BP 18.5
Samtsevych, Artem . . . . . DY 6.12
Samuel, Solomon Birhanu . . •QI 14.18
Samuele, Rebecci . . . . . O 35.3
Sanchez Merlinsky, Luciano . . . O 87.1
Sánchez, Rafael . . . . HL 29.3, TT 58.3
Sanchez Valle, Carmen . . . . . FM 15.2
Sánchez-Barquilla, Raquel . . . . O 10.3, •O 23.3, O 88.9, O 88.10, TT 16.3
Sanchez-Barriga, Jaime . . . . . O 63.4, TT 55.4
Sánchez-de-Armas, Rochio . . . . O 9.4
Sanchez-Fuentes, Ana . . . . . FM 12.3
Sanchez-Manzano, D. . . . . •TT 69.3
Sanchez-Manzano, David . . . . MA 3.1, •TT 69.5
Sánchez-Maqueda, Damián . . . O 47.4
Sánchez-Ramírez, Irián . . . . . TT 14.10
Sand Jespersen, Thomas . . . HL 38.2
Sandaltzopoulou, Elissavet . BP 10.4, CPP 18.4, DY 18.4
Sandbaumhüter, Florian . . . . . MA 6.3
Sandberg, Anna . . . . . TT 23.18
Sandberg, Oskar J. . . . . CPP 25.5
Sande, Muskan . . . MA 43.5, MA 49.8
Sander, Nick . . . . . TT 10.5, •TT 23.33
Sanders, Charlotte . . . . O 66.8, O 76.5
Sandev, Trifce . . DY 42.15, •DY 43.24, TT 63.15
Sandiumenge, Felip . . . . . FM 18.2
Sandner, Daniel . . . . . •HL 46.1
Sandner, Fabian . . . . . O 12.5
Sandoghdar, Vahid . BP 16.9, BP 33.4
Sandonas, Leonardo Medrano CPP 7.1, CPP 7.3, MM 7.1
Sanella, Valentina . . •MM 8.1, MM 8.2
Sanga, Cem . . . . . •HL 24.4
Sangalli, Davide . . . . . HL 8.3, MA 7.31, O 7.2, TT 9.2
Sangeetha, N. S. . . TT 23.10, TT 81.7, TT 81.8
Sänger, Jana . . . . . •CPP 46.13
Sangiovanni, Giorgio . . . . . DS 20.43, HL 24.10, MA 24.1, MA 33.9, O 63.5, O 63.8, O 71.13, O 74.4, O 84.3, TT 3.5, TT 6.4, TT 10.4, TT 11.5, TT 36.1, TT 55.5, TT 55.8, TT 62.8, TT 66.13, TT 68.4, TT 69.8, TT 84.3, TT 95.8
Sankar, Some . . . . . QI 15.5
Sankeshwar, Vijayalaxmi . . . . MA 5.5, TT 7.5
Sanna, Antonio . . . . . FM 6.6
Sanna, Simone . . . . . CPP 46.30, CPP 46.34, CPP 46.35, FM 11.21, FM 11.22, FM 11.27, O 45.10, O 56.1, O 86.6, O 86.8
Sanpera, Anna . . . . . QI 15.5
Santamaria, J. . . . . TT 69.3
Santamaria, Jacobo . MA 3.1, TT 69.5
Santander, Ricardo . . . . . •BP 14.15
Santen, Ludger . . . . . BP 14.6
Santiso, Jose . . . . . FM 18.2
Santoro, Francesca . . . . . •HL 2.3
Santos, Alan C. . . . . TT 22.15
Santos, Alisson Ceccatto . . . . •O 87.1
Santos, Elton . . . . . MA 43.6
Santos, Luis . . . . . QI 15.3
Santos, Paulo V. . . . HL 18.9, TT 32.9
Santra, Ion . . . . . •DY 9.6
Santra, Prosun . . . . . •DS 12.5
Santra, Saswati . . . . HL 12.2, HL 33.5, HL 42.3, HL 42.5
Sanyal, Biplab . . . . . MA 58.12
Sanz de Leon, Alberto . . . . . BP 7.12
Sanz, Diego . . . . . TT 50.6
Saood, Saba . . . . . MM 15.5
Saphiannikova, Marina . . . . CPP 14.6, CPP 31.5, CPP 31.7, CPP 42.3
Sappler, Benjamin . . . . . •TT 51.8
Sarafimov, Blagoj . . . . . MA 7.81
Sarajilic, Edin . . . . . TT 28.5
Sarangi, Arijeet . . . MM 8.6, •MM 12.1
Sarangi, Swosti P. . . . . MA 45.2
Sarantopoulos, Alexandros . . . DS 6.6
Saravanou, Sofia-Falia . . . . . CPP 54.6
Sarcan, Fahrettin . . . . . HL 24.4
Sardinero, Ignacio . . . . . •TT 6.2
Sarebanzadeh, Maral . . . . . •MM 34.2
Sarina, Sarina . . . . . MM 14.1
Sarkanych, Petro . . . . . SOE 5.2
Sarkar, Aranyak . . . •BP 36.5, •DY 57.5
Sarkar, Kanchan . . . . . •AKPIK 6.2
Sarkar, Rajib . . . . . MA 47.11, MA 54.7, MM 12.1, TT 72.3
Sarkar, Ritwick . . . . . •DY 44.2
Sarkar, Sanjay . . . . . MM 19.35
Sarkar, Suchetana . . . . . •O 6.2
Sarker, Partha . . . . . •TT 86.7
Şarlar, Kağan . . . . . MA 52.25
Sarott, Martin . . . . . FM 12.10
Sarott, Martin F. . . . . •FM 12.9
Sarris, Ilias-Marios . . . . . •BP 37.9
Sartipi, Zahra . . . . . •DY 43.3
Sartori, Caterina . . . . . •O 25.2
Sartori, Fabio . . . . . •SOE 10.3
Sartori, Laurin . . . . . •BP 7.55
Sartori, Thomas . . . . . O 38.2
Sarwar, Awais . . •CPP 40.4, CPP 40.6
sasagawa, takao . . . . O 95.9, TT 96.9
Sasaki, Satoshi . . . . . DS 4.2
Sasaki, Shunsuke . . . . . TT 49.4
Sasi, Sarath . . . . . •O 76.3
Sasioglu, Ersoy . . . . . •MA 54.9
Sassenberg, Nils . . . . . DD 16.2
Sastges, Mirco . . MA 20.5, •MA 29.4, MA 51.4, •TT 46.4, TT 88.4
Sathyadharma Prasad, Aniruddha •MA 6.3
sato, haruki . . . . . O 67.7, O 82.3
Sato, Manabu . . . . . TT 6.5
Sato, T. . . . . MA 25.6
Sato, Takuma . . . . . MA 36.1
Sato, Yudai . . . . . TT 73.1
Satoh, Takuya . . . . . MA 45.2
Satoshi, Nishimoto . . . . . TT 94.4
Sattigeri, Raghottam M . . . . . •TT 49.7
Satz, Armin . . . . . MA 55.9
Satzger, Levon . . . . . MM 22.8
Sau, Jyotirmoy . . . . . •MA 7.84
Sauerland, Dennis . . . . . DS 3.1
Saunders, Benedict . . O 33.7, •O 62.4, •TT 54.4
Saunders, John . . . . . TT 22.17
Saunderson, Tom G. . . . . •MA 33.6
Sauter, Gabriel . . . . . •CPP 17.6
Savan, Alan . . . . . FM 6.8
SAVAŞKAN YILMAZ, Sevil CPP 17.30, FM 19.6, •MM 16.4
Savelkouls, Jaqueline . . . . . •BP 14.24, BP 14.75, MM 19.30, MM 19.48
Savich, Yahor . . . . •BP 27.11, BP 32.6, DY 52.6
Savin, Yuri . . . . . FM 11.11
Savino Real, Pablo . . . . . DS 12.6
Savinov, Maxim . . . . . MA 17.3
Savoia, Nathan . . . . . SYBT 1.2
Savoie, Marc . . . . . •O 56.5
Savoini, M. . . . . MA 25.6
Savorana, Giovanni . . . . . BP 11.3
Savvin, Stanislav . . . . . MA 7.2
Saw, Alexander . . . . . AKBP 8.3
Sawant, Pratima . . . . . BP 7.32
Sawatzki, Jakob . . . . . O 46.2, O 46.4
Saxena, Rishabh . . . . . CPP 57.2
Sayama, Hiroki . . . . . PSV I, •SYSC 1.1

Sayar, Mohsin .....•HL 46.2
Sayenko, Dmitry .....•HL 26.42
Saywell, Alex ..... O 95.6, TT 96.6
Sbeih, Suhad .....•O 54.8
Scacchi, Alberto .. BP 26.5, CPP 43.5
Scazzola, Alberto ..... TT 95.5
Schaal, Maximilian ..... O 6.8, O 10.7, O 28.3, O 44.14, O 45.8, O 45.11, O 83.2, TT 16.7
Schaarman, William •MA 5.2, •TT 7.2
Schaate, Andreas ..... HL 48.6
Schabbehard, Tillmann ..... O 14.11, •O 38.5, O 66.5
Schading, Johannes .....•QI 3.4
Schädlich, Philip .... O 40.13, •O 73.5, O 84.2, TT 37.13, TT 84.2
Schaedel, Laura .... BP 12.3, BP 40.2
Schaefer, Joerg .....O 8.5
Schaefer, Karen ..... TT 90.6
Schaefer, Sascha .....MA 38.10
Schaefer, Sébastien .....CPP 26.1
Schaefer, Tobias ..... TT 51.3
Schäfer, Christian ... •HL 38.1, O 57.7
Schäfer, Fabian .....•DD 14.2
Schäfer, Jonas ..... UP 6.3
Schäfer, Jörg ..... DS 14.3, DS 20.43, O 63.5, O 74.4, TT 55.5, TT 68.4
Schäfer, Julien .. •MA 48.4, MA 52.19
Schäfer, Kilian .....MA 50.5
Schäfer, Laura .....DD 38.1
Schäfer, Lukas ...MA 50.5, MA 52.32
Schäfer, Marlon ..... HL 34.1, QI 18.6
Schäfer, Martin .....•MM 14.5
Schäfer, Michaela . CPP 23.1, DY 24.1
Schäfer, Moritz R. .. •MM 19.1, O 24.7
Schäfer, Robin ..... DY 2.2, TT 1.2
Schäfer, Rudolf .. MA 7.80, MA 39.17
Schäfer, Sascha ... HL 18.10, HL 52.1, MA 16.5, O 40.12, O 66.6, TT 32.10, TT 37.12
Schäfer, Sophie .....O 8.7
Schäfer, Thomas ..... TT 13.7
Schäfer, Tim ..... O 4.3, •O 88.2
Schäfermeier, Clemens ..... MA 6.2
Schaffar, Gerald .....MM 36.2
Schäffer, Erik ..... BP 9.4, BP 12.2
Schäffer, Moritz R. ..... CPP 46.54
Schäffer, Tilman E. ..... BP 27.6
Schäffer, Yannick ..... TT 70.2
Schäffner, Karoline .....TT 22.32
Schäfle, Claudia ..... TUT 2.1, DD 1.1, DD 10.3
Schafmayer, Clemens ..... HL 22.4
Schaller, Gernot .... •TT 2.5, TT 18.6, TT 42.5, QI 17.2
Schalling, Marcel .....•O 26.2
Schalling, Marcell ..... O 27.6
Schanzenbach, Dirk ..... CPP 46.37
Schapeler, Timon ..... QI 5.9
Schäpers, Thomas . HL 38.1, TT 73.6, TT 74.3
Schardt, Jan ..... HL 26.17
Schären, Stefan ....MM 8.1, •MM 8.2
Scharf, Dominik ..... O 31.2
Scharf, Florian ..... DD 27.1
Scharf, Gili ..... MA 11.2, TT 21.2
Scharfenstein, Lisa-Marie .. •BP 7.43
Scharff, Konrad .....•MA 9.11
Scharoch, Paweł ..... HL 20.7
Scharpegge, Roxana .....•PSV I
Scharpey, Maximilian ..... •HL 20.8, HL 26.37
Schatt, Leonhard .....•BP 14.80
Schaub, Michael T. ..... DY 8.2
Schauer-Bollig, Ramona ... •DD 20.2, DD 28.1
Schauermann, Daniel .....O 65.12
Schauermann, Swetlana ..... O 34.8, O 81.1, O 88.6
Schauerte, Alexander ..... •HL 45.8
Schaumann, Gabriel . O 40.5, TT 37.5
Schaumburg, F. ..... HL 20.27
Schaumburg, Felix .....•HL 47.1
Schebek, Maximilian ..... •DY 14.2
Schechter, Moshe . MA 11.11, TT 21.11
Scheele, Hauke .....O 34.8
Scheele, Marcus .....HL 4.1
Scheer, Elke ..... HL 18.2, TT 28.1, TT 28.12, TT 29.8, TT 29.10, TT 32.2, TT 78.6, TT 81.3, TT 90.1, •TT 90.6
Scheer, R. ..... HL 45.1
Scheer, Roland .....DS 4.3, DS 8.5
Scheffer, Moritz .....•MA 7.5
Scheffler, Marc ..... TT 5.2, •TT 14.1, TT 14.2
Scheffler, Matthias HL 23.5, HL 40.10, HL 47.4, MM 5.3, MM 5.6, MM 13.6, MM 31.5
Schehr, Grégory ..... DY 49.7
Scheib, Stefan .... •AIW 1.3, •AIW 1.5
Scheibel, F. .....MA 52.22
Scheibel, Franziska MA 13.2, MA 13.4, MA 13.7, MA 50.5
Scheibel, Lucas Andreas .....•O 39.1
Scheibel, Thomas .....•CPP 38.1
Scheidt, Joshua ..... O 61.10
Scheie, Allen O. ..... TT 52.3
Scheiger, Philipp ..... DD 7.1, DD 21.1, DD 30.7, •DD 30.8
Scheiner, Santiago ..... QI 18.9
Schelchshorn, Michael .....•O 17.2
Scheler, Ulrich .. •CPP 13.3, CPP 17.9
Schellenberger, Andreas ..... TT 2.6, •TT 62.10
Scheller, Lukas .....TT 22.12
Schellhammer, Sebastian .CPP 17.12, CPP 17.13, CPP 29.1, CPP 29.3, CPP 37.3, HL 26.16
Schelter, Ingo .....•BP 2.11
Schemmelmann, Sven .....•O 60.4, O 60.7, O 63.5, O 67.5, TT 55.5
Schepers, Anna .....•BP 14.42
Scherb, Sebastian ..... O 99.3
Scherbakov, Alexey .....MA 30.9
Scherbakov, Alexey V. .....HL 39.9
Scherer, Michael M. .. O 62.8, TT 2.7, TT 54.8
Scherer, Theo .....FM 7.2
Scherer, Theo Andreas .....•FM 7.3
Scherf, Nico .....DY 14.7
Scherz, Andreas .....MA 42.3
Scheuchenpflug, Ludwig .•MA 52.37, TT 79.4
Scheuer, C. ..... O 88.11
Scheuermann, Robert ..... TT 52.1
Scheufele, Monika MA 7.48, MA 30.5, •MA 33.11
Scheunemann, Dorothea ..•CPP 37.2
Scheurer, Christoph .....•SYAI 1.2, DY 6.12, DY 14.5, DY 41.12, FM 2.4, FM 5.5, FM 11.13, MM 8.9, MM 19.11, MM 19.12, MM 31.10, MM 41.7, O 23.4, O 23.5, O 55.5, O 81.7, O 85.6, O 88.3
Scheurer, Fabrice ..... O 12.4, O 12.7, O 12.9
Scheurer, Mathias .....TT 24.6
Scheurer, Mathias S. ..... TT 92.5
Scheutzhold, Ralf ..... TT 23.35
Scheve, Clara ..... •UP 2.3
Schewe, Lars ..... SOE 4.6
Schewe, Lukas .....•DS 9.5
Schewin, Coline .....BP 14.49
Schick, Arvid .....•O 26.5
Schick, Daniel ....MA 7.19, •MA 7.68, MA 38.3, MA 39.11, O 40.15, O 98.3, TT 37.15
Schied, Monika .....•O 38.2
Schiegl, Felix ..... O 12.5
Schieler, Merlin .....•MM 40.7
Schiemenz, Sandra .....MA 57.4
Schienbein, Philipp .•CPP 9.2, O 97.2
Schieren, Florian .....MM 40.7
Schießer, Lars .....MA 48.8
Schiesser, Lars .....•MA 52.20
Schiffer, Tobias .....•AKBP 3.5
Schilberth, Felix ...MA 8.9, •MA 23.2, •TT 35.2
Schiller, Karl ..... O 71.3, TT 66.3
Schilling, Benjamin ...•O 24.2, O 97.4
Schilling, Gregor .....AKBP 8.7
Schilling, Henrik .....TT 23.18
Schilling, Marcel ..... HL 37.4
Schilling, Michael ..... QI 16.5
Schilling, Tanja .....•DY 21.7
Schillinger, Phillip ..... QI 20.6
Schillmöller, Finja .. O 71.16, TT 66.16
Schilz, Joshua ..AKBP 6.1, •AKBP 7.5
Schimmel, Sebastian ..... O 63.2, •TT 11.3, TT 11.4, TT 55.2
Schimmel, Thomas ..... MM 40.7
Schimmenti, Vincenzo Maria •BP 3.4
Schimpf, Lennart •MA 29.5, •TT 46.5
Schimpf, Marina ..... UP 3.5
Schindelwig, Jakob .....•BP 29.3, •CPP 45.3
Schindler, Bastian .....•TT 23.26
Schindler, Christina .....DD 4.1
Schindler, Frank ..... TT 61.12
Schindler, Marcel .....•QI 5.10
Schindlmayr, Arno .....HL 26.38, HL 26.43, MA 7.86
Schink, Severin .....•BP 41.3
Schirhagl, Romana .....•HL 11.2
Schirk, Johannes ..... TT 28.7, QI 8.3
Schirmeisen, Andre ... •O 3.1, O 24.1, O 45.10, O 58.1, TT 22.35, TT 22.36, TT 89.1
Schiro, Marco ..... TT 15.7
Schittz, Guido ..... MM 41.2
Schlabes, Arne .....•QI 3.12
Schlachter, Jean-Maxime ... •O 62.3, •TT 54.3
Schlaf, Johannes .....•DD 36.1
Schlagheck, Peter .. DY 13.6, DY 42.4, DY 59.6, TT 19.6, TT 63.4, TT 99.6
Schlaich, Alexander •PSV III, CPP 3.5, CPP 14.3, CPP 14.5, CPP 46.57, DY 44.16, MM 17.3
Schleberger, Marika ..... O 34.4
Schlechtriem, Moritz ..... •O 22.5
Schleenvoigt, Michael .....QI 6.9
Schlegel, Julius .....•MA 38.8
Schleicher, Lukas ....HL 3.9, HL 18.8, TT 32.8
Schleicher, Robin .....•TT 93.19
Schleife, Andre .....HL 35.8
Schlenga, Klaus .. •AIW 2.3, •AIW 2.5
Schlenhoff, Anika .. •MA 5.3, O 40.14, O 71.22, O 71.23, O 72.3, •TT 7.3, TT 37.14, TT 66.22, TT 66.23, TT 67.3
Schlenvoigt, Hans-Peter ... AKBP 6.5
Schlesag, Marcel .....TT 61.14
Schlettwein, Derck .....CPP 17.8, CPP 22.5, CPP 44.4, O 65.1
Schleyer-Thiers, Benjamín . CPP 41.3, •CPP 41.5
Schlichting, Hartmut ... O 9.4, O 45.4
Schlichtung, Hartmut .....O 78.3
Schlickum, Uta ..... FM 5.11, O 19.9, O 35.7, O 43.14
Schliemann, John .. DY 32.3, TT 45.3
Schlierf, Michael ..... BP 14.79
Schliessmann, F. .....AKBP 1.1
Schlipf, Jon ..... O 96.6
Schlipf, Martin .....•MM 22.6
Schlisio, Georg ..... •O 78.1
Schlitz, R. .....•MA 48.11, MA 52.8, MA 59.8
Schlitz, Richard ...MA 7.52, MA 29.8, MA 39.24, MA 45.1, MA 51.8, MA 52.10, MA 52.33, TT 46.8, TT 88.8
Schlögel, Maximilian ..... BP 7.44
Schlögl, R. ..... O 88.11
Schlom, Darrell G. ..... DS 11.3
Schlösser, Magnus ..... DS 21.10
Schlötzer, Samuel DY 42.12, TT 63.12
Schluck, Jakob .... •TT 15.4, TT 15.5, TT 15.6
Schluck, Jonathan .....•TT 42.7
Schlueter, C. . DS 3.4, O 59.2, TT 48.2
Schlueter, Christoph ..... DS 20.41, FM 4.2, FM 23.4, MA 39.9, O 19.2, O 42.9, O 93.2, TT 25.11, QI 6.5, QI 14.23
Schlünz, Dane-Vincent ..... •DD 12.1, DD 26.2
Schlupp, Peter .....HL 26.32
Schlüßler, Raimund BP 27.10, BP 37.7
Schlüter, Henrik ..... DY 13.4, TT 19.4
Schlüter, Julius .....CPP 46.42
Schmalhorst, Jan . MA 7.62, MA 7.63, MA 47.8
Schmalian, Joerg ..... TT 56.8
Schmalian, Jörg .... DY 13.1, MA 8.8, MA 20.4, TT 19.1, TT 56.11, TT 57.11, TT 93.18, TT 95.4
Schmalofski, Timo .....MM 19.25
Schmalz, Holger ..... CPP 41.7
Schmalz, Tim ..... DD 16.2
Schmalz, Veronika ..... O 45.9
Schmalzl, Karin ..... MA 3.6, MA 3.7, MA 47.10
Schmaus, Alexander ..... SOE 6.6
Schmechel, Selina .....•O 28.5
Schmelz, Bruno ..... •BP 7.10
Schmickler, Wolfgang .....O 13.4
Schmid, Alexander .•MA 54.8, O 83.4
Schmid, Almuth ....•BP 8.2, BP 14.19
Schmid, Anna ..... O 96.5
Schmid, Clemens .....•TT 14.12
Schmid, Florian ..... TT 74.12
Schmid, Friederike ... BP 4.2, BP 4.4, BP 4.5, BP 29.4, BP 31.3, CPP 17.4, CPP 45.4, CPP 50.3, CPP 58.3, DY 54.5
Schmid, Harald ...•DY 32.2, •TT 45.2
Schmid, Jonas ..... HL 31.5
Schmid, Judith ....•DD 27.4, DD 30.3
Schmid, Martin .....•DS 3.3, O 2.6
Schmid, Michael .....O 5.6, O 55.4, O 58.7, O 80.1, O 94.5
Schmid, Sebastian .....MA 17.6
Schmid, Sonja ..... •BP 9.1
Schmidbauer, Florian .....•DS 20.9
Schmidhuber, Rabea .....MA 33.1
Schmidmeier, Ramon .....DS 20.40
Schmidt, Annette M. ..... CPP 49.1
Schmidt, Arthur .....•MA 7.70
Schmidt, Bernd .... TT 22.36, TT 89.1
Schmidt, Burkhard ..... TT 52.2
Schmidt, Daniel ..... MM 21.8
Schmidt, Falko •CPP 10.12, •DY 16.12, DY 44.19
Schmidt, Frederik .....•HL 26.43
Schmidt, G. .....HL 37.2, HL 37.6
Schmidt, Georg ..... MA 7.8, MA 9.8, MA 39.10, MA 48.10, MA 52.17, MA 52.21
Schmidt, H. T. ..... TT 22.31
Schmidt, Hauke ..... UP 6.5
Schmidt, Heiko .....DY 28.4
Schmidt, Henri ..... •BP 14.84
Schmidt, Jack-Andre ..... TT 22.35, TT 22.36, TT 89.1
Schmidt, Jonathan .....FM 12.7
Schmidt, Jori F. ..... •MA 6.6
Schmidt, Kai ..... TT 94.8
Schmidt, Kai P. ....TT 23.11, TT 23.12
Schmidt, Kai Phillip ..TT 2.6, TT 23.5, TT 23.6, TT 23.7, TT 23.8, TT 26.2, TT 62.10, TT 70.1, QI 5.4, QI 14.17
Schmidt, Lukas ..... O 26.2, TT 26.5
Schmidt, M. ..... TT 5.9
Schmidt, Marcus ...MA 2.6, MA 8.10, TT 3.3, TT 94.3, TT 98.1
Schmidt, Martina .....UP 7.3
Schmidt, Marvin .....•CPP 17.45
Schmidt, Oliver .....•CPP 17.39
Schmidt, Oliver G. .. HL 55.7, HL 56.5
Schmidt, Paul Philip .. O 35.1, •O 77.1
Schmidt, Richard ...HL 3.1, HL 20.29, O 71.5, TT 56.3, TT 66.5
Schmidt, Robert .CPP 17.46, FM 15.2, HL 20.59, MA 7.7, MA 9.13, MA 12.1, MA 52.5, MA 52.14
Schmidt, Thomas •DS 20.30, MA 7.4, O 65.5
Schmidt, Thomas L. .....MA 37.1, MA 52.15, TT 61.9, •TT 64.5, TT 83.12
Schmidt, Timo ....MA 27.3, MA 37.8, MA 39.17, MA 55.6
Schmidt, Winfried .....•BP 27.5
Schmidt, Wolf Gero ..... FM 11.12, FM 11.20, HL 20.60, HL 26.24, HL 49.3, O 16.1, O 36.2
Schmidt, Wolfgang .....MA 47.10
Schmidt-Grund, Rüdiger ....DS 20.35
Schmidtpeter, Jan MA 49.5, MA 49.7
Schmiedeberg, Michael .. CPP 20.10, DY 23.10, DY 43.6, •DY 47.3
Schmieg, Daniel .....TT 49.4
Schmitt, Cedric .. •DS 14.3, DS 20.43, O 74.4, TT 5.6, TT 68.4
Schmitt, Christin .. MA 2.8, MA 29.10, TT 46.10
Schmitt, Cosima .. •DY 42.2, •TT 63.2
Schmitt, David .....O 14.10, O 40.19, O 66.9, O 98.10, TT 37.19
Schmitt, M. ..... O 59.2, TT 48.2
Schmitt, Markus ...DY 14.13, DY 32.1, DY 53.6, MA 34.10, TT 45.1, TT 51.2, TT 87.6, QI 6.7
Schmitt, Maurice P. ..... •CPP 56.4
Schmitt, Simeon ..... •HL 26.51
Schmitt, Thorsten .MA 11.8, MA 30.4, TT 21.8
Schmitt, Vivien .....QI 2.10
Schmitteckert, Peter .....MA 6.8
Schmitz, Guido ... CPP 15.5, MM 4.7, MM 16.2, MM 19.45, MM 35.4, MM 35.5
Schmitz, Gunnar .... MM 19.1, O 18.3
Schmitz, Jelena .....•BP 14.73
Schmitz, Katja .....•BP 14.14
Schmitz, Stefan .....•QI 3.2
Schmökel, Manuela .....AKBP 9.1
Schmolka, Niklas .•MA 7.54, MA 47.8
Schmoll, David ..... MA 48.2
Schmoll, Philipp .....QI 3.3
Schmölz, Nicolas .....•MA 7.29
Schmuck, Johannes .•HL 8.4, HL 8.7
Schnack, Jürgen .. DY 13.4, MA 42.5,

•MA 42.8, MM 14.2, TT 19.4, TT 51.10
Schnauß, Jörg ..... DD 25.2
Schneble, Dominik ..... DD 40.1
Schneck, Emanuel . CPP 27.1, DY 26.1
Schneider, Andrea ..... •BP 14.56
Schneider, Benedikt ..... TT 51.11
Schneider, C. ..... HL 54.10, HL 54.12
Schneider, Carina ..... •BP 7.5
Schneider, Christian HL 54.8, HL 54.9, QI 2.7, QI 8.3
Schneider, Christian M.F. ..... QI 11.9
Schneider, Christof ..... MA 17.2
Schneider, Claus M. ... MA 5.8, O 2.2, TT 7.8
Schneider, Claus Michael .... MA 5.7, TT 7.7
Schneider, Claus Micheal ..... O 69.2
Schneider, Clemens HL 30.3, TT 59.3
Schneider, D. ..... •AKBP 1.1
Schneider, Dominic ..... AKBP 4.4, AKBP 14.1
Schneider, Ella B. ..... HL 11.6
Schneider, Eric ... BP 14.24, •BP 37.3, MM 19.30, •MM 19.48
Schneider, Florian ..... •O 5.3
Schneider, Hans C. ..... MA 54.8
Schneider, Hans Christian ... MA 8.6, MA 47.3, O 61.7
Schneider, Hans-Christian .. MM 34.2
Schneider, Irina ..... •DD 19.3
Schneider, Konrad ..... CPP 54.2
Schneider, Leonard ..... •HL 20.3
Schneider, M. Alexander ..... O 30.1, O 45.6, O 48.2, O 72.5, TT 67.5
Schneider, Michael .. DS 6.1, MA 7.67
Schneider, Philip ..... •DS 16.6
Schneider, Sebastian ..... •FM 19.1, MA 7.61, MA 7.65, MA 7.82
Schneider, Stefanie ..... •CPP 13.1
Schneider, Thorsten ..... DS 11.6
Schneider, Tim P. ..... •CPP 44.4
Schneider, Xenia ..... BP 15.4
Schnell, Adrian Felix ..... •BP 20.3
Schnelle, Walter .... DS 20.51, O 59.5, O 71.1, O 71.18, TT 48.5, TT 66.1, TT 66.18
Schnermann, Justus ..... •BP 30.7, •CPP 47.7
Schnieber, Timo ..... QI 18.6
Schnipper, Jean-Luc ..... •DY 41.3
Schnitzerlein, Miriam ..... •BP 14.85
Schnitzlein, Matthias ..... O 31.6
Schnorr, Laurin ..... HL 20.35
Schnorrenberg, Johanna .... •O 44.5
Schnorrer, Frank ..... BP 37.12
Schnyder, Andreas .. TT 41.3, TT 61.6
Schnyder, Andreas P. ..... TT 39.7
Schöbel, Susanne ..... AKBP 10.1, AKBP 10.2, AKBP 11.4, AKBP 13.3
Schober, Yannick ..... AKBP 2.4
Schöder, René ..... O 58.3
Schoebel, Susanne ..... AKBP 12.5
Schofield, Ross ..... O 96.10
Schofield, Steven R. ..... O 42.9
Schöll, Eckehard ..•SOE 9.1, SOE 10.1
Schöll, Eva ..... •SYSD 1.4
Scholle, Robin ..... •TT 94.1
Schöllkopf, Wieland ..... O 85.4
Schollmeier, Marius S. ..... AKBP 8.7
Schollwöck, Ulrich ..... TT 83.10
Scholz, Gordon ..... BP 14.24
Scholz, M. ... O 19.10, O 59.2, TT 48.2
Scholz, Markus ..... O 70.3, O 71.17, TT 14.4, TT 25.11, TT 65.3, TT 66.17
Scholz, Sven ..... HL 20.35, HL 20.36
Schölzel, Franziska .•DS 18.1, DS 18.3
Schömig, Richard ..... •CPP 46.57
Schön, Carl-Friedrich ..... DS 7.4
Schönfeldt, Mario ..... MA 52.31
Schöngrundner, Paul ..... O 43.3
Schönhense, G. ..... •O 19.10, O 59.2, O 93.9, TT 48.2
Schönhense, Gerd ..... O 2.4, O 14.3, O 40.20, O 42.9, TT 14.4, TT 37.20
Schönig, Marco ..... •O 87.9
Schönleber, Marco ..... •TT 92.16
Schönleitner, Florian ..... •MA 46.2
Schönwälder, Christopher .. AKBP 6.1
Schoof, Benedikt .... DS 1.2, DS 16.6, •QI 11.10
Schöppl, Florian ..... •DS 8.3
Schöppler, Friedrich ..... HL 26.27
Schorlepp, Timo ..... •DY 15.8
Schormann, Colin ..... DS 16.3
Schörmann, Jörg .. HL 26.3, HL 42.2, HL 45.3
Schorn, Bernadette ..... •DD 19.1
Schorn, Dennis ..... •DY 34.2
Schorr, Lara ..... •DY 42.6, •TT 63.6
Schott, Rüdiger ..... HL 48.1, HL 55.4
Schöttke, Fabian .... O 60.5, •O 60.7, O 63.5, TT 55.5
Schouten, Mette F. ..... HL 17.1
Schowalter, Marco . HL 9.1, HL 20.66, HL 24.1
Schraad, Simon ..... CPP 25.4, CPP 46.45, •CPP 46.51
Schrader, Alexandra ..... •MA 52.16
Schrader, Johanna ..... DD 13.1
Schramm, Dominik ..... •MA 6.5
Schramm, Ulrich AKBP 5.4, AKBP 6.1, AKBP 6.3, AKBP 6.5, AKBP 7.3, AKBP 7.5, AKBP 8.8, AKBP 10.1, AKBP 10.2, AKBP 10.3, AKBP 11.3, AKBP 11.4, AKBP 12.5, AKBP 13.3
Schraut-May, Lisa ..... CPP 22.2
Schrautzer, Hendrik ..... MA 21.5
Schreck, Sabine ..... FM 7.2
Schrefl, Thomas .. MA 34.4, MA 50.2, MA 58.1
Schreiber, Frank . CPP 12.3, CPP 12.5, •CPP 36.1, CPP 48.1, DS 21.4, HL 4.1, AKPIK 6.6
Schreiber, Jörg AKBP 5.1, AKBP 10.4, AKBP 11.1
Schreiber, Lars ..... HL 17.2
Schreiber, Lars R. .... QI 6.2, QI 14.23
Schreiber, Nir ..... •DY 47.2
Schreinemacher, Sophia .... •FM 11.2
Schreyer, Philipp ..... TT 42.6
Schröder, Alexander ..... HL 18.10, O 40.12, O 66.6, TT 32.10, TT 37.12
Schröder, Benjamin ..... HL 8.5
Schröder, Carsten ..... O 34.8
Schröder, Chris O 28.2, O 28.4, O 28.7
Schröder, Christian ..... FM 11.9
Schröder, Jonas ..... CPP 15.6
Schröder, Jörg ..... MA 10.1
Schröder, Malte .... DY 51.1, SOE 6.4, •SOE 6.5, SOE 15.1, SOE 16.1
Schröder, Sarah ..... AKBP 12.4
Schröder, Stefan ..... •CPP 17.48
Schroeder, Carsten ..... O 81.1
Schroedter, Erik .. •DY 42.3, MA 7.59, •TT 63.3
Schröer, Oskar ..... •HL 26.37
Schroeter, Matthias ..... DY 41.1
Schroller, Daniel ..... QI 14.24
Schrön, Martin ..... •UP 7.5
Schröter, Johannes ..... •O 87.3
Schröter, Matthias ..... •AKPIK 2.3
Schröter, Niels O 42.1, O 63.4, O 70.7, TT 55.4, TT 65.7
Schröter, Niels B. M. .. O 42.9, O 64.5
Schubatzky, Thomas ..... PSV I, •SYSC 1.2, DD 14.1
Schubert, Alina ..... HL 20.25
Schubert, Conrad ..... MA 49.7
Schubert, Jonas ..... •PSV VI
Schubert, M. ..... O 57.6
Schubert, Marco ..... TT 28.9
Schubert, Ulrich ..... CPP 48.4
Schubert, Ulrich S. ..... CPP 17.22, CPP 17.25, CPP 17.41, CPP 57.4, CPP 57.5
Schuch, Norbert ..... QI 1.1, QI 1.2
Schuck, Carsten .. HL 26.35, HL 38.7
Schueler, Michael ... MA 11.8, TT 21.8
Schuetzhold, Ralf ..... •QI 17.2
Schüffelgen, Peter ... QI 6.9, QI 14.26
Schug, Alexander BP 14.57, BP 14.65, BP 14.71
Schug, Felix ... •CPP 16.5, CPP 17.38, CPP 17.40
Schuh, Dieter ..... TT 73.7
Schuhmacher, Peter ..... QI 17.1
Schuhmacher, Peter Ken ..... QI 5.5
Schuhmann, Wolfgang ..... FM 6.7, FM 6.10
Schüle, Carolin Sabrina ... •DS 20.44
Schuler, Benjamin ..... BP 20.6
Schuler, Bruno ..... O 9.7
Schüler, Luis ..... •O 26.1
Schüler, Michael . MA 11.7, MA 38.13, O 20.1, O 66.3, TT 21.7, TT 44.9
Schull, Guillaume ..... O 12.4, O 12.7, O 12.9, O 43.16
Schüller, Christian ..... HL 3.8
Schuller, Ivan ..... HL 8.6
Schuller, Marlis ...•MA 31.2, •TT 47.2
Schüller-Ruhl, Aaron ..... UP 8.5
Schulte, Alfons ..... CPP 46.31, •CPP 46.37, CPP 46.39
Schulte, Stefan ..... •O 83.7
Schultheiss, Helmut ..... MA 59.7
Schultheiss, Jan .... FM 4.6, FM 11.4, FM 11.34, FM 18.7
Schultheiss, Katrin ..... MA 59.7
Schultz, Daniel ...•TT 57.11, TT 93.18
Schultz, Johannes FM 19.9, •MA 7.17, MA 27.4
Schultz, Ludwig ..... •DD 24.3
Schultz, Tobias ..... HL 40.2
Schultze, Martin ..... MA 27.11
Schulz, Armin ..... MA 19.8, TT 31.8
Schulz, Camelia ..... MM 34.1
Schulz, Fabian . O 15.5, O 22.1, O 99.7
Schulz, Jannis ..... •AKBP 13.4
Schulz, Michaela ..... •DD 26.2
Schulz, Niklas L. ..... TT 73.8
Schulz, Tommy ... •HL 13.3, HL 54.11
Schulze, Annelie ..... DD 39.2
Schulze, C ..... BP 37.2
Schulze, Dirk ..... HL 31.3
Schulze, Julian ..... AKBP 8.1
Schulze, Manuel ... O 44.12, •TT 61.3
Schulze, Michael ..... TT 79.4
Schumacher, Hans W. ..... HL 25.1
Schumacher, Hans Werner HL 20.54, MA 7.77, MA 7.78, O 95.1, TT 96.1
Schumacher, Henry ..... •DS 3.1
Schumacher, Jonas ..... MA 49.4
Schumacher, Jörg ..... •DY 28.1
Schumacher, Stefan HL 55.4, QI 14.22
Schumacher, Thorsten O 26.2, O 27.6, O 57.2
Schumann, Frank O. ..... •O 64.8
Schumann, Vanessa ..... BP 14.54, BP 14.79
Schumm, Thorsten ..... MA 39.25
Schün, Anton ..... O 68.6
Schunck, J. ..... O 19.10
Schunck, Jan ..... TT 14.4
Schünemann, Volker . O 41.1, TT 38.1
Schuricht, Dirk ..... DY 46.3, TT 75.3
Schürmann, Jannik ..... •HL 39.9
Schurr, Johanna ... •O 74.2, •TT 68.2
Schüßler-Langeheine, Christian MA 7.16, MA 27.2
Schusser, Jakub ..... O 76.3
Schüssler-Langeheine, C. ... MA 27.8
Schüssler-Langeheine, Christian MA 38.2, MA 38.6
Schust, Johannes ..... O 15.7, O 89.1, O 89.5
Schuster, Alexander ..... DD 30.2
Schuster, Constantin ..... TT 82.3
Schuster, Jörg ..... HL 48.8
Schuster, Lukas ..... •BP 40.2
Schütt, Pauline ..... •O 13.7
Schütte, Marc ..... MA 43.2
Schützhold, Ralf ..... O 59.5, O 62.1, O 71.1, O 71.18, TT 2.5, TT 42.5, TT 48.5, TT 54.1, TT 66.1, TT 66.18
Schwab, Dominik ..... FM 15.2
Schwab, Julian ..... •O 79.5, O 85.7
Schwade, Martin •MM 9.3, MM 19.49
Schwager, Anne .... BP 32.6, DY 52.6
Schwaiger, Ruth ..... •MM 32.1
Schwäke, Lynn ..... CPP 17.48
Schwalb, Chris ..... O 44.11
Schwandt-Krause, Johannes HL 24.9
Schwardt, Joachim ..... •DY 47.7
Schwark, Arthur von U.-S. ... MA 48.5
Schwarm, Mica ..... TT 23.30
Schwartz, Rico .... HL 20.25, HL 24.9
Schwartzkopf, M. ..... MA 7.21
Schwartzkopf, Matthias ..... BP 7.9, •BP 11.2, CPP 44.3, CPP 46.64, CPP 48.2, CPP 59.1, CPP 59.3
Schwartzkopff, Sebastian .•CPP 48.1
Schwartzkorpf, Matthias .. CPP 17.42
Schwarz, Denise ..... AKBP 7.3
Schwarz, N. ..... HL 17.7
Schwarz, Nicole ..... BP 7.14
Schwarz, Ulrich ..... BP 1.4, BP 14.67, CPP 1.4, DY 4.4, DY 49.6, TT 5.8
Schwarz, Ulrich S. .. BP 7.37, BP 12.7, BP 14.21, BP 30.3, CPP 47.3, CPP 49.4, DY 54.7
Schwarze, B. V. .... MA 47.7, TT 25.6
Schwarze, Rüdiger ..... DY 19.10
Schwärzer, Kuno ..... CPP 46.39
Schwarzkopf, Jutta ..... DS 20.25, FM 11.3, HL 26.52
Schwarzmaier, Korbinian ..... DS 8.3
Schwarz-Selinger, Thomas .. MM 7.7
Schweers, Sören ..... DY 43.20
Schweicher, Guillaume ..... O 61.8
Schweiger, Florian ..... AKBP 10.4, AKBP 11.1
Schweiß, Sophia ..... •O 3.6
Schweiss, Sophia ..... O 3.4
Schweitzer, Matthias R. ..... MA 52.7
Schweitzer, Pascal ..... CPP 17.8, •CPP 22.5
Schweizer, Matthias R. ..... MA 48.7, MA 48.8, MA 52.3, MA 52.20
Schweizer, Oskar ..... •TT 41.10
Schwendele, Martin ..... TT 22.21
Schwenk, Johannes ... O 3.3, O 15.4, •O 17.7, O 17.9, O 17.11, O 19.7, O 89.3, O 89.12, O 99.10
Schwenke, Philipp MA 52.9, •MA 59.1
Schwerdtfeger, Leah Dorothea •CPP 46.1
Schwierz, Nadine ..... BP 20.3
Schwingenschlögl, Udo ..... MA 13.9
Schwinghammer, Philip .... •HL 40.3
Schwöbel, Gabriel ..... •MA 52.7
Schwoerer, Heinrich ..... HL 26.54
Sciotto, Rachele ..... •MM 8.5
Scodellaro, Riccardo ..... AKPIK 2.3
Scolan, Ivan ..... •FM 22.6
Scoles, Amanda ..... QI 11.9
Scomparin, Luca ..... AKBP 8.10
Scontrino, Emilio ..... O 83.7
Scotti, Andrea .... CPP 35.2, DY 37.2
Seaberg, Mathew ..... HL 8.6
Sebastian, Aland ..... BP 5.5
Sebesta, Jakub ..... •MA 34.3
Sébilleau, Didier ..... O 2.4
Secchi, Eleonora ..... •BP 11.3
Sechovský, Vladimir ..... TT 93.17
Seckin, Melih ..... CPP 39.3
Seddon, Samuel ... FM 12.2, FM 12.6
Seddon, Samuel D. . FM 14.1, FM 14.2, FM 18.3, MA 6.6, O 52.3
Sedghi, Mohammad ..... MA 42.11
Sedighi, Mona ..... O 10.6, TT 16.6
Sedlák, Petr ..... MM 16.6
Sedlmayr, Martyna ..... •DY 8.6
Sedlmayr, Nicholas ..... •DY 32.12, •TT 45.12
Seduk, Farida ..... BP 41.1
Seeber, Phillip ..... BP 14.33
Seemann, Lukas .... DY 6.1, DY 42.12, DY 42.14, TT 63.12, TT 63.14
Seemann, Ralf .... BP 14.26, CPP 8.4, CPP 17.51
Seewald, Felix .. MA 7.50, •MA 47.11, MA 54.7
Segerer, Lina ..... •O 40.18, O 40.21, •TT 37.18, TT 37.21
Segets, Doris ..... HL 20.12
Segovia Gutiérrez, Juan Pablo •CPP 15.2
Sehr, Julian ..... •TT 92.6, TT 92.7
Sehrt, Jan T. ..... MM 19.48
Seibel, Christopher ... O 40.1, O 40.2, O 40.3, O 40.4, O 40.6, •O 98.6, TT 37.1, TT 37.2, TT 37.3, TT 37.4, TT 37.6
Seibel, Johannes ..... •O 23.2
Seibert, Sarah M. ..... BP 14.21
Seibert, Sebastian ..... O 44.11
Seidel, Ralf ..... FM 11.36
Seifert, Tim J. ..... •O 35.7
Seifert, Tom S. ..... O 80.4
Seifert, Udo ..... DY 7.4, DY 21.6
Seifert, Urban ..... TT 98.8
Seifert, Urban F. P. .. TT 6.4, •TT 86.3
Seiffert, Sebastian ..... CPP 54.3, CPP 58.1
Seiler, Anna ..... •HL 13.4, O 98.10
Seiler, Anna M. ..... O 66.9
Seiler, Hélène ..... HL 3.10, HL 8.12, HL 26.53, O 98.7
Seiler, Magdalena ..... •MM 19.18
Seinen, Vito ..... •DY 7.8
Seipel, Simone ..... TT 23.13
Seiter, Marco ..... DD 30.4, DD 32.1, •DD 37.2
Seith, Adrian ..... MA 12.2
Seitz, Franz ..... O 40.7, TT 37.7
Sek, Grzegorz ..... HL 20.34
Sekania, Michael ..... TT 94.9
Sekels, Alexander ..... O 58.1
Sekh, Ankhijur Islam ..... •MA 27.10
Seki, Kazuhiro ..... QI 5.7
Seki, Shinichiro ..... MA 9.1
Seki, Takeshi ..... MA 9.10, MA 30.1
Sekinger, Nils ..... •DS 8.1
Selbach, Sverre M. .. FM 18.8, MA 3.4

Seleznev, Gleb .....•TT 61.13
Sellies, Lisanne .....O 3.2
Selloni, Annabella .....•PLV VIII
Sellschopp, Kai .....MM 13.8
Sels, Dries .....DY 58.1, SOE 17.1
Selyakov, Ivan .....•UP 7.2
Selzer, Christian Erik .....O 77.4
Semeniuk, Konstantin .....TT 29.5, •TT 52.2, TT 94.5
Semenok, D. .....TT 80.6
Semenok, Dmitrii V. .....•TT 80.8
Semisalova, Anna .....MA 50.8
Semprebon, Ciro .....CPP 17.51
Sen, Aritra .....QI 6.4, QI 20.7
Şen, Onur Can .....•MM 34.6
Şen, Sinan .....CPP 15.3
Senarath, A. S. .....O 57.6
Senel, Deniz C. .....•DD 42.3
Senftleben, Arne .. MA 39.22, O 70.4, O 70.5, TT 65.4, TT 65.5
Sengupta, Anirvan . DY 58.1, SOE 17.1
Sengupta, Anupam . •BP 1.11, BP 11.4, •CPP 1.11, •DY 4.11
Sengupta, Kheya .....•BP 40.3
Sengupta, Surangana .....TT 89.4
Senker, Jürgen .....MM 12.4
Senkić, Ana .....HL 13.2, •HL 20.17
Sentef, Michael .....O 98.5, TT 4.12
Sentef, Michael A. ... O 14.9, •O 38.8, TT 44.9, TT 91.3
Senthiappan Vellaiappan Uthayasurian, Vedhanth .....•FM 15.2
Senthilkumar, Suganthan .... •BP 3.2
Sentis, Gael .....QI 21.10
Senyshyn, Anatoliy .....CPP 4.2, CPP 17.37, MM 19.16
Senzier, Pascale .....MM 40.5
Seo, Jun Seok .....MA 59.9
Seo, We-hyo .....O 15.6
Seoane-Souto, Rubén .....TT 6.2
Septembre, Ismaël ... QI 15.9, QI 21.4
Serafini, Giulia .....BP 12.9
Serbyn, Maksym .....•DY 2.1, •TT 1.1, TT 28.11
Serebrennikova, Alexandra .. CPP 6.4
Serényi, Miklós .....DS 6.4
Serga, Aleksander A. .....MA 52.7
Serga, Alexander A. .....MA 48.7, MA 48.8, MA 52.20
Serha, Rostyslav O. .....MA 48.2, MA 48.7, MA 52.7
Seroussi, Inbar .... DY 58.8, SOE 17.8
Seshappan, Arabi .. •TT 17.11, •QI 4.11
Sessoli, Roberta .....O 42.4
Šesták, Petr .....•MM 16.6, MM 16.7
Sesti, Giacomo .....•O 84.7, •TT 84.7
Setescak, Alexander .....•MA 58.2
Setescak, Christoph . O 41.2, TT 38.2
Setescak, Christoph Stephen •O 63.10, •TT 55.10
Sethi, Harshit .....O 12.2, O 44.4, •AKPIK 5.11
Šetina, Janez .....O 78.5
Setlur, Girish .....•DY 54.6
Settanni, Giovanni ... BP 4.2, BP 31.3, CPP 50.3
Sette, Andrea .....O 58.3
Setti, Yassine ..... HL 29.2, TT 58.2
Setty, Abhishek .....•QI 1.3
Setvin, Martin .....O 93.8
Setz, Jeremi .....O 96.12
Sevilla, Mauricio •CPP 48.3, DY 43.10
Sevinchan, Yunus . BP 14.90, BP 36.8, DY 57.8, SOE 5.2
Sevriuk, Vasilii .....•TT 22.17
seyed heydari, mahsa .....•MA 54.5
Seyller, Thomas .... DS 20.42, O 31.1, O 66.2, O 73.5, O 74.8, O 84.2, O 93.1, TT 68.8, TT 84.2
Seyve, Lilian ..... HL 29.2, TT 58.2, •TT 74.11
Sezik, Emir .....•DY 62.6
Shabala, Natalia .....•MA 40.7
Shabalin, Anatoly .....HL 8.6
Shabani, Faezeh ... DS 18.4, •DS 18.5, DS 18.6
Shabani, Javad .....O 48.6
Shabaz, Abdul Qadir ..... •DS 20.23
Shabbir, Huzaifa .....CPP 59.5
Shaebani, Reza .....BP 14.6, BP 40.2
Shaffer, Milo S. P. .....CPP 26.1
Shah, Shreya .....AKPIK 6.6
Shahbazi, Farhad .....SOE 8.4
Shahi, Farzad .....QI 12.5
Shaikhaidarov, Rais .....TT 22.17
Shaju, Sandra C. .....MA 7.71
Shakhayeva, Billura .....•CPP 17.49
Shakirov, Timur .....CPP 46.60
Shalaby, Ahmed .....TT 93.4
Shalaby, Mustafa .....•TT 93.4
Shallcross, Sam .....MA 38.14
Shallcross, Samuel ..... MA 35.10, TT 60.10
Shalloo, Rob .....AKBP 12.3
Shalloo, Rob J. .....AKBP 8.4
Shameem, Raufar .....•FM 11.36
Shampa, Maharun Nesa ....•DY 28.4
Shamrovska, Polina .....•DS 20.19
Shan, H. .....HL 54.12
Shan, Hangyong .....HL 54.8
Shan, Jie .....•PLV III
Shanbhag, Shridhar .....HL 54.2
Shanbhag, Shridhar Sanjay .•HL 54.3
Shandi, Asaad .....MA 7.42
Shang, Yuanyuan .....MM 34.7
Shankar, Suraj .....BP 37.11
Shanmugam, Maheswaran . MA 42.6
Shannon, Nic .....MA 19.10, TT 31.10
Shao, Wei .....MM 36.5
Shao, Ziming .....HL 8.6
Shapiro, D. .....MA 50.3
Shapiro, Dmitrii .....•AKPIK 5.15
Shapiro, Dmitriy S. .....QI 3.9
Sharan, Sanchita .....AKBP 8.7
Sharif, Reza .....MM 19.20
Sharifi-Aghili, Azadeh ..... CPP 8.3
Sharifian, Ali .....•BP 14.65
Sharikow, Eugen .....O 69.7
Sharipov, Rustem .....QI 17.8
Sharma, Abhinav . CPP 49.2, DY 34.8, DY 55.4, DY 55.6, DY 55.8
Sharma, Abhishek ..... BP 26.11, CPP 43.11
Sharma, Anand .....•DY 14.11
Sharma, Anjali .....AKPIK 5.5
Sharma, Ankit ..... MA 6.2
Sharma, Avdhesh Kumar ..•MM 40.3
Sharma, Chithra .... MA 7.67, O 71.17, TT 66.17
Sharma, Chithra H. .....•TT 64.4
Sharma, Deepali ..•MA 11.5, •TT 21.5
Sharma, Gargee .....•MM 26.4
Sharma, Mayank •CPP 34.3, •DY 36.3
sharma, meenakshi •TT 5.3, TT 22.23
Sharma, Mira .....QI 8.1
Sharma, Nand Lal ... HL 34.1, QI 18.6
Sharma, Niyorjyoti ..... FM 18.8
Sharma, Rahul ..... HL 20.14, O 10.6, TT 16.6
Sharma, Rati ..... BP 15.9
Sharma, Rohit ..... TT 23.14, TT 61.2
Sharma, Sangeeta .....•MA 14.1, MA 27.11, MA 35.10, MA 38.5, MA 38.14, MA 58.6, TT 60.10
Sharma, Shubham ..•DY 14.9, O 72.6, TT 67.6
Sharma, Suhani ... TT 64.3, TT 93.16
Sharma, Veerendra Kumar .. CPP 7.2
Sharp, Ian ...DS 8.1, DS 12.3, HL 12.2, HL 40.3
Sharp, Ian D. . DS 9.3, DS 11.1, DS 11.2, HL 1.1, HL 9.4, HL 12.5, HL 12.7, HL 33.5, HL 42.1, HL 42.3, HL 42.5, MM 4.2, MM 4.3, O 97.8
Shatruk, M. .....TT 5.9
Shayduk, Roman .... O 40.15, O 98.3, TT 37.15
Shchepetilnikov, Anton .....HL 10.5, TT 20.5
Shchukin, Konstantin O 10.11, •O 54.4, TT 16.11
Shea, Jeanine .....DY 55.5
Shee, Amir .....CPP 11.7, DY 17.7
Shee, Payel .....•TT 25.1
Sheehy, Daniel .....TT 56.11
Shehada, Sufyan .....•O 17.1
Sheikhan, Ameneh . DY 59.9, TT 99.9
Sheina, Valeria ....MA 43.5, MA 49.8
Sheka, Denis D. .... MA 44.7, TT 76.7
Shekar, Chandra .....MA 40.8
Shekarabi, Sahar .....CPP 46.43, HL 26.41
Shekhar, Chandra MM 40.1, MM 40.3, O 63.4, TT 49.5, TT 55.4
Shemerliuk, Yuliia .....•TT 4.9
Shen, Bin ...MA 8.5, TT 57.5, TT 98.2
Shen, Chen .....BP 14.24, CPP 19.4, DY 20.4, MA 33.7
Shen, K. M. .....TT 69.6
Shen, Lingjia .....MA 33.11
Shen, Qin Xin .....TT 69.1
Shen, Zhiqi .....BP 3.3
Shen, Zhi-Xun ..... O 84.8, TT 84.8
Sheng, Shaoxiang .....O 12.3
Shengelaya, A. .....TT 5.9
Shera, Kumrie .....TT 22.32
Sherjan, Areso .....•AKBP 7.4
Shevtsova, Olga .....•TT 92.4
Shi, Lifen .....•TT 93.11
Shi, Qing .....•O 48.3
Shi, Shan MM 3.2, MM 3.4, MM 19.19, MM 19.21
Shi, Yunli .....•MM 4.8
Shibahara, Haruto ..•O 72.2, •TT 67.2
Shick, Alexander ..•MA 11.4, •TT 21.4
Shimanovich, Ulyana .....BP 3.3
Shimizu, Makoto ...MA 11.1, MA 11.2, TT 21.1, TT 21.2
Shimizu, Yusei .....TT 2.1
Shimokawa, Takaya .....O 61.11
Shin, Dong Hoon .....BP 9.1
Shin, Dongho ....HL 20.23, HL 20.24
Shin, Soohyeon ..MA 47.10, •TT 25.5
Shinwari, Tauqir .....•DS 12.9
Shiota, Yoichi .....MA 59.4, MA 59.9
Shiotari, Akitoshi ... O 12.10, •O 43.2, O 45.1
Shipunov, Gregory .....TT 11.4
Shipunov, Grigory ..MM 40.4, TT 11.3
Shipunov, Grisha .....MA 24.3, O 2.5, TT 36.3
Shitotari, Akitoshi .....O 45.7
Shiversky, Denis .....MM 19.15
Shkodich, Natalia .....MA 50.1
Shnirman, Alexander TT 85.6, QI 17.5
Shojaee, Pejman .....BP 33.6
Shokeen, Vishal ... MA 24.4, TT 36.4
Shokrani, Morteza .....DS 7.3
Shokri, Hamed .... MA 13.7, MA 50.1
Shokri, Sina TT 13.1, •TT 71.5, TT 71.6
Shondo, Josiah Ngenev ....CPP 15.3
Shpyrko, Oleg ..... HL 8.6
Shradha, Sai .....•HL 13.7, HL 20.5, HL 20.6, HL 20.13, HL 39.5
Shrestha, Binamra .....•HL 48.7
Shrestha, Sulabh ..... HL 20.45
Shubbak, Yahya ....DY 41.13, MA 5.1, MA 7.23, •MA 36.4, MA 36.5, TT 7.1
Shukla, Atul ..... CPP 40.2
Shukla, Chinmay ..... O 36.4
Shukla, Gaurav ..... MA 13.6
Shukla, Nidhi ..... MA 13.6
Shumaly, Sajjad .....CPP 8.5
Shuvaev, Alexey .... HL 10.5, MA 4.5, MA 17.11, TT 20.5
Shvartsman, Vladimir .....•FM 4.4, FM 11.18, FM 11.32
Shysho, Oleksandr ..... HL 53.4
Si, Liang ..... TT 69.2
Si, Wen .....O 42.5
Sibille, R. .....TT 25.9
Sich, Annemarie .....•DD 18.1
Sicheler, Niklas .....MA 33.9
Sichelschmidt, J. .....TT 5.9
Sichelschmidt, Jörg TT 61.3, TT 94.3
Sick, Bernhard .... DY 41.13, MA 7.23
Siday, Tom ..... O 12.5
Sidis, Yvan ..... MA 3.6
Sidorenko, Anna .....•O 26.3
Sidorova, Mariia .....TT 82.3
Siebenhofer, Matthäus ..... •O 52.4
Siebenkotten, Dario ..... •O 96.5
Siebigs, Leo .....•HL 15.2, O 96.1
Siebold, Mathias ..... AKBP 7.3
Siecker, Karla .....•O 68.2
Siegert, Marie ..... CPP 22.2
Siegert, Sandra .....BP 3.7
Siegl, Julian ..... DY 32.3, TT 45.3, TT 56.13
Siegl, Markus .....•DY 42.5, •TT 63.5
Siegmund, Malte . BP 26.8, BP 26.10, CPP 43.8, CPP 43.10
Siemann, Gesa .....O 66.8, •O 76.5
Sievers, Philipp ..... •BP 11.1
Sievers, Sibylle .... MA 7.77, MA 7.78
Siewert, Jens .....•QI 21.10
Siewirska, Katarzyna ..... TT 14.5
Sifft, Markus .....•QI 14.27, QI 21.3
Sigel, Reinhard .....•CPP 46.63
Signorell, Ruth .... CPP 19.5, DY 20.5
Šikola, Tomáš .....O 27.1, O 96.7
Silber, Robin .....MA 39.6, MA 39.7, MA 39.13
Silly, Mathieu G. .....O 11.4
Silva Dias, Leonardo ..... BP 14.96
Silva, Jadson ..... TT 26.4
Silveira Junior, Orlando .....O 44.4
Silveira, Orlando ..... AKPIK 5.11
Silveira, Orlando J .....•O 12.2
Silverman, Kevin ..... HL 55.2
Sim, Junyoung ..... O 43.6, •O 43.9, O 80.4
Simitsis, Leonidas .....O 94.11
Simkovic, Fedor ..... TT 17.5, QI 4.5
Simmel, Friedrich .. BP 8.4, BP 14.23, CPP 20.2, DY 23.2
Simmel, Friedrich C. ..... BP 5.1
Simon, David .....UP 6.3
Simon, Florian ..... TT 74.10
Simon, Hannes .....HL 16.7
Simon, Pascal .....DS 12.4, TT 83.2
Simon, Seyfferth ..... DD 12.2
Simoncelli, Michele ..... MM 31.4
Simonov, Kyrylo .....QI 12.3
Simperl, Florian .....O 93.1
Simpson, Grant J. ..... O 46.7
Šindler, Michal ..... TT 93.12
Singer, Andrej ..... HL 8.6
Singer, Mirko . BP 1.4, CPP 1.4, DY 4.4
Singer, Moritz .....•DS 1.2, DS 16.6, QI 11.10
Singewald, Tanja D. .....BP 7.12
Singh, Abhishek .....MM 31.6
Singh, Aditya .....FM 12.11
Singh, Akriti ..... •MA 3.9
Singh, Aman .... MA 13.3, •MA 39.17
Singh, Anisha .....O 84.8, TT 84.8
Singh, Ankit ..... •MM 41.1
Singh, Anuj Kumar .....HL 20.30
Singh, Anupam ..... DS 11.8
Singh, Chandan ....O 40.15, TT 37.15
Singh, Deepak .....TT 14.9
Singh, Diwakar .....HL 24.4
Singh, Gyanendra .....TT 81.1
Singh, Hansveer .....•QI 3.11
Singh, Haribrahma •MA 7.26, TT 41.7
Singh, Jayant k. .....CPP 17.47
Singh, Karan .....•TT 61.2
Singh, Karnika ..... DY 62.5
Singh Negi, Devendra ..... MA 3.11
Singh, Nisha .....MM 21.1
Singh, Prabhdeep .....•O 27.4
Singh, Puloma .....•MA 27.11
Singh, Rajendra .....HL 40.4
Singh, Ravi Prakash MA 11.5, TT 14.9, TT 21.5, TT 64.3, TT 93.16
Singh, Ravi Shankar ..... MA 11.5, MM 21.7, TT 21.5
Singh, Rohan ..... QI 13.9
singh, sandeep .....TT 5.3
Singh, Sanjay ..... MA 13.6
Singh, Satya Veer .... O 10.4, TT 16.4
Singh, Shobha .....•TT 61.4
Singh, Shraddha ..... QI 6.10
Singh, Shubham Rakesh ... •MA 13.9
Singh, Sonika .....•HL 40.4
Singh, Suhani .....•O 48.6
Singh, Sujata .....MA 31.5, TT 47.5
Singh, Sunil P. ..... BP 1.6, •BP 10.1, CPP 1.6, •CPP 18.1, DY 4.6, •DY 18.1
singh, surinder ..... TT 5.3
Singh, Tavinder .....MM 8.7
Singh, Utkarsh .....•HL 45.7
Singha, A. .....TT 24.7
Singha, Aparajita ... TT 40.2, TT 92.1, TT 92.2, TT 92.4
Singla, Sakal .....O 40.12, TT 37.12
Singleton, John .....FM 10.5
Sinha, Aritra .....•MA 34.8
Sinha, Kshitij .....•AKjDPG 1.4
Sinha, Mangalika ..... BP 14.30
Sinha, Sakshi .....•BP 7.11
Sinha, Swarnshikha ..... TT 14.5
Sinigaglia, Chiara .....BP 3.3
Sinn, Alexander .....AKBP 12.2, AKBP 12.3
Sinner, Anton . •CPP 46.49, CPP 59.6
Sinner, Tun .....O 5.6
Sinnhuber, Björn-Martin .....UP 6.2, UP 8.4
Sinnis, Photini BP 1.4, CPP 1.4, DY 4.4
Sinnott, Pierce .....O 78.6
Sinova, Jairo MA 2.3, MA 2.5, MA 2.7, MA 7.53, MA 7.55, MA 8.5, MA 8.6, MA 20.2, MA 20.6, MA 47.6
Sinz, Björn ..... HL 8.4
Sinzinger, Stefan .....AKPIK 4.3
Sipos, Marcell .....MA 58.3
Siretanu, Igor .....•O 36.4
Sirk, Timothy W. ..... MM 41.1
Sirotti, Elise ..... HL 42.1
Sirotti, Fausto .....O 38.2
Sirt, Serkan .....•HL 25.4, HL 40.1
Sitierle, Andreas ..... CPP 15.1

Sitter, Daniel ..... QI 14.24
Sivasubramaniyan Sudandiradevi, Vishak ..... MM 19.44
Siverin, Nikita ..... HL 49.3
Sivianes, Javier .....•O 7.4, •TT 9.4
Siviero, Matilde ..... HL 26.2
Sivis, Murat ..... FM 11.33, HL 8.5, MA 27.3, O 79.7
Sjølin, Benjamin H. ..... MM 5.2
Skála, Tomáš ..... O 65.12, O 94.4
Skalli, Anas .....•AKPIK 3.4
Skandalis, Athanasios ....CPP 46.26
Skerk, Rudy ..... •DY 58.9, •SOE 17.9
Skibitzki, Oliver ..... O 96.6
Skobjin, Gregor .....•MA 7.52
Skok, Gregor ..... UP 5.5
Skokov, K. MA 18.1, MA 18.5, MA 23.5, MA 50.3, TT 30.1, TT 30.5, TT 35.5
Skokov, Konstantin ..... MA 18.2, MA 50.4, MA 50.5, MA 50.6, MA 50.7, MA 50.8, MA 52.23, MA 52.27, MA 52.32, TT 30.2
Skolaut, Julian .... MA 37.2, •O 17.10
Skopnik, Anna ..•DY 42.14, •TT 63.14
Skoropota, E. ..... MA 25.6
Skourski, Y. MA 23.5, TT 35.5, TT 74.5
Skourski, Yurii ..... MA 2.6, MA 23.4, TT 35.4
Skrotzki, Werner .....•MM 7.9
Skrzypczyk, Paul . MA 19.10, TT 31.10
Škvára, Jan ..... O 65.12
Slanovc, Florian ..... MA 34.6
Slautin, Boris ..... FM 11.18
Sławiński, W. ....•CPP 32.3, •DY 35.3
Sleziona, Vivien .....O 22.1, O 43.4, O 43.10
Slipchenko, Mykola ..... MA 13.8
Slobodianiuk, Denys ..... MA 48.2
Slobodkins, Arkadijs ..... MA 34.1
Slopianka, Cissie ..... O 8.7
Smallenburg, Frank ..... DY 62.7
Smart, Thomas ..... TT 93.6
Smart, Thomas J. ...•QI 6.9, QI 14.26
Šmejkal, Libor ..... MA 8.5, MA 8.13, MA 20.2, MA 20.6, MA 29.7, MA 33.13, MA 47.6, MA 54.6, MA 54.10, TT 46.7
Smerzi, Augusto ..... QI 15.3
Smet, Jurgen .....TT 24.6, TT 92.5
Smid, Sabrina .....•BP 14.66
Smidman, Michael . MA 19.3, TT 31.3
Smiri, Adlen .....•DS 12.8, HL 3.12
Smirne, Andrea ..... QI 7.4
Smirnova, Daria ..... MM 7.4
Smith, Jack .....•MA 34.6
Smith, Rodney .....O 34.4
Smoliarova, Tatiana ..... MA 50.1
Smyczek, Jan .•O 34.8, O 81.1, O 88.6
Sneh, Sneh .....TT 61.4
Snoeken, Michiel .....•HL 26.48
Snowden, Henry T. .....•O 98.8
Soares, Gustavo ...•O 95.2, •TT 96.2
Soavi, Giancarlo .. DS 13.2, HL 20.18, HL 20.21, HL 20.31, HL 26.47, HL 30.3, HL 35.6, HL 54.1, HL 54.2, HL 54.3, TT 59.3
Sobierajski, Ryszard ..... MM 19.3, MM 19.22
Sobisch, S. ..... HL 45.1
Sochiera, Simon .•MA 29.2, •TT 46.2
Sochiera, Simon J. ..... MA 37.2
Sochor, Benedikt CPP 15.1, CPP 17.15, CPP 17.42, CPP 25.4, CPP 46.17, CPP 46.51
Sodemann Villadiego, Inti .. TT 44.11, TT 44.12, TT 72.2, TT 83.11
Söderberg, Daniel ..... CPP 32.4, CPP 46.17, DY 35.4
Södergren, Lasse ..... QI 8.3, QI 11.6, QI 11.9
Sodjargal, Tulga-Erdene ..... MM 9.2
Soe, We-hyo .....O 89.10
Soe, We-hyon .....O 15.9
Soederberg, D. ..... MA 7.21
Sofer, Zdenek .....HL 20.5, HL 20.13, HL 20.22, HL 25.2, HL 35.6, HL 39.3, HL 39.4, HL 39.5, HL 39.6, HL 39.7, HL 39.8, HL 39.11, MA 39.22, MA 46.5, O 38.4, O 76.5
Soffiati, Gabriela .. CPP 2.3, SOE 3.3, UP 1.3
Soh, Yeong-Ah .....MA 11.8, TT 21.8
Sohn, Seoyun .....•MM 39.2
Sokaras, Dimosthenis ..... FM 11.31
Sokolov, Aleksey .....•O 30.4
Sokolowski, Moritz ..•O 46.5, O 46.6
Solbrekken, Edvard .O 95.11, TT 96.11
Soldatov, Ivan ....MA 7.80, MA 39.17
Solé, Andrés Pinar ..... O 17.4
Soleimani, Mahmoud .....•HL 26.16
Sollich, Peter .....BP 7.18, BP 7.39, DY 7.10, DY 43.15, DY 44.17, DY 44.20, DY 49.5
Sologub, Sergii .....•O 33.4, O 73.1
Solomakhin, Ivan ...•QI 14.7, QI 14.8, QI 18.3
Solomons, Naomi R. ..... QI 18.9
Solovev, Ivan .....•HL 16.1
Solov'yov, Ilia ..... BP 14.70
Soltanmohammadi, Mina .....O 23.9
Sommer, Jens-Uwe BP 29.5, BP 31.4, BP 39.2, •BP 42.1, CPP 45.5, CPP 50.4, CPP 54.4, CPP 55.2, CPP 59.5, •CPP 61.1, DY 55.4, DY 55.6, •DY 64.1
Sommer, Marco ..... MA 7.73
Sommer, Maximilian .....•JOB 1.1
Sommer, Michael ..... CPP 17.43, CPP 59.2, O 82.5
Sommers, David .....O 48.6
Sondermann, Holger .....BP 11.2
Sonderrmann, Holger ..... BP 7.9
Song, Bo .....MA 57.1
Song, Geonho ..... BP 7.12
Song, Haoyu ..... BP 31.1, CPP 50.1
Song, Jitong ..... TT 52.4
Song, K. W. .....HL 54.10, HL 54.12
Song, Lulu .....•FM 6.11
Song, Moojune .. MA 52.12, MA 59.9
Song, Qi ..... MA 27.7
Song, Qian .....HL 24.10
Song, Xiaohong ..... HL 1.3
Song, Y. ..... O 88.11
Song, Yefan ..... CPP 54.6
Song, Yihua ..... •MM 41.7
Song, Young-Joon .....•FM 10.1
Song, Zijian ..... DD 40.1
Sonnenberger, Jan Ole .... •TT 22.36
Sonnweber-Ribic, Petra .... MM 34.3
Soomro, Romesa ..... •BP 7.1
Soon, Youngseon .....•MA 52.12
Sopinska, Katarzyna ..... FM 12.11
Şopu, Daniel .....MM 18.2, MM 18.4
Sorba, Lucia .....HL 20.34
Sorgenfrei, Felix .....MM 37.5
Sorn, Sopheak ....•MA 54.4, TT 23.4
Sorrentino, Andrea .MA 44.6, TT 76.6
Sortino, Luca ..... HL 20.18
Sosa Barth, Fiona •MA 51.8, •TT 88.8
Sosa-Lizama, Pablo ..... TT 39.7
Sosniok, Tom .....•BP 7.29
Sostina, Daria ..... O 17.5
Sotgiu, Simone ..... HL 20.26
Sothmann, Björn ... HL 20.41, O 89.9, O 98.4, TT 2.5, TT 42.3
Sotiriadis, Spyros ..... QI 3.3
Soubatch, Serguei .... O 45.9, O 61.1, O 83.2
Soufla, Aliki .....O 83.1
Souliou, Michaela ..... TT 95.2
Souliou, Sofia. M ... TT 23.31, TT 71.1
Soultati, Anastasia . DS 16.2, DS 20.5
Sourd, J. ..... MA 23.5, TT 35.5
Sourd, Jeremy ..... MA 2.6, MA 23.4, •TT 25.6, TT 35.4
Souri, Somayeh ..... HL 46.3
Sourjik, Viktor ..... BP 14.51
Sousa Barbosa, Ricardo Manuel •MA 24.5, •TT 36.5
Sousa, David ..... O 44.17
Souza, Ivo .....MA 5.6, TT 7.6
Sovic, Karlo ..... •O 34.2
SÖYLEMEZ, Saniye .....MM 16.4
SÖYLER, Dilek .....MM 16.4
Spagna, Stefano ..... O 44.11
Späh, Peter ..... •FM 7.4
Spaldin, Nicola ... FM 12.7, •MA 25.2
Spaldin, Nicola A. ... FM 7.7, MA 25.7
Spallek, Domenik .. DS 20.18, •FM 7.8
Spanheimer, Kai Luca .... •CPP 20.3, •DY 23.3, DY 44.3
Spantzel, Lukas ..... BP 14.33
Sparmann, Tobias . MA 21.1, MA 55.8
Spartz, Franz ..... O 14.2, O 40.16, TT 37.16
Späth, Thomas ..... O 44.12
Spatz, Verena .....DD 8.3, DD 29.1, DD 30.5
Spears, Alexander .....•O 66.10
Specht, Rahel .....FM 19.5, O 46.1
Speck, Thomas ... BP 29.6, CPP 11.2, CPP 14.7, CPP 45.6, DY 9.3, DY 17.2, DY 43.11
Speed, Sarah K. ..... CPP 54.4
Speier, Stephan ..... BP 14.10
Speliotis, T. ..... MA 47.7
Speller, Sylvia .....BP 14.25, BP 33.9, O 27.2, O 44.13, O 46.9, O 68.6
Spencer, Michael ..... MA 25.3
Spencer, Michael S. ..... •O 49.2
Spencer, Russell .....•BP 16.8
Sperlich, Andreas .....CPP 17.16, CPP 25.2, CPP 57.5, FM 11.20, HL 16.6, HL 20.61, HL 24.3, HL 26.29, HL 49.2
Sperling, Jan .....QI 5.9
Spickmann, Florian . FM 11.33, O 22.2
Spiecker, Martin .....TT 43.6, QI 11.4, QI 11.5
Spiegelberg, Noah .....MA 7.86
Spiegler, Stefanie ... BP 7.34, BP 7.38
Spies, Johannes ..... •MM 9.8
Spies, Maximilian •CPP 44.6, HL 45.5
Spiller, Peter .....AKBP 7.3
Spindler, Ephraim •MA 6.1, MA 52.39, TT 24.3
Spirito, Davide ..... HL 38.9
Spitzer, Nikolai ..... HL 26.31
Spitzner, Noah .....•HL 18.5, HL 26.1, •TT 32.5
Splettstoesser, Janine .....•TT 18.4, TT 53.2
Splith, Daniel ..... HL 26.40
Spolenak, Ralph .. DS 16.1, •MM 32.4, MM 35.3, O 96.12
Spörk-Erdely, Petra ..... MM 21.5
Sporkett, Melina ..... •HL 26.33
Sprafke, Alexander ..... CPP 46.9
Spree, Lukas ... O 8.6, O 17.4, O 77.6, O 89.10
Spree, Lukas Emanuel ..... •O 77.5
Spreitzer, Axel ..... AKBP 1.2
Sprengel, Carla .....BP 14.47
Springate, Emma ..... O 66.8
Springborn, J. Richard .....MM 19.1
Springborn, Johann Richard ..•O 18.3
Spruce, Kieran ..... O 42.9
Spruijt, Evan .....BP 29.1, CPP 45.1
Sprung, Michael .....HL 4.1
Spuri, Alfredo ..... •TT 29.10
Spyrantis, Alexander ..... FM 11.28
Squires, David .....•AKBP 8.3
Squires, Oliver .....TT 62.7
Sridhar, Gautam .....BP 14.68
Sriluckshmy, PV .... •TT 17.5, •QI 4.5
Srinivasan, Harish .....•CPP 7.2
Srivastava, Ashutosh .....MM 31.6
Srivastava, Diksha •CPP 17.47, O 10.4, TT 16.4
Srivastava, Shashank .....•TT 14.9, TT 64.3, TT 93.16
Srolovitz, David J. ..... MM 30.1
Srowik, Kilian .....TT 5.7, TT 40.3, •TT 92.3
Srpak, Ilija .....•DY 14.10
Staab, Torsten ..... FM 19.7
Staab, Torsten E.M. ..... FM 5.3
Staabs, Maximilian •MA 7.10, O 40.17, TT 37.17
Staacks, Sebastian . DD 24.2, DD 36.1
Staats, Max ..... DY 58.4, SOE 17.4
Stacchiola, Dario ..... •O 94.1
Stach, Oliver ..... CPP 14.7
Stadermann, Kirsten ..... DD 36.3
Stadler, Andreas .....MA 7.25
Stadler, Georg ..... DY 15.8
Stadler, Oliver ..... DD 7.2
Stadler, Pascal ..... QI 14.4
Stadler, Sebastian .....•BP 14.78
Stadler, Tristan ..... TT 42.6
Stadtmüller, Benjamin .....MA 8.6, MA 38.7, MA 47.3, MA 54.8, O 8.1, O 9.1, O 14.2, O 40.16, O 41.1, O 42.2, O 57.4, O 83.4, TT 37.16, TT 38.1
Stadtmüller, Till ..... FM 7.5
Staffieri, Gregorio .....•TT 14.6
Stagge, Pascal ..... MA 49.4
Stagni, Alessandro ..... DY 28.3
Stahlberg, Linus P. .....TT 5.5
Stähler, Anne .....•AKBP 7.2
Stähler, Cosima .....O 69.11
Stählke, Susanne ..... BP 33.9
Staiger, Lukas ..... O 41.1, TT 38.1
Stallberg, Klaus ..... O 58.6, •O 83.9
Stallmach, Frank ..... DD 16.1
Stampfer, Christoph . HL 3.3, HL 10.3, HL 20.26, MA 43.2, •TT 12.1, TT 20.3, DD 36.1
Stampfl, Catherine FM 23.2, MM 14.1
Ständer, Christian TT 22.19, TT 22.22
Stange, Daniel E. ..... BP 37.7
Stanger, Michael .....TT 22.25
Stangier, Veronika .....•TT 56.11
Stanionytė, Augustė .....MA 3.3, •MA 52.35
Stankevych, Andrei ..... CPP 57.2
Stanković, Igor .....MM 32.5
Stannarius, Ralf ....DY 25.3, DY 25.4, •DY 25.5
Stanzel, Silke ..... TUT 2.1, DD 1.1, •DD 10.3
Stará, Veronika ..... O 6.3
Starikov, Sergei ..... MM 7.4
Stark, Alexandra ..... MM 34.3
Stark, Holger BP 1.3, CPP 1.3, DY 4.3, •DY 55.5, DY 62.8
Stark, Máté .... O 15.4, O 17.7, O 17.9, O 17.11, •O 89.3, O 89.12, O 99.10
Stärk, Philipp .....CPP 3.5, CPP 14.3, CPP 14.5, MM 17.3
Stark, Wojciech G ..... O 66.10
Starke, Jens .....O 44.13
Starke, Ulrich ..O 19.1, O 33.3, O 62.6, O 66.8, O 74.5, TT 54.6, TT 68.5
Starkov, Dmitry .•BP 36.10, •DY 57.10
Starkov, Grigorii ...•HL 10.2, •TT 20.2
Starostin, Vladimir .....CPP 12.5, AKPIK 6.6
Starykh, Oleg A. ..... TT 86.3
Stastny, Simon .....•QI 6.6
Staszewski, Luke .•DY 46.6, •TT 75.6
Staub, U. ..... MA 27.8
Staub, Urs HL 8.10, MA 7.16, MA 25.6, MA 27.2
Staude, Isabelle .... DS 16.7, DS 20.8
Staudenmayer, Patrik O 10.11, O 54.4, TT 16.11
Staufer, Oskar .....•BP 16.4
Stauffenberg, A. ..... HL 45.1
Staunton, Julie B ..... MM 41.3
Stavale, Fernando ..... O 94.4
Stavans, Joel BP 1.9, CPP 1.9, DY 4.9
Stavraka, Theodora .....•UP 3.3
Stavropoulos, P. Peter ..... •MA 31.3, •TT 47.3, TT 51.1
Stavropoulos, Panagiotis ....TT 72.5
Stavropoulos, Panagiotis P. MA 33.10
Stechemesser, F. .....•HL 20.27
Stecher, Leon .....HL 10.3, TT 20.3
Steck, Thomas .....MM 19.20
Steeger, Paul ..... FM 15.2
Steen, Malcolm ... CPP 10.4, DY 16.4
Stefan, Karpitschka ..... BP 14.8
Stefancu, Andrei ..... O 96.10
Stefanini, Matteo ..... DD 7.2
Steffen, Fabio D. ..... BP 14.54
Steffens, Ana Katharina ..•AKBP 9.2
Steffens, Paul .....MA 3.6, MA 3.7, TT 95.7
Stehling, Till-Jakob ..... TT 61.14
Steiakakis, Konstantinos .... BP 20.2
Steidel, Jakob ..... O 46.2
Steiglechner, Peter .....•SOE 2.8
Steil, Daniel .....MA 7.10, •MA 55.6, O 14.3, O 14.10, O 19.6, O 40.17, O 40.19, O 40.21, O 66.9, O 98.10, TT 37.17, TT 37.19, TT 37.21
Stein, David .....MA 7.7, •MA 12.1, MA 52.33
Stein, Louis .....TT 57.5, •AKBP 2.5
Stein, Markus .....HL 23.8, HL 26.28
Stein, Quentin .....•O 12.4, O 12.7
Steinacker, Christoph .....•SOE 6.4
Steinbach, Claudia ..... O 52.4
Steinbach, Felix ..... MA 38.4
Steinbach, Florian .....•BP 20.9
Steinbauer, Michael Karl ...•MA 7.44
Steinbrecher, Luca ..... HL 15.2
Steinbrecher, Manuel .....O 99.3
Steinbrecher, René .....CPP 31.4
Steinbrück, Smilla ... BP 1.4, CPP 1.4, DY 4.4
Steiner, Alex .....QI 16.1
Steiner, C. ..... HL 20.27
Steiner, Corinne ..... HL 47.1
Steiner, Emil .....MA 38.8
Steiner, Maria .....•O 99.12
Steinfurth, Andrea .....DY 48.6
Steingelb, Genrietta ..... HL 12.3
Steinhart, Martin ..... CPP 46.9
Steinhöfel, Tara .....•DY 44.8
Steinhoff, Alexander ..... HL 13.3, HL 54.11
Steinhuber, Mathias .DY 13.6, TT 19.6

Steiniger, Klaus ..... AKBP 10.1, AKBP 10.2, AKBP 10.3, AKBP 12.5
Steinigeweg, Robin DY 46.3, DY 46.4, TT 53.8, TT 75.3, TT 75.4
Steinkirchner, Katharina .....•O 70.3, •TT 65.3
Steinkopf, Lars ..... DS 20.36
Steinkühler, Jan .....•BP 16.5
Steinmann, Johannes ..... AKBP 4.2
Steinmetz, Tilmann •DD 13.2, DD 24.1
Steinrück, Hans-Peter .. O 4.2, O 87.1, O 87.6, •O 100.1
Steinweh, Jimmy .....•FM 11.15
Stekiel, Michal ..... MA 9.11
Stella, Attilio L. ..... DY 15.5
Stelzer, Ernst H.K. ..... BP 37.5
Stelzl, Lukas ..... BP 14.27, BP 14.74, BP 29.6, BP 39.6, •CPP 17.4, CPP 45.6, CPP 55.6
Stemer, Dominik .....O 42.4
Stemler, Ralf .....AKPIK 4.2
Stemmler, René .....AKPIK 3.3
Stemplinger, Manfred ..... DS 11.1
Stengler, Timo .....AKBP 14.3
Stenz, Christian ..•DS 20.24, FM 11.2
Stepanenko, Vladimir ..... O 96.1
Stepanov, Evgeny .. TT 13.3, •TT 53.5
Stepanov, Evgeny A. ..... TT 53.1
Stepanova, Mariia ..... MA 37.6
Stephan, Dominic ..... O 61.7
Stephan, F. ..... BP 27.8, BP 37.2
Stephan, Rebecca .....•CPP 49.1
Stephan, S. ..... HL 54.12
Stephan, Sven ..... HL 54.9
Stephen, David T. ..... TT 17.6, QI 4.6
Stephens, Greg ....•TUT 4.1, •SOE 1.1
Steppke, Alexander ..... TT 62.6
Sternemann, Christian .... MM 19.30, MM 19.48
Sternemann, Lasse .. O 71.3, •O 84.4, TT 66.3, •TT 84.4
Stetsovych, Oleksandr O 10.2, TT 16.2
Stetter, Markus G. ..... BP 21.5
Stettner, Monja .....O 45.9
Steuer, Oliver .....AKBP 3.6
Stevens, Callum ..... TT 93.17
Stevens, Laurie .....•CPP 9.5
Stewart, Ross ..... MA 19.3, TT 31.3
Sticlet, Doru ..... DY 46.10, TT 75.10
Stief, Ann-Kristin .....•O 54.5
Stiehm, Noah .....•DS 20.35
Stier, Andreas V. ..... O 38.4
Stierle, Andreas ... CPP 46.17, O 34.6
Stiewe, Finn-F. .....MA 39.7
Stiller, Karolin ..... SOE 6.6
Stilp, Fabian .....•O 4.6
Stinken Rösner, Lisa ..... DD 26.2
Stinken-Rösner, Lisa ..... DD 26.5, •DD 39.1, DD 41.3
Stocco, Antonio .....•BP 16.10, CPP 46.22, CPP 46.23
Stocco, Elia .....•DY 14.8
Stöcher, Paul ..... O 87.2
Stock, Taylor J. Z. ..... O 42.9
Stockburger, Jürgen ..... •DY 47.10, QI 13.1
Stöcker, Hartmut CPP 16.3, CPP 16.6, CPP 17.36, CPP 17.39, FM 12.8
Stocker, Lidia ..... •TT 2.11, TT 62.10
Stockert, O. .....•TT 25.9
Stockert, Oliver ..... TT 52.1
Stockert, Ulrike .....•TT 79.3
Stödter, Leonie ..... TT 23.1, TT 57.1, •TT 57.2, TT 57.3
Stoehr, Rainer ..... TT 92.5
Stoer, Angelina .....•CPP 17.20
Stoffel, Wieland G. ..... TT 5.5
Stöhler, Jörn ..... O 37.6
Stöhlker, Thomas .....AKBP 7.3
Stöhr, Meike .. O 35.1, O 35.2, O 35.3, O 77.1
Stojkovic, Marija .....•MM 12.2
Stolarek, David ..... O 96.6
Stoll, Alexander .. TT 22.20, •TT 28.2
Stoll, Enrico ... AKPIK 4.4, AKPIK 5.8
Stoll, Mareike .....•BP 7.56
Stollberg, Isabella ..•O 72.5, •TT 67.5
Stollenwerk, Tobias .....•QI 1.7
Stolte, Matthias ..... CPP 17.20
Stolterfoht, Martin .....HL 4.7
Stolz, Rony .....TT 93.6
Stommel, Markus ..... CPP 46.19, CPP 59.1
Stoodley, Matthew ..... O 4.1
Stooß, Henrik .. CPP 14.3, •CPP 14.5, MM 17.3
Stopp, Silvan ... •DY 42.12, •TT 63.12
Störmer, Heike ..... MM 3.6
Stosch, Rainer ..... O 95.1, TT 96.1
Stosiek, Matthias ..... •CPP 38.2, MM 19.9, TT 93.13, AKPIK 2.1
Stottmeister, Alexander ..... QI 10.9
Stötzner, P. .....•HL 45.1
Strachan, John Paul .....DY 43.9
Strahl, Janina .....•TT 25.10
Stråka, Emil .....•DY 41.11
Strand, Hugo ..... TT 27.4, TT 53.5
Strand, Hugo U. R. .....•TT 51.12
Stranik, Ondrej ..... BP 14.58
Strasberg, Philipp .....•QI 9.3
Straßheim, M. .... MA 18.1, •MA 18.4, MA 52.24, TT 30.1, •TT 30.4
Straßheim, Marc ... MA 18.2, TT 30.2
Straßner, Marius M. ..... QI 14.10
Stratmann, Frank ..... UP 6.3
Stratmann, Nadine .....MA 13.7
Straub, Dennis .....•CPP 17.18
Strauch, Hannah .....•O 19.6
Strauß, Kilian .... DS 14.3, •DS 20.43, O 74.4, TT 68.4
Strauss, Dirk ..... FM 7.2
Strauss, Fabian ..... HL 4.1
Strauss, Kilian ..... TT 5.6
Strauss, Raimund ..... TT 22.32
Strebel, Oliver .....•DY 41.4
Strecka, Jozef .... MA 31.6, MA 36.2, •MA 36.11, TT 47.6
Street, Mike ..... O 60.6
Streibel, Verena .....DS 11.2, HL 9.4, HL 12.5, HL 12.7, HL 33.5, HL 40.3, •HL 42.1, HL 42.3, HL 42.5
Streil, Thomas . AKBP 6.1, •AKBP 6.4
Streit, Julian O. .... BP 39.1, CPP 55.1
Streller, Matthias ..... BP 33.5
Streun, Johannes ..... DD 16.3
Strickler, Christine .....•MA 52.19
Striebel, Moritz ..... BP 12.8
Strik, Julian H. ..... O 89.7, O 99.9
Striker, Nele N. ..... CPP 46.5
Strinic, Ana .....•TT 43.9, QI 2.4
Strittmatter, André .. DS 11.4, HL 33.2, HL 33.3, HL 34.3, HL 37.5
Strkalj, Nives .....•FM 18.5
Strobel, Johannes ..... HL 20.54
Strobel, Tim .....•HL 34.1, QI 18.6
Strobel, Urs .....TT 22.16, •TT 43.4
Strobl, Frederic .....BP 37.5
Strobl, Klara .....BP 2.4
Strobl, Timo ..... HL 16.6, •HL 20.61
Strocov, Vladimir N. ..... O 42.9
Stroh, Lukas .....•MA 7.62
Strohbeen, Patrick .....O 48.6
Strohmair, Simone ..... DS 21.8
Strohmeier, Marcel . TT 29.8, TT 78.6, •TT 90.1
Strohsack, Jaka .....O 64.4
Strokov, Vladimir .... O 63.4, TT 55.4
Strolka, Onno .....CPP 26.2
Stroppa, Alessandro ..... MA 17.5
Strothmann, Robert .....•CPP 15.7, CPP 46.66
Strubbe, David A. ..... MM 37.3
Strüber, Christian ..... MA 7.12
Strugatsky, Alon .....•TT 57.8
Strungaru, Mara ..... MA 14.5
Strunk, Christoph .... TT 5.1, TT 14.2, TT 22.24, TT 64.2, TT 73.7, TT 97.1, TT 97.2
Strunskus, Thomas .....CPP 17.15, CPP 17.48
Strunz, Walter . QI 7.3, QI 9.5, QI 10.3, QI 10.5, QI 14.3, QI 14.6
Strunz, Walter T. ..... QI 17.4
Struve, M. .....HL 54.10, HL 54.12
Struve, Marti .....•HL 54.9
Struzhkin, Viktor V. ..... TT 80.8
Strydom, A. M. ..... TT 62.5
Strzalka, Malgorzata .....•QI 14.2
Stubenrauch, Jakob .....•DY 33.8
Stüber, Nils .....•MA 39.2
Stubhan, Samuel .....•BP 20.8
Studart, André .. •BP 26.7, •CPP 43.7
Stühn, Lukas .....•O 44.11
Stumpp, Nico .....•O 66.6
Stupakiewicz, Andrzej ..... MA 27.5
Sturm, Chris ..... HL 1.7, HL 26.40, HL 26.42
Su, Yixi ... MA 5.8, MA 7.6, MA 47.10, O 2.2, TT 7.8, TT 25.5
Suárez-Dou, Sergio .....•BP 15.6
Suárez-Morell, Eric ..... O 67.3
Subach, Sergey .....O 46.5
Subbiah, Jegadesan ..... CPP 48.5
Subedi, Arjun .....O 60.6
Subramanya, Chinmayi .....DY 51.5, SOE 15.5
Suchomel, Lisa ..... HL 20.31
Sudana, Sai Durga Prasad . CPP 17.41
Sudarsan, Akhil ... BP 26.4, CPP 43.4
Sudbø, Asle ..... DY 43.19, MA 6.11, MA 21.6, TT 56.6
Sudzius, Markas .... DS 16.5, HL 1.12
Suen, Cissy ..... TT 40.1
Suess, Dieter .....MA 7.41, MA 9.9, MA 34.6, MA 55.6, MA 58.2
Suetin, Mikhail .....•O 18.2
Sugimoto, Hiroshi ..... BP 9.4
Suhak, Yuri ..... FM 14.4
Suhak, Yuriy ..... FM 11.30
Suhr, Ellen ..... FM 6.7
Suhr, Maximilian ..... MM 7.7
Sukhanov, Aleksandr ..... MA 11.3, MA 16.1, TT 21.3, •TT 81.6
Sukhanov, Alexander .....MA 19.3, TT 31.3
Sulaiman, Cathy .....O 10.3, TT 16.3
Sulaiman, Vanessa .....TT 23.11, •TT 23.12, TT 94.8
Suleiman, Abdulsalam Aji .. •HL 20.1
Sulliger, Marc ... CPP 10.12, DY 16.12
Sullow, Stefan ..... MA 7.3, TT 23.1, TT 57.1, TT 57.2, TT 57.3, TT 81.5
Sulpizi, Marialore CPP 9.5, CPP 30.3, •CPP 39.1, •O 36.1
Sulyma, Oleksandr .....•TT 51.11
Sumeet, Sumeet .....•QI 5.4
Sumić, Barbara .....•O 65.8, O 97.11
Summa, Lena ..... BP 7.44
Sun, Benyao .....•FM 11.8
Sun, Daxiao ..... BP 16.2
Sun, He ..... TT 52.4
Sun, Jiale .....DS 20.33
Sun, Jiaxing ..... CPP 15.4
Sun, Jun .....•SOE 2.7
Sun, Kun ..... CPP 4.6, CPP 44.5, CPP 48.2
Sun, Ningwei ... O 6.5, O 45.5, O 58.4
Sun, Peijie ..... TT 29.6, •TT 52.4
Sun, Qiang ..... O 43.2
Sun, W. ..... TT 69.6
Sun, Xiaoxiao ..... HL 17.5
Sun, Yan ..... TT 61.4
Sun, Yihui .....AKPIK 6.4
Sun, Ying ..... CPP 57.3
Sun, Yuxuan .....HL 17.5
Sun, Zhuotong ..... FM 18.5
Sunada, Satoshi ..... AKPIK 3.4
Sundaramurthy, Vignesh ... MA 33.4, •TT 39.6, TT 39.7
Sündermann, Eric . •BP 7.38, BP 7.40
Sundermann, Martin .....TT 3.2
Sundermeyer, Jörg .... O 61.4, O 69.7
Sunil, John C. .....•DY 7.7
Sunkel, Torben .. •BP 10.6, •CPP 18.6, •DY 18.6
Sunny, Joe ..... MA 7.65, MA 7.70
Sur, Saikat ..... QI 7.5
Sur, Shouvik ..... TT 41.11
Surendran, Anudeep ..... •SOE 2.4
Suresh, Akshey ..... CPP 21.5
Sürgers, Christoph ..... O 3.3, O 15.4, O 17.7, O 17.9, O 17.11, O 89.3, O 89.12, O 99.2, O 99.10
Suri, Dhavala .....TT 74.12, TT 97.1
Surówka, Piotr ....•SYBS 1.5, TT 40.1
Suruga, Taichi ..... O 67.9, •O 82.4
Suryansh, Suryansh .....•O 94.6
Susanne, Susanne ..... FM 11.19
Suthar, Abhi ..... TT 39.6, TT 39.7
Suvorov, Oleksandr ..... O 2.3
Suyolcu, Y. Eren ..... TT 39.7
Suzart, K. ..... BP 27.8, BP 37.2
Svaneborg, Amalie ..... O 76.5
Svanidze, E. ..... TT 5.9
Svanidze, Eteri .....TT 5.8, TT 17.2, TT 42.12, QI 4.2
Svastits, Domonkos ..•QI 6.4, QI 20.7
Švec, Martin .....O 43.17
Svedlindh, Peter ..... MA 12.6
Svyrydenko, Mariia .....HL 45.4
Swami, Jeel .....•O 29.2
Swaraj, Bhageerath TT 23.31, TT 71.1
Swatosch, P. .....•TT 93.7
Świetek, Rafał .... •DY 32.6, •TT 45.6
Switka, Michael •AKBP 1.2, AKBP 1.3, AKBP 2.4, AKBP 3.5, AKBP 7.2, AKBP 7.6, AKBP 14.2
Sychev, Dmitrii ..... HL 3.5
Syga, Simon .....•DY 33.9
Sykes, E. Charles H. ..... O 81.2
Sykora, Steffen .....TT 93.14
Syljuåsen, Erlend .•MA 51.5, •TT 88.5
Syljuåsen, Olav Fredrik ..... TT 73.12
Syrrokostas, George .....DS 16.9
Syskaki, Maria Andromachi . MA 21.4
Syskaki, Maria-Andromachi . MA 21.6
Szabo, Andras .....•DY 60.6
Szabó, Dorothée Vinga .... MM 30.2, MM 30.3
Szachniuk, Marta ..... BP 14.54
Szalay, Szilárd .....•QI 10.8
Szaller, Dávid .....MA 16.8, MA 17.7, •MA 17.11
Szameit, Alexander ..... DY 48.6, HL 20.25
Szangolies, Jochen .....•QI 12.9
Szász, Bence .... MA 17.7, •MA 17.10
Szczefanowicz, Bartosz ..... O 35.3
Szczurek, Kamila .....•MA 7.35
Széchenyi, Gábor ..... QI 2.8
Szentpéteri, Bálint ..HL 30.2, TT 59.2
Szewczyk, Aleksander .... •CPP 26.3
Szokoll, Stefan ..... BP 14.91
Szombathy, Dominik .TT 41.9, QI 21.9
Szopa, Wiktoria .....•FM 11.10
Szot, Kristof ..... MM 27.4
Szot, Michal ..... HL 26.45
Szpak, Nikodem ... TT 18.6, •TT 42.5, TT 92.14
Szpara, Dominik ..DY 32.12, TT 45.12
Szpytma, Marcin ..... O 10.3, TT 16.3
Sztucki, Michael ..... BP 20.8
Szunyogh, László MA 21.2, •MA 42.2, MA 58.5, TT 15.12, TT 15.13
Szymański, Konrad . QI 10.11, •QI 13.8
Szymiczek, Martin P. ..... •DY 48.4
T. B. Goennenwein, Sebastian HL 18.1, TT 32.1
T. Corredor, Laura .....FM 11.25
T. Costa, Antonio .... DS 1.3, MA 5.9, TT 7.9
Tabaru, Emre Timuçin .....DS 20.2
Tabaru, Timuçin Emre ..... DS 20.14, •MA 42.9, MM 12.9
Taboada-Gutiérrez, Javier .... O 52.3
Tacon, Matthieu Le .TT 23.31, TT 71.1
Tadjeugue-Nangmo, Junior-Wilfried •DS 8.4
Tafida, Usman .....•O 24.4
Tafti, Fazel ..... MA 59.1
Taga, Kotaro ..... MA 52.13, MA 59.4
Tagliente, Antonio Maria ....•TT 13.8
Taguchi, Yasujiro .. MA 16.6, MA 17.4
Taheriniya, Shabnam .....MA 52.5, MA 52.14
Taherpour, Saba ..... •O 15.2, O 64.2, O 89.2
Tai, Bo .....•MA 54.3, MM 40.3
Tajik, Mohammad ..... O 98.4
Tajima, Shimon .....•MA 17.8
Tajkov, Zoltan ..... DS 12.7, MA 58.3, •MA 58.10
Takagi, Hidenori .....TT 49.3
Takahashi, Hidefumi .....FM 9.2
Takahashi, Kazutoshi .....O 42.5
Takahashi, Takuya ..... MA 59.4
Takaki, Ryota ....•BP 10.7, •CPP 18.7, •DY 18.7
Takamura, Yayoi ..... HL 8.10
Takano, Hayato ..... FM 9.5
Takatsu, Hiroshi ..... FM 22.9
Takayama, Akari ..... O 42.5
Takenobu, Taishi ..... O 82.4
Takeuchi, Kazumasa A. .. •CPP 28.5, •DY 29.5
Takeya, Jun ..... CPP 17.45
Takeyasu, Koutarou .....O 61.11
Taleb, Masoud •HL 1.9, O 27.3, O 27.4
Talebi, Nahid HL 1.9, •HL 49.1, O 27.3, O 27.4, O 37.2, QI 2.5
Talei, Roham .....MM 35.4
Talukdar, Saswata .....•MM 21.7
Tan, Hark Hoe ..... HL 35.4
Tan, Hengxin .....O 63.11, TT 55.11
Tan, Ryan ..... HL 39.7, HL 39.11
Tan, Tao-Lin DY 2.4, •DY 32.11, TT 1.4, •TT 45.11
Tan, Xin L. .....MA 24.3, TT 36.3
Tan, Xin Liang ...•O 2.1, O 2.5, O 76.6
Tanaka, Hiroki ..... FM 23.6
Tanaka, Katsuya ....DS 16.7, DS 20.8
Tanaka, Yukio ..... TT 83.6, TT 98.5
Tancogne-Dejean, Nicolas ... HL 8.10
Tang, Chuan .....BP 31.1, CPP 50.1

Tang, Nan .....•TT 79.4
Tang, Qiyun ..... BP 31.1, •CPP 24.5, CPP 50.1
Tang, Weizhen ... •CPP 11.7, •DY 17.7
Tang, Wenxuan .....O 96.10
Tang, Xiankang .....•MM 13.1
Tangi, Malli ..... DS 11.8
Tani, Shuntaro .....O 60.7
Taniguchi, Hiroki ..•FM 22.7, FM 22.8
Taniguchi, Takashi ... HL 3.3, HL 3.8, HL 10.1, HL 10.3, HL 18.7, HL 20.25, HL 24.9, HL 30.2, HL 47.2, MA 43.2, MA 49.2, O 95.2, O 95.11, TT 20.1, TT 20.3, TT 32.7, TT 59.2, TT 96.2, TT 96.11
Taniwaki, Michiki ..... •AKPIK 5.6
Tanzilli, Sébastien .....QI 18.1
Tao, Ran TT 23.15, TT 93.17, •TT 95.7
Tao, Shuxia ..... DS 18.1
Tapia, Franco .....•DY 19.2, DY 19.5, DY 19.8
Tappertzhofen, Stefan ..... O 84.4, TT 84.4
Tapşin, Ömer S. ..... HL 16.4
Tarabunga, Poetri Sonya ..... QI 15.6
Tarakci, E. ..... BP 27.8, •BP 37.2
Tarannam, Naziha .....•BP 20.1
Tarasov, Ivan .....•MA 18.6, MA 50.1, •TT 30.6
Tarczewska, Maria .....•BP 7.53
Tardieux, Marie .....MA 39.19
Tarek, Mona ..... BP 26.2, CPP 43.2
Tarrach, Lena .....•CPP 46.25
Tarzia, Marco ..... DY 60.3
Tarzikhan, Antonio ..... BP 14.47
Tas, Niels ..... TT 28.5
Tasquier, Giulia .....•PLV V
Tasto, J. ..... MA 7.14
Tasto, Janosch .....•FM 11.31
Taubenberger, Anna .....BP 27.10
Taubenberger, Anna V. ..... BP 37.7
Täuber, Daniela .. BP 14.29, BP 14.33, BP 14.37, BP 14.45, •BP 33.7, CPP 46.65
Taubert, Oskar ..... BP 14.71
Taubner, Thomas ..... O 26.1, O 26.5, O 57.5, •O 79.4, O 96.3, O 96.4, O 96.9, O 96.11
Taucer, Marco ..... O 56.5, O 56.6
Taufour, Valentin ..... TT 2.1
Tautz, F. Stefan ..... MA 43.3, O 9.5, O 17.1, O 41.4, O 54.3, O 61.10, O 63.9, O 67.9, O 69.8, O 83.7, TT 38.4, TT 55.9, TT 93.6
Tautz, Frank Stefan .... O 3.7, O 45.9, •O 61.1, O 83.2
Tautz, Stefan .....O 17.5, O 31.3
Tavagnacco, Letizia ..... CPP 58.5
Tavakkoli, Fatemeh .....•DY 43.7
Tavakoli, Ariyan .....•O 61.7
Tavakoli, Armin ..... QI 15.2
Taychatanapat, Thiti .....TT 4.6
Taylor, Victoria .... O 40.10, TT 37.10
Taylor, Victoria C. A. MA 27.2, O 22.5, •O 71.11, •TT 66.11
Tcakaev, Abdul-Vakhab ....•MA 24.1, •TT 36.1
Tchernyshyov, Oleg . MA 19.1, TT 31.1
te Vrugt, Michael ... DY 43.1, DY 44.7, •DY 49.10, O 18.2
team, FAIRmat .... FM 6.5, MM 22.3, AKjDPG 1.2, AKPIK 6.3, AKPIK 6.5
team, the W7-X ..... O 78.1
Tebano, Antonello ..... TT 14.5
Tebbe, David ..... HL 3.3
Tegeder, Petra .... CPP 17.6, DS 21.2, O 46.2, O 46.3, O 46.4
Tegenkamp, Christoph ..... DS 18.2, DS 18.4, DS 20.47, DS 20.48, O 33.4, O 62.7, O 66.2, O 73.1, O 74.9, O 79.6, O 84.2, TT 54.7, TT 68.9, TT 84.2
Tegtmeyer, Felix .....•DS 16.10
Tehei, Moeava .....MA 7.3
Teheriniya, Shabnam ..... MA 9.13
Tehranchi, Ali ....MM 25.3, MM 34.4, MM 34.7, •MM 39.9
Teichert, Christian .....MM 4.4
Teichert, Jochen AKBP 2.2, AKBP 2.5
Teichgreber, Robin M. .....•HL 53.5
Teinor, Nene Narh .....•MA 13.4
Teistler, Anja .....DD 26.4
Tekgül, Atakan .....•MA 52.25
Telle, Helmut H. ..... DS 21.10
Temirov, Ruslan . O 3.7, •O 9.5, O 17.1, O 31.3, O 69.8, O 83.7
Temmen, Finn ..... TT 17.3, QI 4.3
ten Haaf, Sebastiaan ..... TT 15.3
Tenne, Ron ..... FM 4.2
Teodoro, Marcio ..... HL 47.2
Teppe, Frederic .....HL 29.5, TT 58.5
Tepper, Lucas ..... O 87.7
Tepper, Lukas .....•BP 14.75
ter Glane, Jan .... CPP 17.21, •O 72.3, •TT 67.3
Terakawa, Shigemi .....•O 64.5
Terbeck, Manuel ..... HL 25.2
Tereshchenko, Oleg .....MA 12.2
Terfort, Andreas ..... O 46.11
Ternes, Markus MA 43.3, O 3.7, O 17.5
Teröde, Thomas ..... TT 93.10
Terörde, Thomas .....•MM 19.44
Teruzzi, Luca ..... CPP 46.6
Terzi, Aybike ..... O 23.4
Tesař, Roman ..... •TT 93.12
Tesei, Giulio .....•BP 39.1, •CPP 55.1
Teslenko, Kirill .....•TT 74.4
Tessarek, Christian .....HL 24.1
Teubler, Raimund ..... CPP 6.4
Teuerle, Laura ... CPP 38.5, •HL 22.3
Teurle, Laura ..... HL 22.1
Tewordt, Teresa .....•DD 41.3
Teza, Gianluca .... DY 15.5, MA 31.12, TT 47.12
Thaemer, Martin ..... O 61.3, O 95.5, TT 96.5
Thake, Henry .....•O 4.1, O 31.3
Thakur, Balaram .....•MM 19.2
Thakur, Gohil S. .... MA 24.1, TT 36.1
Thakur, Sangeeta ..... MA 7.47, •MA 36.10, MA 38.4, MA 38.6
Thakur, Shagun ..... DS 16.10
Thakuria, Dimpi .....•QI 10.11
Thalakulam, Madhu ..... TT 64.4
Thaler, Marco ..... O 6.6, •O 58.5
Thalmann, Fabrice ..... CPP 46.22
Thalmann, Karin S. ..... •CPP 53.5
Thalwitzer, Robert ..... HL 4.1
Thämer, Martin ..... O 51.2, O 87.7
Thamizhavel, Arumugam .... TT 25.1
Thamm, Matthias ..•TT 64.1, TT 83.9
Thanabalasingam, Bheeshmon O 56.5, O 56.6
Thangavel, Muthu ..... MA 7.75
Thao, LTP ..... MA 7.30
Tharmalingam, Mithuss ... MA 30.11
Thavayogarajah, Yasothaa . CPP 58.1
Thawany, Priyanka .....•O 96.3
Theile, Jannik ..... •CPP 22.4
Thein, Marinus ..... BP 14.4
Theiss, Tobias ..... FM 15.2
Thelen, Felix ..... FM 6.7, FM 6.10
Thelen, Marc ..... CPP 46.9
Thelge, Yoon .... •DY 58.3, •SOE 17.3
Themlin, Jean-Marc ..... •O 67.4
Thery, Manuel .....•SYGF 1.3
These, Albert ..... HL 23.4
Thessalonikios, Christos ... FM 11.28
Thevenet, Maxence ..... AKBP 12.2, AKBP 12.3
Thewes, Filipe C. .....DY 33.4
Thiel, Maximilian ..... MA 52.3
Thiel, Maximilian Alexander ..MA 9.2
Thiele, Uwe .....CPP 10.5, DS 20.6, DY 16.5, DY 22.3, •DY 41.10, DY 44.15
Thielemann-Kühn, Nele ..... MA 38.2
Thiemann, Fabian .. HL 52.4, •O 86.9
Thiemann, Franz .....•O 11.8
Thieme, Josua .....QI 14.26
Thieme, Marc .... MM 17.2, •MM 17.6
Thiering, Christian ..... BP 14.24
Thiering, Nicola .....MM 19.30
Thierkopf, Ina ..... DD 16.3
Thiersch, Heiner .....•CPP 15.6
Thies, Andreas ..... HL 20.25
Thiesbrummel, Jarla ..... •HL 4.8
Thijssen, Kristian ..CPP 10.9, DY 16.9
Thimm, Norman .....•DD 30.6
Thirion, Louis .....TT 51.5
Thirolf, Peter G. . AKBP 5.1, AKBP 8.5
Thole, Lars .....•HL 10.4, HL 24.5, •TT 20.4
Thomale, Ronny .... FM 22.6, O 63.3, TT 55.3
Thomas, Andy .....MA 39.7
Thomas, John .....O 16.2
Thomas, Natascha .....BP 14.47
Thomas, Sean M. ..... TT 52.3
Thomas, T. R. ..... TT 23.10
Thomassin, Jean-Luc .....TT 82.1
Thome, Leonardo ..... AKBP 1.3, AKBP 7.2, •AKBP 7.6
Thompson, Amelia .. O 95.6, TT 96.6
Thomsen, Fenja ..... HL 20.40
Thomsen, Joachim Dahl ...•MA 46.5
Thorid, Rabe ..... DD 15.3
Thorwart, Michael . CPP 23.1, DY 24.1
Thoss, Michael ..CPP 53.5, DY 46.12, TT 42.9, TT 42.10, TT 53.4, TT 75.12
Thremer, Luis ..... •TT 92.13
Thulasiram, Parasar .....•TT 98.7
Thum, Lukas ..... O 81.7
Thümler, Moritz ....•DY 8.3, SOE 16.1
Thümmler, Martin .....HL 1.11
Thunström, Patrik MA 34.9, MA 50.7, MM 37.5
Thurner, Stefan ... SOE 9.4, SOE 11.3, SOE 11.4
Thuruthiyil Jose, Amala ....•MA 7.25
Thy, Dominik .....•DY 44.15
Thygesen, Kristian .....O 76.5
Thygesen, Kristian S. .....MM 17.7, O 59.4, TT 48.4
Thyzel, Tim ..... TT 23.17
Tian, Chuanshan .....•O 51.3
Tian, Haoyang .....•TT 4.7
Tian, Sicheng ..... •BP 14.29
Tian, Yu .....•DY 51.5, •SOE 15.5
Tichy-Rács, Éva .....•FM 14.4
Tickoo, Nainish ...•TT 23.14, TT 25.1
Tiebe, Carlo ..... DS 9.4
Tiebel, Jessica AKBP 10.1, AKBP 10.2, •AKBP 10.3, AKBP 12.5
Tierney, Jordan .....•TT 5.8
Tietjen, Finja .....•DY 60.5, DY 61.1
Tiginyanu, Ion ...HL 20.23, HL 20.24, HL 26.10, HL 26.23
Tik Man, Erlina .....O 61.11
Tilger, Thomas ..... CPP 29.4
Tilgner, Niclas O 66.2, O 73.5, •O 84.2, •TT 84.2
Timewell, Tim .....UP 8.5
Timm, Adina . O 7.5, •O 71.16, O 71.19, O 71.21, TT 9.5, •TT 66.16, TT 66.19, TT 66.21
Timm, Carsten ..... FM 6.3, TT 15.9
Timm, Jörg ..... BP 14.56
Timm, Matthew J. ....•O 43.7, O 46.7
Timm, Nora ..... •MA 49.4
Timme, Marc DY 8.3, DY 51.1, DY 51.2, DY 51.4, SOE 6.4, SOE 6.5, SOE 15.1, SOE 15.2, SOE 15.4, •SOE 16.1
Timmer, Daniel ..... HL 46.3, DD 33.1
Timmermann, Tiemo ..... CPP 2.1, SOE 3.1, UP 1.1
Timr, Štěpán ..... BP 2.5, •BP 15.3
Timrov, Iurii .....MM 8.1, MM 8.2
Tindall, Joseph ..... O 14.9, O 38.8
Tinhofer, I. ..... BP 27.8, BP 37.2
Tippner, Felix ..... •DY 21.4
Tirasutt, Tassaphon •O 84.5, •TT 84.5
Tirler, Peter ..... QI 15.2
Titkov, Ilya E. ..... HL 26.46
Titl, Maximilian ..... O 3.5
Titov, Ivan ..... MA 46.1
Titov, Mikhail ..... O 89.7
Tittl, Andreas .....HL 20.18, O 85.7
Titus, Michael S. ..... MM 36.5
Titze, Tim MA 7.10, MA 55.6, O 40.17, TT 37.17
Tiunov, Egor ..... DY 28.2, QI 5.6
Tiwari, Achyut ..... O 96.1, TT 12.6
Tiwari, Apoorv ..... TT 53.3
Tiwari, Chandranshu ..... •BP 1.6, •CPP 1.6, •DY 4.6
Tiwari, Dhruv .....•TT 44.7
Tiwary, Tiark .....•TT 29.8
Tjardts, Tim ..... CPP 15.3
Tjeng, Liu H. ..... MA 19.5, TT 31.5
Tjeng, Liu Hao ..... HL 42.4, O 84.5, TT 3.2, TT 3.3, TT 25.2, TT 84.5
Tkach, O. ... O 19.10, O 59.2, •O 93.9, TT 48.2
Tkach, Olena ..O 2.4, O 14.3, O 40.20, TT 14.4, TT 37.20
Tkatchenko, Alexandre .....BP 2.10, BP 14.63, BP 15.6, CPP 9.3, CPP 29.2, DY 14.11
Tobias, David ..... DY 43.17
Tobiassen, Andrea .....•FM 11.4
Tobin, Siobhan .....MA 7.3
Tobisch, Sarah .....•O 94.5
Tocchio, Luca F. .....•TT 95.5
Todenhagen, Lina M. ..... HL 26.34, MM 4.2
Todorov, Tchavdar ..... FM 12.5
Todorova, Mira ....MM 9.1, MM 26.3, MM 39.6, •MM 39.7, O 13.3, O 13.6, O 65.7, O 65.9
Todorović, Milica ..... O 47.2
Todorovski, Ljupco .....UP 5.5
Tödter, Sophia ..... O 11.2
Toepfer, Hannes ..... TT 28.8
Toffenetti, Davide ..BP 12.8, •DY 22.4
Togo, Atsushi .....HL 23.9
Tohamy, Hossam TT 22.14, TT 22.15, •TT 43.7
Tohyama, Takami ..... TT 23.2
Toichi, Yuichiro ..... O 60.4, O 67.5
Tokita, Alea Miako .....MM 19.1
Tokiwa, Yoshifumi . MA 31.2, TT 47.2
Tokle, Egil ..... FM 11.34
Tokunaga, Yusuke ..... MA 17.4
Tokura, Yoshinori . MA 16.6, MA 17.4, MA 37.6
Tolan, Metin .....BP 14.24, BP 14.75
Tolić, Iva ..... BP 2.3
Tölle, Johannes ..... CPP 17.35
Tolmachev, Dmitry BP 26.5, CPP 43.5
Tomancak, Pavel .....BP 12.9
Tomaník, Lukas ...CPP 23.4, DY 24.4
Tomáš Novotný, Tomasz .... TT 85.8
Tomašić, Lucija .•BP 32.11, •DY 52.11
Tomizuka, Hitoshi ..... O 82.6
Tomoscheit, Maximilian ... HL 20.21, HL 26.47
Tomut, Marilena .. MM 3.5, MM 18.3, MM 18.5
Tonauer, Christina M. .....•CPP 32.1, •DY 35.1
Toncian, Toma ..... AKBP 8.8
Toncich, Nensi .....•DS 16.1
Tong, Daniel ..... TT 43.8
Tong, Junwei ..... MA 27.1
Tong, Shanyin ..... DY 15.8
Tonhäuser, Johann ..... TT 61.14
Tönjes, Ralf ..... •DY 63.2
Tonner-Zech, Ralf ..... O 11.4, O 11.8
Tonolo, Tommaso .....DY 33.12
Topmöller, Jan-Phillip .....•O 61.2
Topstad, Mats ..... FM 18.8
Toquer, Damien .....•CPP 14.3
Toral, Raúl ..... DY 33.10, DY 48.3, •DY 60.1, SOE 10.2
Torchia, Laura ..... •TT 10.2, TT 13.9
Tormann, Constantin ..... CPP 37.4
Tornatzky, Hans ...HL 24.6, •HL 35.1, HL 40.2, HL 40.6, HL 57.5
Tornow, Marc DS 1.2, DS 16.6, QI 11.10
Tornow, Nele ..... •HL 30.3, •TT 59.3
Török, Mátyás ..... MA 21.2
Torres Boy, América Yareth ... O 85.4
Torres-Diaz, Daniela ..... CPP 19.5, •CPP 23.2, CPP 27.3, DY 20.5, •DY 24.2, DY 26.3
Torta, Pietro .....DY 14.12
Toschi, Alessandro . TT 13.4, TT 13.7, TT 62.8
Tosi, Leandro ..... TT 22.24, TT 73.7, TT 97.2
Tosoni, Sergio ..... O 65.5
Tóth, Géza . QI 14.11, •QI 15.3, QI 20.5
Toubin, Céline ..... UP 6.1
Touge, Kenta ..... MA 3.10
Tounsi, Tfyeche .....O 17.12
Tounsi, Tfyeche Y. .....•O 89.8
Tour, James M. .....O 46.7
Tournie, Eric ..... HL 29.5, TT 58.5
Tovar, Michael ..... TT 57.2
Tovey, Samuel .....DY 6.1
Toyfl, Johann .....•AKBP 9.6
Tozer, Stanley .....•TT 80.7
Tozman, Pelin .....MA 50.6
Traeger, Georg .....O 12.7
Traeger, Georg A. •O 71.20, •TT 66.20
Trahms, Martina ...•TT 50.8, TT 82.1
Trajanovski, Pece DY 42.15, TT 63.15
Trambly de Laissardière, Guy •O 62.2, O 74.6, TT 4.2, TT 4.3, •TT 54.2, TT 68.6
Tran, Ann Kathrin .....•O 24.3
Tran, Duc .....MA 29.9, •MA 55.5, TT 46.9, TT 93.4
Tran, Duc M. ..... MA 55.3
Tran, Duc Minh ... MA 51.2, MA 55.9, TT 88.2
Tran, Duong .....•O 23.1
Tran, Fabien .....•MA 34.13
Tran, Lan Maria .....MA 7.27
Tran, Loi V. ..... O 55.1
Tran, N .....MA 7.30
Trassin, Morgan .... FM 4.7, FM 23.5
Trautschold, Sebastian .....•MM 4.5
Trautwein, Ulrich .....DD 27.7
Trauzettel, Björn .... MA 7.51, O 63.8,

TT 11.5, TT 22.5, TT 55.8
Travac, Enes ..... AKBP 8.7
Trebst, Simon ..... TT 33.4
Trefflich, Lukas ..... HL 1.7, HL 26.21
Trefzger, Thomas ... DD 4.2, DD 14.3, DD 23.4, DD 24.3
Tremel, Luc-Fabrice MM 4.2, •MM 4.3
Trenczek, Anton ... HL 3.10, HL 26.53
Trenins, George .....•O 11.6, O 14.7
Trényi, Róbert .....•QI 20.5
Trepat, Xavier ..... BP 27.2
Trepl, Thomas ..... BP 2.11
Tresca, Cesare ..... HL 36.2
Treska, Nicholas .....•AKBP 14.2
Tress, Martin .....•CPP 3.3
Tress, Wolfgang ..... CPP 40.6
Tretiak, Sergei .... CPP 53.3, HL 46.3
Treu, Tim MA 18.7, TT 22.34, TT 30.7, •TT 89.2
Tricarico, Roberto ..... QI 3.10
Trif, Mircea ..... MA 39.5, TT 15.2
Trifonova, Yordanka ..... HL 20.64
Trigo, M. ..... MA 4.4
Trillot, Salomé ..... MA 16.7
Trinter, Florian . CPP 23.4, •CPP 34.2, DY 24.4, •DY 36.2
Tripathi, Anshuman .....•MA 39.5
Tripathi, Anuvrat .....•MA 7.20
Tripathi, Ashutosh Kumar .. MA 49.9
Tripathi, Rishabh .....•QI 13.9
Tripathi, Sarthak ..... HL 55.1
Tripathi, Shivani ..... MM 21.7
Trippelsdorf, Lina ..... HL 26.33
Trishin, Sergey ..... O 80.4
Trittel, Torsten ..... DY 25.4, DY 25.5
Trittschanke, Niko .....•QI 16.3
Trivedi, Nisarg .....•DS 20.45
Trivini, Stefano O 15.5, O 89.6, O 99.7, •TT 73.5
Troeger, Lucas ..... BP 7.23
Trofimov, Pavel ... HL 3.10, HL 26.53, O 98.7
Trofimov, Sergei .....•FM 11.28
Trommer, Clara W. A. ..... MA 36.10
Trommer, Elisabeth .....•PSV VI
Tropmann-Frick, Marina .. CPP 46.24
Troue, Mirco .....•HL 13.2, HL 13.5
Troyan, Ivan A. ..... TT 80.8
Trujillo-Mulero, Jara .....•O 3.7
Trukhan, Elena .....•MM 31.8
Trunschke, A. ..... O 88.11
Truong, Charles ..... BP 9.2
Trushechkin, Anton .. QI 14.9, QI 18.4, •QI 18.8
Truzzolillo, Domenico ..... CPP 31.2, •CPP 35.2, CPP 46.33, CPP 46.38, •DY 37.2
Trzewik, Daniel .....•O 24.7
Tsabedze, Sebenzile .....•DY 44.7
Tsai, Yi-Chen .....•BP 14.60, TT 4.1
Tsaloukidis, Lazaros ..... SYBS 1.5
Tsanda, Artyom ..... SOE 10.1
Tschakert, Jalmar ..... O 58.1
Tschammer, Rudi ...•DS 9.4, DS 11.5, O 88.7, O 96.6
Tschernig, Konrad .....AKPIK 4.4, AKPIK 5.8
Tschirner, Teresa ..... O 73.3, O 95.1, TT 96.1
Tschisgale, Paul .....DD 37.1
Tschulik, Kristina ..... O 94.9
Tschurl, Martin O 65.6, O 81.6, O 94.8, •O 94.10
Tsen, Adam Wei ..... MA 43.6
Tseplyaev, Vasily ..... O 64.3
Tserkovnyak, Yaroslav ..... TT 74.12
Tsintsaris, Michalis .....CPP 29.4
Tsirkin, Stepan .... MA 35.9, TT 60.9
Tsirlin, Alexander ....MA 8.9, TT 98.1
Tsirlin, Alexander A. MA 2.6, MA 8.10, TT 5.11, TT 57.5, TT 72.6, TT 72.9, TT 94.6
Tsitsilianis, Constantinos .. CPP 54.6
Tsitsilin, Ivan .. QI 8.3, QI 11.6, QI 11.9
Tsuchiura, Hiroki ..... MA 50.7
Tsud, Nataliya ..... O 65.12, O 94.4
Tsujikawa, Y. ..... O 85.2
Tsunaki, Lucas .....FM 11.28
Tsurkan, Vladimir . MA 17.6, MA 54.2
Tsurkan, Vladirmir ..... MA 16.8
Tsuzuki, Takahiro ..... FM 15.3
Tubiana, Luca ... CPP 24.4, CPP 29.5
Tuchkov, Yehor ..... DY 49.10
Tucker, Victoria ..... MM 36.5
Tuczek, Felix .... MA 36.10, MA 42.3, O 83.8, O 89.9
Tuero, Pablo ..... TT 73.9
Tügen, Alperen ..... HL 13.4
Tumino, Francesco ..... O 11.8
Tümmler, Johannes .....MA 7.19
Tunn, Isabell ..... BP 7.12, •BP 26.5, •CPP 43.5
Turchanin, Andrey ..... BP 26.11, CPP 43.11, DS 14.9, HL 13.7, HL 20.6, HL 20.14, HL 30.2, O 10.6, O 10.7, O 54.7, O 70.1, O 72.4, O 73.2, O 95.12, TT 16.6, TT 16.7, TT 59.2, TT 65.1, TT 67.4, TT 96.12
Turek, Ilja .....•MA 7.83
Türken, Samuel .....•BP 7.34
Turnbull, Luke ..... MA 6.4, TT 40.1
Turrini, Alexandra ..... MA 17.2
Tusche, Christian ..... MA 5.7, TT 7.7
Tüysüz, Harun ..... MA 36.1
Twiehaus, Clara ..... CPP 46.9
Tworzydło, Jakub .... O 63.6, TT 55.6
Tyler, Jamie .....SOE 11.2
Tymoshenko, Yuliia .....•TT 49.1
Tysoe, Wilfred ..... O 78.4
Tzalenchuk, Alexander ..... TT 22.17
Tzegazab, Yizak ..... CPP 21.5
Tzschaschel, Christian .... •MA 27.7, MA 45.2
Tzvetkov, Peter ..... MA 7.27
U.B. Wolter, Anja ..... FM 11.25
Ubbelohde, Niels ..... HL 25.1
Ubben, Malte ..... DD 30.3
Ubben, Malte S. ..... DD 22.2
Ucar, Mehmet Can .....•BP 3.7
Uchida, Yoshihito . CPP 28.5, DY 29.5
Uddin, Masum ..... TT 22.12
Uderhardt, Stefan BP 14.50, BP 14.85
Udina, Mattia ..... MA 25.8
Udvardi, László ...•MA 21.2, MA 58.5
Uebele, Hagen ..... CPP 12.4
Ueberholz, Ken ..... AKBP 7.3
Ueda, H. .....MA 25.6
Ueda, Hiroki .....•MA 25.5, MA 38.13
Uehlein, Markus ..... O 40.1, O 40.3, O 40.4, O 40.6, O 98.6, TT 37.1, TT 37.3, TT 37.4, TT 37.6
Uehli, Daniel ..... O 44.15
ueno, teppei ..... O 95.7, TT 96.7
Ufer, Ariane ..... AKBP 8.6
Ufer, Patrick .. AKBP 10.2, AKBP 11.4, AKBP 12.5, AKBP 13.3
Ugartemendia, Andoni ....•CPP 29.6
Ugeda, Miguel ..... TT 49.6
Ugeda, Miguel M. .... O 86.4, TT 74.1
Ugokwe, Chikezie Williams CPP 17.41
Uhlarz, M. ..... MA 47.7
Uhlig, Joshua .....•SOE 12.1
Uhlir, Vojtech ..... O 98.3
Uhlirova, K. ..... MA 23.5, TT 35.5
Uhlířová, Klára ..... MA 8.3
Uhlmann, Petra .•CPP 12.1, CPP 13.6, CPP 17.9
Uhrig, Götz .. MA 58.8, TT 94.8, QI 1.6
Uhrig, Götz S. .....DY 46.9, MA 7.9, TT 23.11, TT 23.12, TT 56.5, TT 75.9
Újfalussy, Balázs .. TT 15.12, TT 15.13
Ukleev, V ..... MA 19.7, TT 31.7
Ukleev, Victor ..... DS 12.9, MA 16.4
Ukulov, Denis ..... MA 8.9
Ulaga, Martin .....•TT 23.2
Ulbrich, Knut .....DS 20.28
Ulbrich, Marek ..... DS 20.28
Ulcakar, Iris .....•QI 17.8
Ul-Hassan, Jawad ..... QI 20.6
Ulhe, Abhilash ..... HL 8.7, HL 57.4
Ullmann, Fabian ...•DS 4.4, DS 20.23
Ullrich, Aladin ....MA 37.8, MA 52.33
Ullrich, Anna .....•MA 57.4
Ullrich, Jasper .....•HL 20.44
Ullrich, Mark .....DD 6.1
Ullrich, Yannis ..... TT 61.6
Ullsperger, Tobias ..... MM 33.1
Ulm, Laura .....•O 4.2
Ulrich, Rössler ..... TT 94.4
Ulstrup, Søren ..... O 66.8, O 95.11, TT 96.11
Uluca, Ahmed .....•O 78.6
Ulugöl, Alptuğ .....BP 14.80
Ulybyshev, Maksim .....•MM 26.5, O 62.10, TT 54.10, TT 92.13
Umansky, Vladimir ..... HL 25.4
Umetsu, Rie Y. ..... MA 7.26, TT 41.7, TT 61.4
Ünal, Ahmet ..... TT 40.3, TT 92.3
Unfried, J. .....•HL 55.9
Unfried, Jakob .....TT 51.7
Unfried, Justus ..... HL 20.42
Unfried, Justus A. .....HL 20.37
Unger, Daniel .... TT 22.27, TT 22.29, TT 82.2
Unger, Frederik .....BP 14.44
Ungermann, Christian ..... BP 20.9
Unigarro, Andres ....•O 62.5, O 74.2, •TT 54.5, TT 68.2
Unikandanunni, Vivek .....•MA 14.4
Unkelbach, Ulla .....BP 7.14
Unnikrishnan, Arjun .....•TT 72.4
Unold, Thomas ..... DS 20.36
Unruh, Tobias ..... BP 16.11
Unterkofler, Florian ..... MM 19.36, •MM 22.5
Untiedt, Carlos .....MM 40.8
Ünzelmann, Maximilian .... MA 47.5, O 42.7, O 48.5, O 76.1, •O 80.5
Uohashi, Toshiya ..... FM 22.8
Upadhyay, Utkarsh ..... BP 14.71
Uraganase, Masayuki ..... FM 15.3
Urban, Alexander .....HL 4.3
Urban, Alexander S. HL 45.2, HL 48.4
Urban, Alexander Skyrme .....HL 4.2
Urban, Birgit ..... CPP 13.6
Urban, Daniel F. .... MM 3.7, MM 8.3, •MM 14.3, MM 39.5, MM 39.8, QI 1.8
Urban, Joanna ..... MA 25.3
Urban, Joanna M. ..... O 49.2
Urbanek, Michal ..... MA 9.9
Urban-Klaehn, Jagoda .....•MM 12.7
Urbanska, Marta ..... BP 7.40
Urbaszek, Bernhard HL 13.7, HL 20.5, HL 20.6, HL 20.13, HL 20.22, HL 26.36, HL 26.39, HL 39.5, HL 39.7, HL 39.11
Urbina, Cristian ..... TT 50.6
Urbina, Juan Diego . DY 13.6, DY 42.4, DY 42.13, DY 59.5, TT 19.6, TT 63.4, TT 63.13, TT 99.5, QI 21.8
Urbina, Juan-Diego .....QI 12.10
Urdaniz, Corina ..... MA 43.5, O 15.2, O 17.1
Uredat, Stefanie ..... CPP 31.2, CPP 46.33, •CPP 46.38
Urich, Yannis .....•TT 41.3
Ursaki, Veaceslav .....HL 26.10
Usachov, Dmitriy ..... MA 5.8, TT 7.8
Usanov, Dmitry ..... O 19.8
Ushakov, Ivan .....FM 4.6
Ushakov, Ivan N. .....•FM 18.8
Ustimchuk, Daria .....•FM 5.7
Ustinov, Alexey .....TT 43.2
Ustinov, Alexey V. ... O 19.7, TT 22.11, TT 22.13, TT 22.14, TT 22.15, TT 22.16, TT 43.3, TT 43.4, TT 43.7
Utegulov, Zhandos .....HL 40.5
Utesov, Oleg .....TT 81.6
Utsch, Felix .....MA 27.7
Utz, Sebastian .....•MM 8.8
Uykur, Ece MA 2.6, •MA 8.10, TT 57.5, TT 57.6, AKBP 2.5
Užulis, Janis .. O 18.4, •O 47.3, O 84.1, TT 84.1
Uzulis, Max Vincent .....•DD 10.2
V. Astakhov, Georgy .....HL 11.7
V. Dinh, Duc ..... HL 11.7
V. Guzman, Horacio .....•BP 18.6, •CPP 41.2
v. Klitzing, Regine ..... CPP 46.18, HL 20.13
V. Krasheninnikov, Arkady ..... O 7.7, TT 9.7
V. Novikov, Sergey ... O 95.6, TT 96.6
V. Pourovskii, Leonid MA 11.9, TT 21.9
V. Roth, Stephan CPP 17.19, CPP 44.5, CPP 46.17, CPP 58.2
V. Vyalikh, Denis .... O 40.11, TT 37.11
Vacchini, Bassano ..... QI 7.4
Vadakkeputhanmadom Subramanian, Krishna Iyer .....•BP 14.2
Vahid, Hossein .....•DY 55.6
Vahland, Jörn .....CPP 57.1
Vaibhav, Vinay ....•DY 49.5, MM 41.1
Vaidya, Shroya ..... TT 22.12
Väinö Hevelke, Valentin ..... HL 25.3
Vaitsi, Alkisti O 22.1, O 43.4, •O 43.10
Vakhnin, Alexander ..... CPP 57.2
Valadkhani, Adrian . TT 81.7, •TT 95.6
Valecha, Bhavesh .....•DY 55.8
Valencia, Ana M. CPP 22.2, HL 26.25
Valenti, Agnes ...•DY 58.1, •SOE 17.1
Valentí, Roser ..... FM 10.1, MA 31.3, MA 33.10, TT 33.2, TT 47.3, TT 51.1, TT 57.8, TT 72.5, TT 81.7, TT 83.1, TT 95.6, TT 98.3
Valentin, Sascha R. HL 26.7, HL 26.9, HL 26.12, HL 55.4
Valentin, Sascha René ..... HL 20.41
Valentin, Thomas .....TT 14.2
Valentin, Wilhelm .....TT 50.7
Valentinis, Davide .....•TT 56.8
Valenzuela Reina, Javier ....•FM 5.5
Valenzuela, Sergio ..... MA 7.46
Valeriani, Chantal ..... DY 62.8
Valiera, Francesco ..... TT 23.27
Valigi, Pietro ..... DY 33.12
Vališka, Michal ..... TT 93.17
Valiullin, Rustem . CPP 6.2, CPP 46.7, CPP 46.8
Vallant, Willi ..... TT 5.5
Vallejo Bay, Álvaro .....•CPP 7.4
Valleriani, Angelo .....BP 14.81
Valles, Adam ..... QI 15.5
Valli, Angelo .....•DY 46.10, TT 17.7, •TT 75.10, QI 4.7, QI 21.9
Vallini, Elisa .....•DY 59.11, •TT 99.11
Valls Boix, Meritxell .....•MA 9.7
Valls Mascaro, Francesc .... O 13.10, O 97.9
Valtiner, Markus BP 14.91, MM 19.20, O 22.4, O 30.3, O 65.7, O 87.2, O 87.5
Valvidares, Manuel . MA 37.8, O 84.9, TT 84.9
van Aken, Peter A. .....TT 39.7
van Buel, Reinier .....•CPP 10.10, •DY 16.10
van de Krol, Roel ... HL 12.4, HL 26.11
van de Loo, Maximilian ..... MA 33.4
Van de Walle, Anka ..... TT 51.6
Van Den Brink, Jeroen ..... FM 22.6, HL 8.11, MA 2.11, MA 20.1, MA 47.4, TT 11.4, TT 83.3, TT 98.4
van der Ham, Stijn ..... DY 34.2
van der Meer, Jann .....•SYSD 1.5, •DY 21.1
van der Schoot, Paul ..... BP 2.4
van der Veen, Dennis .....FM 12.10
van der Veen, Renske M. .... HL 8.10
van der Veer, Ewout .....•FM 12.10
van der Vegt, Nico .....•CPP 9.1, CPP 10.3, CPP 13.2, DY 16.3
van der Vegt, Nico F. A. ..... BP 4.3
Van der Vorst, Elena .....BP 7.24
van Dorp, Maarten .....•O 28.1
van Duin, Adri ..... MM 25.1
van Efferen, Camiel .....O 89.8
van Gent González, Johanna FM 12.10
van Hassel, Shen .....•TT 92.18
van Helvoort, Antonius T.J. ..FM 18.8
Van Hulle, Joséphine ..... BP 14.83, •BP 32.12, •DY 52.12
van Kan, Adrian .....•DY 8.10
van Kuiken, B. ..... MA 7.14
van Loon, Erik .....TT 27.4
Van Loon, Erik G C P ..... TT 44.10
van Luijk, Lauritz .....QI 10.9
van Mullekom, Niels P. E. ..... O 99.9
van Niekerk, Marthinus ...•CPP 59.4
Van, Phuoc Cao ..... MA 52.12
van Rossum, Aernout ..... DD 36.3
van Steensel, Alwin ..... QI 2.2
van 't Westende, Esra ..... TT 41.1
van Veen, Feike .....•TT 6.1
van Vliet, Nicole .....BP 27.7
van Weerdenburg, Werner M.J. O 71.4, •O 99.5, TT 66.4, TT 73.3
Van Wezel, Jasper . FM 22.6, TT 98.4
van Wingerden, Bent . O 14.3, O 14.10, O 40.19, •O 40.20, TT 37.19, •TT 37.20
Vanakalapu, Varun .... MA 5.1, TT 7.1
Vandersypen, Lieven M.K. ... HL 38.4
Vandewalle, Nicolas .....DY 19.7
Vaníčková, Elena ..... O 80.1
Vanmaekelbergh, Daniel ..... TT 6.1
Vannada Puleri, Anusree ...•MA 7.36
Vano, Viliam ..... TT 56.13
Vanselow, Moritz .....•DS 14.4
Vardar, Alptekin .....AKPIK 6.4
Varga, Szabolcs .....DY 47.4
Vargas, Patricio ..... O 67.3
Varjas, Dániel .....•HL 17.4, HL 38.6, QI 2.8, AKPIK 5.12
Varma, Kaarthik .....BP 20.6
Varoutis, Stylianos .....O 78.1
Varri, Akhil .....MA 9.13, MA 52.5, MA 52.14
Varsano, Daniele .... O 84.7, TT 10.6, TT 84.7
Vartanyants, Ivan .....HL 4.1
Vartanyants, Ivan A. ..... O 34.6

Varvaro, Gaspare .. MA 44.7, TT 76.7
Vasconcellos, Steffen Michaelis de HL 20.59, MA 7.7
Vasconcelos, Vítor ..... SOE 16.3
Vasilaki, Eleni ..... •SYBT 1.4
Vasiljević, Jovana . BP 31.2, CPP 50.2
Vasilopoulos, Alexandros .... DY 15.5
Vasilopoulou, Maria ..... DS 16.2
Vasin, Kirill ..... •MA 54.2
Vasina, Timothée ..... TT 2.1
Vašina, Vojtěch ..... •QI 14.16
Vásquez-Sepúlveda, Sebastián BP 7.50
Vassaux, Maxime ..... •BP 20.2
Vasudevan, Amrutha ..... •UP 8.2
Vasylkovskyi, Volodymyr . CPP 17.10, FM 11.20, HL 26.24, •MA 13.8
Vasyuchka, Vitaliy ..... MA 52.9, MA 52.13, MA 52.20, MA 59.1
Vasyuchka, Vitaliy I. ..... MA 48.7, MA 48.8, MA 52.7
Vaxevani, Katerina ..... O 99.7
Vayalil, Sarathal Koyiloth .. CPP 17.15
Vayalil, Sarathlal ..... CPP 17.42
Väyrynen, Jukka I. . TT 64.5, TT 83.12
Vaz, Carlos A F ..... MA 7.81
Vaz, Elishka ..... •O 31.6
Vaz, Inês C. M. ..... CPP 21.1
Vazquez, Hector ..... •O 50.5
Véber, Tamás ..... •MA 58.3
Vecchietti, Julia ..... O 88.5
Vecchione, Antonio . HL 23.1, O 80.3, TT 81.3
Vedel, Ida M ..... BP 20.7
Vedel, Ida Marie ..... BP 18.3
Vedmedenko, Elena ..... MA 30.7, MA 55.7
Veena Uday, Nandana ..... •O 22.2
Vehse, Martin ..... DS 20.4
Veis, Martin ..... MA 39.6
Veith, Joaquin ..... DD 13.1, DD 27.4
Velasquez, Nicolas CPP 23.4, DY 24.4
Veldman, Lukas ..... •O 15.7, O 17.2, O 89.1, O 89.5
Veldman, Lukas M. .... O 99.1, O 99.8
Velja, Stefan ..... CPP 26.2
Veloza-Diaz, Diego DY 43.10, •DY 54.5
Velpuri, Usha ..... HL 33.2, HL 33.3, HL 34.3
Vendolsky, Luis ..... O 4.6
Venkatasubramanian, Varun MA 11.1, TT 21.1
Venkatesh, Karan ..... •DY 43.8
Venkatraman, Jaya ..... QI 6.10
Vennéguès, Philippe ..... HL 57.5
Vennettilli, Michael BP 10.2, CPP 18.2, DY 18.2
Ventura, Enrico .. •DY 45.2, •SOE 14.2
Ventura-Macias, Emiliano ..... O 3.7
Venturi, Giacomo ..... O 57.3
Venugopal, Rakshith ..... DS 20.10
Vera, Alexander ..... HL 20.11
Verba, Roman ..... MA 9.9, MA 48.2
Verbakel, Jort ..... TT 41.1
Verbeek, Xanthe ..... •MA 20.2
Verbiest, Gerard J. ..... O 97.9
Verdi, Carla ..... FM 23.2, HL 49.4
Vereijken, Arne ..... MA 5.1, MA 36.4, MA 36.5, TT 7.1
Veremchuk, Igor .. •HL 23.1, MA 7.20, MA 30.8
Veremchuk, Ihor ..... MA 49.6
Vergionry, Maia G. ..... HL 8.11
Vergniory, Maia ..... O 63.4, TT 55.4
Verheijen, Marcel A. ..... HL 17.1
Verhoeven, Marcus ..... •PSV IX
Verhoff, Leonard . FM 11.22, •TT 69.2
Verlhac, Ben ..... O 99.9
Verma, Jyoti ..... •MM 11.2, MM 12.8
Verma, Nishchhal ... DY 13.1, TT 19.1
Verma, Sandeep ..... O 46.10
Verma, Sonu ..... HL 39.11
Vermeer, Benjamin ..... BP 9.1
Versok, Evelyn ..... •O 31.5, O 35.4
Vértesi, Tamás ..... QI 20.5
Vertruyen, Benedicte ..... MA 7.27
Verusheski, Kristijan ..... •TT 62.3
Vervelaki, Andriani ..... MA 49.2
Verzola, Ina Marie .... MA 5.7, TT 7.7
Vescan, Andrei ..... O 96.3
Vescovi, Milenko ..... AKBP 5.4
Vescovo, Elio ..... HL 24.10
Veslin, Timo ..... •DS 21.1
Vesti, Anders ..... •MM 9.7
Veuillen, Jean-Yves ... O 15.1, O 62.2, TT 54.2
Vewinger, Frank ..... HL 12.1
Veyan, Jean F. ..... O 67.3
Veyrat, Arthur ..... MM 40.4
Veyret, Noemie .... •BP 7.25, BP 7.49
Vézian, Stéphane .... O 62.3, TT 54.3
Veziroglu, Salih ..... CPP 15.3
Vezzani, Alessandro ..... DY 7.2
Vicente-Arche, Luis M. ..... TT 81.1
Vidmar, Lev ..... DY 32.6, TT 45.6
Vie Jørgensen, Sindre ..... •MA 6.11
Vieira, Rafael ..... MM 41.3
Vieira, Rafael M. ..... MA 50.2
Vierck, Paula ..... •DS 20.18
Vieweg, Maximilian TT 23.6, •TT 70.1
Vigliotti, Lucia ..... •TT 28.11
Vignale, Giovanni ..... TT 74.7
Vignesh, Kuduva ..... MA 7.74
Vijay, Sudarshan ..... MM 22.6
Vijayan, Nikhil ..... MA 39.1, MA 55.9
Vijayan, Ponraj .. HL 20.37, HL 20.38, HL 20.42, HL 34.2, HL 34.4, HL 34.5
Vijayan, R. ..... HL 55.9
Viji, Priya ..... CPP 37.4
Vila, Laurent ..... MA 51.3, TT 88.3
Vilardi, Demetrio .... TT 13.4, TT 94.1
Vilas-Varela, Manuel ..... O 9.10
Vilfan, Andrej ..... •SYBS 1.3
Vilhena, Guilherme .. MM 31.2, O 87.8
Villadiego, Inti Sodemann ... TT 83.5
Villamarin, Maria ..... BP 7.46
Villani, D. ..... BP 27.8, BP 37.2
Villaos, Rovi Angelo Beloya .. MA 5.7, TT 7.7
Villar Guerrero, Jorginho .. •TT 22.34
Villaseñor, David .. •DY 32.9, •TT 45.9
Villegas, Javier E. ..... TT 69.3
Villoro, Ruben Bueno ..... MM 34.7
Vilquin, Alexandre CPP 20.9, DY 23.9
Vilquin, Bertrand ..... •FM 4.1
Viña-Bausá, Beatriz ..... •O 15.1
Viñas Boström, Emil .. O 49.5, O 79.1
Vinnemeier, Elena ..... •HL 39.2
Vinnichenko, Mykola ..... MA 44.6, TT 76.6
Virnau, Peter ..... BP 2.4, CPP 34.3, CPP 56.4, DY 36.3, MA 21.1, MA 21.6, MA 55.8
Viscaya, Sanber ..... O 67.3
Vishart, Andreas Lynge ..... O 18.1
Vishina, Alena ..... MA 50.7, MA 58.1
Vishwakarma, Aditya ..... •MM 7.2
Vishwanath, Ashvin ..... TT 4.5
Visscher, Maria ..... •O 76.7
Visser, Amber ..... TT 98.4
Vít, Jakub ..... DS 7.5, •MA 57.5
Vitagliano, Giuseppe . TT 17.9, QI 4.9, QI 10.11, QI 21.5
Vitartas, Valdas ..... MM 9.4, O 62.4, TT 54.4
Vitek, Marco ..... O 3.2
Vitusevich, Svetlana ..... BP 20.9
Vizcaya, Sanber ..... O 67.11
Vlasiuk, Ekaterina ..... •TT 56.3
Vlcek, Vojtech ..... HL 35.2
Vliem, Jara ..... TT 6.1
Vo, T.-P. ..... O 93.9
Vo, Trung-Phuc ..... •O 2.4
Vocaturo, Riccardo ..... TT 11.4
Vocks, Elin ..... MA 39.15
Voehringer, David ... BP 14.7, BP 14.9
vöelkel, simeon ..... DY 19.3
Vogel, Alexander ..... BP 9.1
Vogel, Bärbel ..... UP 5.3
Vogel, Carola ..... BP 16.11
Vogel, Clemens ..... •HL 26.49
Vogel, Michael .. •CPP 56.1, MA 21.3, MM 14.5
Vogel, Nicolas .... CPP 20.3, DY 23.3
Vogel, Tim ..... •MA 39.14
Vogl, Lilian ..... FM 2.1
Vogt, Christopher ..... CPP 46.27
Vogt, Patrick ..... DS 11.3, HL 9.1
Vogt, Sofie . HL 9.3, HL 9.6, HL 26.20, HL 26.21, HL 26.22, HL 40.7, HL 40.9
Vogt, Sonja ..... SYTP 1.1
Voigt, Alexander ..... DD 10.1
Voigt, Axel BP 1.2, CPP 1.2, CPP 10.8, DS 14.5, DY 4.2, DY 16.8
Voigt, Fabian F. ... BP 14.38, •BP 33.1
Voigtländer, Bert ..... O 41.4, O 54.3, TT 38.4
Voits, Julian B. ..... •DY 54.7
Vojácek, Libor ..... MA 51.3, TT 88.3
Vojta, Matthias ..... TT 2.2, TT 86.1
Volavka, Dominik ..... •O 35.3
Volk, Christian .... HL 10.3, HL 20.26, TT 20.3
Volkamer, Andrea ..... BP 15.6
Volkau, Ivan •TT 41.6, TT 61.6, TT 62.1
Völkl, Timo BP 1.10, CPP 1.10, DY 4.10
Volkmann, Ulrich ..... BP 5.3
Volkmer, Lukas ..... •MM 7.1
Volkov, Dmitriy ..... QI 8.5
Volkov, Oleksii ..... MA 49.1
Volkova, Kseniia ..... FM 11.28
Völler, Jonas ..... •TT 2.10
Vollmer, Doris ..... •CPP 5.1, CPP 8.1, CPP 8.3
Vollmer, Ina ..... AKPIK 3.2
Vollmer, Sergej .. HL 20.37, HL 20.42
Vollus, Tara ..... •HL 53.4
Völter, Constantin ..... CPP 12.5
Volz, Kerstin CPP 4.4, MM 4.6, O 10.9, O 70.1, O 95.12, TT 16.9, TT 65.1, TT 96.12
von Appen, Alexander ..... BP 27.11
von Bassewitz, Alice ..... •JOB 1.2
von Coelln, Nadine ..... •DS 21.2
von Delft, Jan ..... TT 51.11
von Delius, Max ..... HL 53.4, O 54.7
von den Driesch, Nils ..... HL 12.1, HL 38.1, QI 6.2
von der Lehr, Fabrice ..... BP 14.57
von Destinon, Richard ..... •MM 18.5
von Eysmondt, Hendrik ..... BP 27.6
von Freymann, Georg ..... HL 52.5, MA 45.5, MA 48.8, TT 24.3, AKPIK 5.3
von Helden, Gert ..... O 85.4
von Klitzing, Regine . BP 7.5, CPP 5.5, CPP 26.4, •CPP 28.3, CPP 29.4, CPP 30.4, CPP 39.5, CPP 46.11, CPP 46.13, CPP 49.1, CPP 49.5, •DY 29.3, DY 44.14, HL 20.22, HL 39.5, HL 39.7, HL 39.11
von Kltizing, Regine ..... CPP 21.2
von Korff Schmising, Clemens MA 7.15, MA 27.11, MA 38.4
von Milczewski, Jonas ..... HL 3.1
von Oppen, Felix ... DY 32.2, TT 45.2, TT 50.5
von Plessen, Gero ..... O 57.5
von Reppert, Alexander .... MA 38.9, O 40.15, TT 37.15
von Rohr, Fabian O. ..... FM 11.23
von Rueden, Alexander ..... •O 65.10
von Savigny, Christian ..... CPP 2.1, SOE 3.1, UP 1.1, UP 3.4, UP 6.4, UP 6.5, •UP 6.6
von Seggern, Aaron ..... O 34.5
von Seggern, Rieke ..... HL 52.1
von Selzam, Nick ..... •QI 12.1
von Wattenwyl, Noel ..... O 96.12
von Wenchstern, Holger ... HL 26.44
von Wenckstern, H. ..... HL 46.6
von Wenckstern, Holger .... FM 10.2, HL 9.3, HL 9.5, HL 9.6, HL 26.19, HL 26.20, HL 26.21, HL 26.22, HL 26.32, HL 26.40, HL 40.7, HL 40.9
Vonbun-Feldbauer, Gregor ... •O 94.2
Voneshen, David ..... TT 95.7
Vonhoff, Frederik .. •HL 23.7, MM 9.3
Vonhusen, Annika ..... •DY 43.20
Vonk, Vedran ..... DS 9.5
Vonka, Jakub ..... TT 62.6
Vool, Uri . MA 6.12, MA 7.36, MA 24.2, MA 58.2, TT 5.3, TT 17.2, TT 22.23, TT 36.2, TT 40.1, TT 40.3, TT 57.10, TT 92.3, QI 4.2
Vorac, David ..... DY 61.5
Vorobyov, Vadim ..... QI 20.6
Voronov, Andrey ..... •MA 9.9
Vorwerk, Maximilian ..... MA 10.1
Vos, Bart .. BP 7.27, BP 7.32, DY 43.5, DY 43.18
Voss, Florian .... •CPP 10.5, •DY 16.5
Voss, Jan Nicolas ..... TT 43.2
Voss-Böhme, Anja . BP 33.5, •BP 33.6
Vowinckel, Bernhard ..... DY 19.5, •DY 19.6, DY 19.8
Vranic, Ana ..... SYTP 1.4
Vrellou, Maria ..... MM 36.4
Vucelja, Marija ..... •DY 9.7
Vucicevic, Jaksa ..... TT 51.1
Vuijk, Hidde ..... •DY 55.3
Vuijk, Maurits ..... •O 85.6
Vuković, Filip ..... MM 14.2
Vural, Hüseyin ..... QI 14.1
Vutukuri, Hanumantha Rao .. DY 34.2
Vyalikh, D.V. ..... MA 27.8
Vyalikh, Denis ..... MA 7.16, MA 8.5
Vyas, Dhyey ..... BP 15.9
Vyas, Kuber ..... •O 17.12, O 89.8
Vyborny, K. ..... MA 47.7
Vyvlecka, Michal ... HL 34.1, HL 34.5, QI 18.6
W. Claeys, Pieter ..... QI 7.1
Waack, Jan M. ..... •HL 37.1, HL 48.2
Wachtel, Rowena . MA 47.11, MA 54.7
Wachter, Christoph ... O 30.2, O 30.4, O 69.6
Wächter, Hendrik ..... •MA 52.2
Wächter, Matthias ..... DY 41.5
Wächter, Metthias ..... DY 15.11
Wächtler, Christopher ..... •DY 46.5, •TT 75.5
Wächtler, Maria ..... TT 24.3
Wäckerlin, Christian ..... O 9.11
Wackermann, Rainer ..... DD 14.1
Waclaw, Bartlomiej ..... DY 33.2
Wadewitz, Victoria ..... •QI 16.4
Wadsack, Myriam ..... O 9.8
Wagatha, Peter ..... MM 17.1
Waghmare, Umesh ..... DS 7.4
Wagner, Andreas DS 20.22, MM 12.8, •AKBP 2.1, AKBP 2.2, AKBP 2.5, AKBP 8.2
Wagner, Barbara ..... CPP 8.4
Wagner, Bettina ..... HL 20.20
Wagner, Chiara ..... •O 87.2
Wagner, Christian ... BP 7.7, BP 7.20, BP 7.21, BP 14.28, BP 14.32, BP 14.36, BP 14.41, BP 14.83, BP 32.12, BP 36.7, DY 52.12, DY 57.7, O 9.5, O 31.3, •O 61.10, O 69.8
Wagner, Daniel ..... •FM 5.3
Wagner, Glenn ..... O 63.3, TT 55.3
Wagner, Jakob ..... •MA 52.4
Wagner, Joachim ..... CPP 20.11, CPP 46.21, DY 23.11
Wagner, Koloman ..... HL 3.7
Wagner, Laura I. .... DS 11.2, HL 33.5, HL 42.1, MM 4.2
Wagner, Lukas ..... HL 34.5, UP 8.5
Wagner, M. R. ..... O 57.6
Wagner, Margareta ... •O 58.7, O 94.5
Wagner, Markus ... HL 40.2, HL 55.11
Wagner, Markus R. HL 35.1, •HL 40.6
Wagner, Martin ..... •DY 63.4
Wagner, Matthias ..... MA 39.14, •MA 48.3, MA 48.9
Wagner, Ralph ..... TT 93.10
Wagner, Stefan MM 19.18, MM 19.47, MM 30.2, MM 30.3, MM 35.2, MM 39.3
Wagner, Susan ..... BP 33.3
Wagner, Thorsten ..... O 4.7
Wagner, Tim ..... DS 20.43
Wagner, Timo ..... •DY 44.4, HL 17.6, O 68.2
Wagner, Tobias ..... MA 2.4
Wagner, Tolga ..... FM 15.1
Wah, Lavoisier ..... •TT 53.9
Wahada, Amine .... O 40.11, TT 37.11
Wahada, Mohamed A. ..... O 38.4
Wahl, Dennis ..... HL 22.4
Wahl, Peter .. O 80.3, O 93.5, •O 93.7, TT 5.10, TT 29.2, TT 94.2
Wahlström, Niklas ..... MA 34.11
Wakatsuki, Taiki ..... •SOE 9.2
Walbrunn, Valentin ..... •DS 11.2
Walczak, Aleksandra ..... BP 32.5, DY 52.5
Waldecker, Lutz ..... HL 3.3, MA 43.2
Waldmann, Jannis ..... •DY 43.2
Waldmann, Oliver MA 36.13, MA 42.1
Walker, Benjamin J. ..... DY 44.13
Wallauer, Robert ..... O 38.6
Wallden, Petros ..... QI 5.3
Wallerberger, Markus ..... TT 23.23
Wallis, Sandra ..... UP 6.4, •UP 6.5
Walliser, Nils-Ole . •BP 36.4, •DY 57.4
Wallmersperger, Thomas .. CPP 24.2
Wallner, Hannes ..... O 44.13
Walowski, Jakob .. MA 21.3, MA 39.7, MA 39.12, MA 54.11
Walsh, Aron ..... MM 13.5
Walter, Marcel ... MA 7.47, MA 36.10, MA 38.6
Walter, Michael .... CPP 17.43, O 31.4
Walter, Niklas ..... •HL 3.9
Walther, Andreas BP 14.27, •CPP 31.1
Walther, Clemens ..... DD 16.2
Walther, Franziska . MA 7.56, MA 8.3, •MA 8.5, MA 27.2, TT 98.2
Walther, Luis ..... •TT 64.6
Walther, Matthias R. ..... TT 23.11, TT 23.12

Walther, Thomas ..... AKBP 7.3
Walther, Tobias ..... BP 7.37
Walz, Andreas . O 9.4, O 45.4, •O 78.3
Walz, Constantin ..... •MA 38.9
Walz, Michael ..... O 78.3
Wan, Caihua ..... AKPIK 6.4
Wandall, Lau H. ..... O 88.4
Wang, B. Y. ..... TT 69.6
Wang, Bihan ..... HL 4.1
Wang, Bosen ..... TT 93.11
Wang, Boyi ..... •DY 34.7
Wang, Cheng ..... •O 14.8
Wang, Chenxi BP 1.9, CPP 1.9, DY 4.9
Wang, Chin-Wei .. MA 31.10, TT 47.10
Wang, Dongfei ..... O 99.7
Wang, Fu-Ming ..... MM 8.7
Wang, H. ..... MA 4.4
Wang, Hai ..... FM 10.4
Wang, Hai I. ..... MA 39.1
Wang, Hao ..... MA 8.7, MA 33.7
Wang, Henry MM 19.1, O 24.4, •O 24.6
Wang, Huabing ..... TT 71.2
Wang, Huimin ..... •O 98.5
Wang, Jiaju ..... •O 63.4, •TT 55.4
Wang, Jiaozi ..... DY 46.4, DY 59.10, TT 53.8, TT 75.4, TT 99.10
Wang, Jiaying ..... •AKBP 11.3
Wang, Jinhua ..... O 45.4
Wang, Jipeng ..... HL 31.4
Wang, Jue ..... •O 45.4
Wang, Kaize ..... TT 57.7
Wang, Peijiang ..... CPP 46.46
Wang, Pengjie ..... AKBP 5.4
Wang, Pushi ..... CPP 17.45
Wang, Qi ..... MA 9.9, TT 57.6
Wang, Qian ..... CPP 59.2
Wang, Rui Ning ..... QI 2.6
Wang, Ru-Pan ..... BP 9.6
Wang, Shengqiao ..... MA 33.7
Wang, Shuanglong ..... FM 10.4
Wang, Shuhan ..... MA 19.8, TT 31.8, TT 49.5, •TT 74.6
Wang, Shu-Jen ..... CPP 15.6
Wang, Sitao ..... CPP 54.2
Wang, Siyu ..... •QI 14.15
Wang, Tong ..... BP 20.6, •MM 25.4
Wang, Wen ..... TT 86.3
Wang, Wenbo ..... CPP 15.1
Wang, X. ..... HL 37.2
Wang, Xia ..... •FM 22.2
Wang, Xianjie ..... MA 57.1
Wang, Xiaotao ..... MA 49.6
Wang, Xiaoyang ..... QI 7.2
Wang, Xinran ..... MA 39.2
Wang, Xuejian ..... FM 15.3, •FM 18.4
Wang, Xusheng ... TT 29.12, TT 95.3
Wang, Yandong •CPP 46.31, CPP 54.6
Wang, Yang •DS 16.4, MM 5.4, QI 13.5
Wang, Yibo ..... •MA 24.6, •TT 36.6
Wang, Yifan ..... •MA 36.13
Wang, Yihua ..... QI 20.1
Wang, Yijun ..... BP 14.38
Wang, Ying ..... O 52.2
wang, Yingwen ..... BP 14.13
Wang, Yingxiao .. •BP 30.1, •CPP 47.1
Wang, Yizhen ..... •CPP 8.2
Wang, Yongjan ..... TT 61.2
Wang, Yongsong ..... •TT 74.1
Wang, Yu ..... •TT 85.2
wang, yuandong ..... •MM 19.11
Wang, Yu-Chiun ..... BP 3.5
Wang, Yuemin . O 55.6, O 81.4, O 88.5
Wang, Zhe ..... MA 7.46, MA 12.4, MA 35.6, O 94.9, TT 23.14, TT 41.2, TT 60.6, TT 71.2
Wang, Zhenbo ..... O 4.4
Wang, Zhenyu ..... •O 13.6
Wang, Zhiwei ..... O 41.4, TT 38.4
Wang, Zixuan ..... HL 55.2
Wang, Ziying ..... O 59.7, TT 48.7
Wanjura, Clara ..... •QI 21.1
Waqas, Muhammad ..... •HL 15.8
Waqee Ur Rehman, Muhammad HL 23.1
Warburton, Richard J. ..... HL 55.4
Ward, Ciara ..... •FM 11.16
Warkotsch, Dustin ..... •DY 43.12
Warnken, Nils ..... MM 34.4
Warren, Patrick ..... DY 21.7
Waseda, Osamu ..... MM 5.5
Waseem, Muhammad O 76.4, TT 27.4
Wasem, Marius ... HL 26.3, •HL 45.3
Waßmer, Elias ..... •CPP 37.6
Wasser, Philipp ..... TT 22.32
Wastl, Leon ..... •TT 23.20
Waszkiewicz, Radost ..... SOE 4.2
Watanabe, Hirotaka ..... HL 57.1
Watanabe, Kenji ..... HL 3.3, HL 3.8, HL 10.1, HL 10.3, HL 18.7, HL 20.25, HL 24.9, HL 30.2, HL 47.2, MA 43.2, MA 49.2, O 95.2, O 95.11, TT 20.1, TT 20.3, TT 32.7, TT 59.2, TT 96.2, TT 96.11
Watanabe, Yoshito ..... TT 33.4
Wätjen, Timo ..... O 2.6
Watschke, Anselm ..... •HL 20.32
Watson, Freya ..... •FM 12.11
Watson, Matthew ..... DS 14.3
Watson, Matthew D. ..... O 76.5
Watts, Benjamin ... MA 7.81, MA 46.4
Watzka, Bianca ..... •DD 2.1, DD 25.1, •DD 27.6, DD 42.3
Wdowik, Urszula D. ..... DS 7.2
Weatherby, Thomas Sean ... •DD 4.3
Weaver, Bruce ..... O 66.8
Weber, Christoph .. BP 14.86, BP 16.2, BP 29.1, CPP 45.1
Weber, Christoph A. BP 5.6, BP 14.96
Weber, Daniel ..... TT 78.4, •TT 92.8
Weber, Elke ..... SYTP 1.1
Weber, Frank ..... TT 49.1, TT 95.2
Weber, Fried-C. ..... MA 38.9
Weber, Fried-Conrad ..... •MA 7.39
Weber, Heiko ..... AKjDPG 1.3
Weber, Jens P. ..... HL 2.5
Weber, Johannes •MA 45.1, MA 52.18
Weber, Jonas H. ..... HL 34.1
Weber, Jonathan ..... MA 38.10
Weber, Manuel ..... •TT 2.9
Weber, Marius ..... MA 47.3
Weber, Mirko ..... •BP 14.54
Weber, Sebastian ..... MM 34.6
Weber, Sebastian T. ..•O 40.1, O 40.2, O 40.3, O 40.4, O 40.5, O 40.6, O 98.6, •TT 37.1, TT 37.2, TT 37.3, TT 37.4, TT 37.5, TT 37.6
Weber, Sophie ..... MA 5.2, TT 7.2
Weber, Thomas ..... HL 20.18
Weber, Timur ..... MA 49.3
Weber, Yannik ..... AKPIK 5.15
Webster, Preston T. ..... DS 21.3
Weckhuysen, Bert Marc ... AKPIK 3.2
Wedlich-Söldner, Roland ... BP 14.59
Weeber, Rudolf ... BP 7.13, CPP 49.1, CPP 49.3
Weerda, Erik Lennart ..... •TT 73.12
Weffling, David ..... MA 59.1
Wegbünder, Lucia . BP 7.36, •BP 7.40
Wegener, Simon A. ..... CPP 31.4, CPP 53.2
Wegener, Simon Alexander •CPP 44.2
Wegerich, Alexander . O 30.1, •O 48.2
Wegewijs, Maarten ..... •TT 18.5
Wegner, Daniel ..... O 89.4, O 89.7
Wegner, Gino ..... O 44.12
Wegner, Hermann ..... O 3.1
Wegner, Hermann A. CPP 22.5, O 58.1
Wegner, Juliette ..... •DY 44.6
Wegner, Mathias ..... TT 82.3
Wegner, Muriel ..... O 28.5, •O 55.1
Wegscheider, Werner ..... HL 10.5, HL 29.4, HL 48.1, TT 20.5, TT 58.4
Wehling, Philip ..... •BP 9.6
Wehling, Tim O 62.7, TT 54.7, TT 69.8
Wehling, Tim O. ..... O 84.2, O 86.4, O 86.5, O 95.8, TT 23.24, TT 84.2, TT 96.8
Wehrenberg, Felix ..... BP 15.10
Wehrspohn, Ralf ..... CPP 46.9
Wehrstein, Katharina ..... •FM 23.4, O 93.2
Wei, Chen ..... •DY 42.10, •TT 63.10
Wei, Fengkai ..... •DS 16.8
Wei, Peijia ..... •BP 2.9
Wei, Shihao ..... DS 6.2, MM 35.4, •MM 35.5
Wei, Tzu-Chieh ..... DD 40.1
Wei, Ye ..... QI 13.5
Wei, Yizhou ..... •TT 82.4
Wei, Yuan ..... MA 30.4
Wei, Zhengqing . •MM 3.9, MM 19.33
Weickhardt, Till ... DS 13.2, HL 20.18, HL 20.31
Weidemann, Sebastian ..... DY 48.6
Weidenhiller, Franz ..... DS 20.17
Weidgans, Christian ..... •HL 39.8
Weidig, Daniel . •CPP 20.11, •DY 23.11
Weidt, Nikolai .... DY 41.13, •MA 7.23, MA 36.4, MA 36.5, MA 52.40
Weig, Eva ... HL 3.9, HL 18.1, HL 18.4, HL 18.6, HL 18.8, HL 31.5, MA 59.5, TT 32.1, TT 32.4, TT 32.6, TT 32.8
Weig, Eva M. ..... HL 18.7, TT 32.7
Weigand, Markus ..... MA 8.13
Weigel, Martin ..... •DY 15.2, DY 15.4, DY 15.6, DY 43.21, DY 43.22, DY 43.23, DY 47.5, DY 60.2
Weigel, Tina ..... CPP 17.36
Weigl, Leonard ..... O 98.9
Weiler, Mathias ..... MA 6.1, MA 9.2, MA 9.4, MA 9.5, MA 48.8, MA 52.3, MA 52.7, MA 52.9, MA 52.11, MA 52.13, MA 52.20, MA 59.1, MA 59.9, TT 24.3
Weimann, Nils ..... HL 26.5
Weimar, Jens ..... DY 14.1, DY 41.14
Weinberger, Theodore ..... TT 93.17
Weindl, Adrian ..... •O 41.2, O 63.10, •TT 38.2, TT 55.10, TT 74.12
Weindl, Anna ..... •HL 3.8
Weinel, Kristina ..... O 70.2, TT 65.2
Weinelt, Martin ... MA 7.12, MA 38.2, O 42.4
Weiner, Orion D. ..... BP 3.11
Weinert, Hendrik ..... O 4.6
Weinhagen, Lennart ..... O 14.10, •O 40.19, •TT 37.19
Weinhold, Tillmann ..... MA 47.11, •MA 54.7
Weinmann, Max ..... •DY 14.3
Weinstock, Daniel ..... HL 8.6
Weintz, Leon ..... •CPP 17.10
Weiß, Christopher .... O 27.5, •O 57.4
Weiß, Leonie ..... O 40.8, TT 37.8
Weiß, M. ..... HL 55.9
Weiß, Matthias ..... HL 18.5, HL 36.1, TT 32.5
Weiß, Michelle .. HL 20.38, •HL 20.42
Weiß, Niklas ..... •DD 26.3
Weißbach, Alexander ..... MA 47.8
Weißenberger, Philipp ..... •MA 12.2
Weißenhofer, Markus ..... •MA 14.3, •MA 40.10
Weiser, Maximilian J. ..... AKBP 5.1, •AKBP 5.2, AKBP 8.5
Weiske, Hendrik ..... O 11.4
Weismann, Alexander O 17.10, O 69.4, •O 83.8, O 89.11
Weißmantel, Steffen ..... DS 4.6
Weißmüller, Jörg ..... MM 15.7
Weisrock, Tobias ..... •JOB 2.2
Weiss, Benedikt ..... •DD 30.5
Weiss, Carl ..... •AKBP 9.1
Weiss, Daniel. K. ..... QI 6.10
Weiss, Dieter ..... HL 30.2, TT 59.2, TT 97.2
Weiss, Klaus-Peter ..... MM 34.1
Weiss, M. A. ..... MA 52.8, MA 59.8
Weiss, Marco ..... O 4.6
Weiss, Marvin Alexander ... MA 38.8
Weiss, Matthias .... BP 14.1, BP 14.4, BP 27.9, BP 36.5, DY 57.5, HL 26.1
Weiss, Michelle ..... HL 20.37
Weiss, Paul ..... •DY 46.1, •TT 75.1
Weissenhofer, Markus ..... MA 7.11, MA 38.6
Weissitsch-Reiner, Lukas ... MM 24.1
Weissmüller, Jörg MM 15.6, MM 21.3, MM 21.10, MM 30.4, MM 39.2
Weisweiler, Hardy ..... TT 22.35
Weitz, R. Thomas ... O 40.21, O 66.9, O 98.10, TT 37.21, TT 92.15
Weitz, Thomas .. DS 20.50, HL 20.32
Weitz, Tobias ..... SYFC 1.5, O 74.1, TT 68.1
Weitzel, Alexander ..... TT 64.2
Weitzel, Karl-Michael ..... MM 14.5, •MM 16.3
Weizel, Alexander ..... TT 5.1
Welberg, Julia ..... DD 15.2
Welker, Till ..... •DY 21.8
Welle, Alexander ..... HL 4.5
Wellecke, Gerrit .. BP 14.95, •BP 32.1, •DY 52.1
Wellens, Thomas .... QI 13.3, QI 16.7, QI 16.9
Wemheuer, Niklas ..... HL 8.5
Wemhoff, Piotr Igor ..... O 52.2
Wen, Hai-Hu ..... •TT 39.5
Wende, H. ..... MA 7.14, MA 23.5, MA 50.3, TT 35.5
Wende, Heiko .... FM 11.31, MA 13.2, MA 36.1, MA 42.3, MA 50.8, MA 52.26, MA 52.27
Wende, Vincent . AKBP 2.3, AKBP 8.1
Wendel, Andreas ..... HL 22.3
Wendeln, Andreas MA 16.5, •O 40.12, O 66.6, •TT 37.12
Wenderoth, Martin .. O 28.8, O 71.20, O 73.3, O 73.4, O 74.9, TT 66.20, TT 68.9
Wendland, D. ..... HL 55.9
Wendler, Elke ..... DS 13.2
Wendler, Frank .... •FM 15.3, FM 18.4
Wendler, Nicolas ..... BP 20.8
Wendt, Klaus ..... DD 14.2, DD 23.2
Wendt, Mirco ..... •O 68.6
Weng, Ruiling ..... DY 22.9
Wenger, Christian .. DS 14.8, HL 23.3, O 96.6
Wenig, William L. ..... •MM 31.3
Wenskat, Marc .. FM 11.29, AKBP 9.1, AKBP 9.2
Wentzell, Nils ..... TT 13.4, TT 51.12
Wenzel, Maxim ... •MA 33.4, TT 12.6
Wenzel, Sabine ..... O 8.7
Wenzel, Volker ..... DD 31.1
Wermann, Caroline ..... •DD 9.2
Werner, Carsten ..... BP 27.10
Werner, Julius ..... •TT 82.1
Werner, Marco ..... •CPP 59.5
Werner, Miklos Antal ..... DY 46.10, TT 75.10, •QI 3.1
Werner, Paul . O 14.3, O 38.1, O 40.18, O 40.21, O 66.9, •O 98.10, TT 37.18, TT 37.21
Werner, Peter ..... DY 15.3
Werner, Stephan ..... CPP 16.4
Werner, Wolfgang ..... O 93.1
Wernicke, Pascal ..... •MA 7.19
wernicke, tim ..... HL 26.6, HL 37.3, HL 37.4
Werninghaus, Max ..... QI 2.7, QI 8.3
Wernsdorfer, Wolfgang ..... MA 42.6, O 3.3, O 15.4, O 17.7, O 17.9, O 17.11, O 89.3, O 89.12, O 99.2, O 99.10, TT 92.6, TT 92.7, QI 11.4, QI 11.5, QI 14.24
Wertz, Florian ..... MM 40.7
Wesch, Stephan ..... AKBP 12.2, AKBP 12.4, AKBP 13.2
Weschke, E. ..... MA 23.5, TT 35.5
Weschke, Eugen .. MA 8.13, MA 24.1, MA 36.1, TT 36.1
Weßels, Teresa ..... DS 20.32
Weshcke, Eugen .... MA 11.3, TT 21.3
Wessel, Stefan ..... TT 2.4, TT 2.10
Westenfelder Gil, Eva .... •CPP 46.34
Westerbeck, Nico ..... SOE 4.6
Westphal, Andrea ..... DD 39.2
Westphal, Carsten ..... O 94.9
Westphal, Lea ..... •CPP 4.2
Westrich, Sebastian ..... TT 24.3
Wetzel, J. ..... O 57.6
Wetzel, Jakob ..... FM 18.3, •O 52.3
Wetzelaer, Gert-Jan ..... HL 15.4
Weyandt, Julia ..... CPP 17.6
Weyer, Henrik ..... BP 14.51, DY 22.4, DY 41.8
Weyers, M. ..... HL 37.6
Weymann, Ireneusz .TT 78.3, TT 85.8
Weymouth, Alfred ..... O 3.6, O 56.2
Weymouth, Alfred J. ..... O 3.4
Weymouth, Alfred John ..... •O 3.5
Weymouth, Jay ..... O 40.8, TT 37.8
Wharam, Katrina ..... •BP 12.5
Wheeler, Edward ..... BP 14.42
Wiche, Miguel ..... O 56.1
Wichmann, Tobias . MA 43.3, O 86.5, O 95.8, TT 96.8
Wickenhäuser, Tom ..... MM 19.13
Wicker, Joris ..... •O 40.17, •TT 37.17
Widaa, Abdulrahman ..... TT 22.9, TT 28.9, TT 28.10
Widdra, Wolf .. O 14.5, O 28.5, O 38.3, O 40.9, O 42.1, O 55.1, TT 37.9
Widera, Artur ..... TT 24.3
Widera, René ..... AKBP 10.3
Widmann, Simon ..... O 42.7
Widstam, Joppe ..... •QI 12.8
Wiebe, Jens ..... O 15.8, O 99.6
Wiechers, Paul ..... O 43.6, O 80.4
Wieck, Andreas . HL 20.35, HL 20.36, HL 26.2
Wieck, Andreas D. .. HL 17.8, HL 26.7, HL 26.9, HL 26.12, HL 55.4, HL 55.8
Wieck, Andreas Dirk ..... HL 20.41
Wiede, Anja ..... •AKC 1.1
Wiedemann, Christian ..... TT 29.10, •TT 98.6
Wiedemann, Philipp ..... TT 92.6
Wiedenhofer, Dominik ..... SOE 6.3
Wieder, Benjamin ..... TT 10.7
Wiedmann, Raymond ..... TT 23.11

Wiedwald, Ulf ..... DS 14.4, MA 18.6, MA 50.8, MA 52.26, TT 30.6
Wiegand, Thomas ..... CPP 46.42
Wieland, Florian ..... BP 14.72
Wieland, Philipp .....•CPP 17.13
Wielert, Isabelle ... •BP 11.5, BP 14.16
Wiersema, Roeland ..... QI 5.8
Wiersig, Jan ..... DY 59.4, TT 99.4
Wiersma, Guido ..... TT 41.1
Wierzchalek, Ladislas ..... DY 25.1
Wiesendanger, Roland ..... MA 55.7, O 15.8, O 99.6
Wiesener, Philipp ..... O 23.1, O 72.3, TT 67.3
Wieser, Sandro ... MM 22.5, MM 31.4
Wiesner, Fabian .....•QI 18.5
Wiesner, Karoline . DY 58.10, SOE 4.2, SOE 12.1, SOE 16.2, SOE 17.10, AKPIK 2.5, AKPIK 5.9
Wießner, Sven .... CPP 54.2, HL 25.3
Wietek, Alexander . DY 46.6, MA 11.9, MA 34.8, TT 21.9, TT 75.6
Wietfeld, Alexander ..... BP 5.1
Wigger, Daniel ..... HL 3.6, HL 20.8, HL 20.58, HL 26.37, HL 35.7
Wiggers, Hartmut ..... HL 20.12
Wigren, Torbjörn ..... MA 34.11
Wijaya, Edward ..... CPP 17.25
Wijekoon, Himal .....•FM 11.6
Wijitpatima, Setthanat ..... HL 55.1
Wild, Johannes . •MM 30.2, MM 30.3
Wildbichler, Sarah ..... •DD 14.1
Wilde, Gerhard .... MM 3.5, MM 14.4, MM 18.1, MM 18.3, MM 18.5, MM 35.6
Wilde, Marc A. ..... TT 23.3, TT 41.6, TT 61.6, TT 62.1
wildenburg, leonardo ..... •HL 26.6, HL 37.3
Wilder, Jan ..... BP 7.38
Wilhelm, Fabrice .... MA 51.1, TT 88.1
Wilhelm, Frank ..... QI 17.1
Wilhelm, Frank K. ..... AKPIK 5.15
Wilhelm, Jan ..... BP 14.73, HL 24.8, HL 30.3, HL 54.1, HL 54.2, HL 54.3, MA 12.2, TT 59.3
Wilhelm, Richard A ..... O 93.1
Wilhelm, Thomas ... DD 4.3, DD 17.3, DD 20.1, •DD 27.3, DD 31.1
Wilhelm-Mauch, Frank •PSV V, QI 3.9, QI 13.6
Wilkins, David .... CPP 14.1, MA 42.7
Willems, Moritz ..... •HL 35.5
Williams, Federico J. ..... O 87.1
Williams, Travis ..... TT 95.7
Willke, Philip .... O 3.3, O 15.4, O 17.7, •O 17.9, O 17.11, O 19.7, O 89.3, O 89.5, O 89.12, O 99.2, O 99.10
Willsher, Josef ..... MA 19.11, TT 2.3, TT 31.11, TT 64.6, TT 79.4
Wilmar, Quentin ..... QI 18.1
Wilming, Henrik ..... QI 10.9
Wilson, Justin H. ... DY 46.2, TT 75.2
Wilson, Matthew .. SOE 4.2, SOE 12.1, SOE 16.2
Wilson, Nathan P. ..... O 38.4
Wilson, Nicholas ..... HL 20.12
Wilson, Russell J. ..... BP 14.81
Wilson, Stephen ... TT 57.9, TT 57.12
Wimmer, Michael .. HL 17.4, •TT 15.3
Wimmer, Tobias ... MA 51.8, TT 88.8
Wimmi, Stephan ... BP 11.5, BP 14.16
wind, nils ..... TT 25.11
Windes, William ..... MM 12.7
Windischbacher, Andreas ..... O 9.1, O 69.2, O 83.6
Windsor, Y.W. ..... MA 27.8
Windsor, Yoav W. ... MA 27.2, O 71.11, TT 66.11
Windsor, Yoav Will .. O 40.11, TT 37.11
Windsor, Yoav William ..... •MA 7.16, O 22.5, O 40.10, TT 37.10
Wing, Matthew ..... AKBP 12.2, AKBP 12.4, AKBP 13.2
Wingenbach, Jan ..... QI 14.22
Winidischbacher, Andreas .... O 61.7
Winkel, Patrick ..... TT 43.6
Winkelmann, A. ..... O 59.2, TT 48.2
Winkelmann, Clemens ..... O 74.6, TT 68.6, TT 82.1, •QI 2.10
Winkelmann, Clemens B ..... O 62.3, TT 50.8, TT 54.3, TT 73.3, TT 78.1
Winkelmann, Jan ..... DD 15.2
Winkelmann, Larissa ..... O 46.2
Winkelmann, Lutz ..... AKBP 11.2
Winkelmann, Stefanie ..... SOE 8.3
Winkler, Benjamin ..... DY 22.5
Winkler, Christina ..... MA 58.1
Winkler, Conrad ..... CPP 57.3
Winkler, Franz .....•MM 26.1
Winkler, Jonas ..... MA 58.1
Winkler, Louis Conrad .... CPP 17.24, CPP 40.4, •CPP 40.6
Winkler, Lucy .....•CPP 29.3
Winkler, Maximilian ..... MA 17.6
Winkler, Nils O. ..... •BP 14.21
Winkler, Roland G . BP 10.1, CPP 18.1, DY 18.1
Winkler, Thomas ..... AKPIK 5.6
Winkler, Thomas B. ..... MA 55.2
Winnerl, Stephan ... HL 17.5, HL 52.2, HL 52.3, MA 8.10, O 62.1, TT 54.1, TT 57.6, AKBP 2.5
Winte, Katrin ..... HL 46.2, HL 46.3
Winter, Antonia ..... BP 14.51
Winter, Benedikt ..... HL 24.3
Winter, Bernd ... CPP 19.5, CPP 23.2, CPP 23.4, DY 20.5, DY 24.2, DY 24.4
Winter, Steve M. ..... TT 72.9
Winterott, Moritz .....•MA 6.7
Winters, Danyal .....•AKBP 7.3
Wintz, Sebastain ..... MA 37.8
Wintz, Sebastian .. MA 8.13, MA 24.1, MA 59.6, TT 36.1
Winzer, Andreas T. ..... FM 7.1
Wipf, Oliver ..... •MM 35.3
Wippermann, Stefan .. O 13.3, O 13.6, O 86.7
Wirsdörfer, Vincent ..... MA 30.9
Wirth, Anneliese ..... •CPP 46.47
Wirth, Felix ..... •MA 3.6, MA 3.7
Wirth, Konstantin ..... O 79.4
Wirth, Ludger .....•DD 28.1
Wirth, Luise ..... CPP 13.6
Wirth, Martin ..... UP 7.4
Wirth, Nicolas ..... O 4.6
Wirth, Steffen ..... TT 62.3
Wisniewski, Piotr ..... FM 11.10
Witmans, Femke ..... TT 6.1
Witt, Niklas . O 62.7, TT 54.7, TT 62.8, TT 69.8, •TT 91.1, TT 95.8
Wittbrodt, Dustin .....•HL 17.2
Witte, Arthur .....•HL 26.32
Witte, Gregor ..... •O 32.1
Witte, Luis .....•O 28.2, O 28.4
Witte, Tobias ..... O 98.4
Witteveen, Catherine ..... FM 11.23
Witteveen, Olivier ..... •SOE 2.10
Witthaut, Dirk ..... DY 8.2, SOE 4.6
Wittigschlager, Simon ..... SYFC 1.5
Wittkowski, Raphael ..... BP 7.48, •BP 30.4, BP 30.6, BP 30.7, •CPP 47.4, CPP 47.6, CPP 47.7
Wittmann, Angela •MA 29.1, MA 29.2, MA 36.8, MA 36.9, MA 37.2, MA 39.3, O 61.8, •TT 46.1, TT 46.2
Wittmann, Gilles ..... CPP 46.45
Wittmann, Ludwig ..... O 38.6
Wittmann, Lukas .....•TT 51.9
Wittrock, Steffen ..... MA 37.8
Wittwer, Felix .....•BP 14.44, FM 19.2
Witzmann, Thomas ..... CPP 41.7
Wodtke, Alec ..... O 11.5, O 34.7
Wodzinski, Rita ..... DD 13.3, DD 23.5
Wohlgemuth, Marcus ..... DS 6.6
Wöhrl, Nicolas ..... O 68.2
Wojcieszak, Damian ..... DS 11.5
Wójcik, Jan ..... DY 34.10
Wójcik, Krzysztof .. TT 42.1, •TT 94.2
Wójcik, Krzysztof P. ..... TT 90.4
Wojnar, Piotr ..... HL 26.45
Wolanksy, Jakob ..... CPP 57.3
Wolansky, Jakob ..... CPP 17.20, CPP 40.1, •CPP 57.6, HL 22.6
Wolf, Christoph ..... MA 43.5, O 15.2, O 17.1, O 17.9, O 64.2, O 89.2, O 89.10, •O 99.4, O 99.11
Wolf, Daniel ..... FM 11.15, FM 19.5, FM 19.9, MA 44.6, MA 57.4, O 70.2, TT 65.2, TT 76.6
Wolf, Elisabeth H. ..... CPP 4.3
Wolf, Erasmus ..... TT 28.9
Wolf, Henrik ..... SOE 6.4
Wolf, Jan ..... FM 19.4
Wolf, M. ..... O 57.6
Wolf, Marcell .. CPP 32.4, CPP 46.37, DY 35.4
Wolf, Martin ..... MA 7.18, MA 25.3, O 12.10, O 22.1, O 38.4, O 38.7, O 40.11, O 43.2, O 43.4, O 43.8, O 43.10, O 45.1, O 45.7, O 49.2, O 51.2, O 66.3, O 71.10, O 71.11, O 85.4, O 87.7, O 95.5, O 96.8, O 98.7, TT 37.11, TT 66.10, TT 66.11, TT 96.5
Wolf, Maximilian .....•HL 20.29
Wolf, Melanie A. R. ..... •TT 23.7
Wolf, Niklas ..... •CPP 10.3, •DY 16.3
Wolf, Oliver .....•DS 8.5
Wolf, Ramona ..... AKPIK 6.1
Wolf, Robin .....•AKBP 3.1
Wolf, Stefan ..... DY 47.11
Wolfertz, Max ..... O 10.5, •O 10.8, TT 16.5, •TT 16.8
Wolff, Alexander ..... AKPIK 4.2
Wolff, Jakob .....•O 59.6, •TT 48.6
Wolff, Marion ..... O 44.11
Wolff, Niklas .... HL 20.23, HL 20.24, HL 26.23
Wolff, Susanne ..... DS 20.42, O 31.1, •O 74.8, •TT 68.8
Wolfgang, Belzig ..... TT 50.7
Wolfram, Lorenz ..... TT 94.4
Wolfthaler, Laura M. ..... •BP 14.81
Wölk, Sabine ..... QI 5.10
Wolke, Nathalie .....•DD 9.3
Wöll, Christof DS 21.2, O 55.6, O 81.4, O 88.5
Wöll, Dominik .....•CPP 58.6
Wollenberg, Wiebke ..... BP 33.9
Wollenweber-Bienerth, Yan Ravil •DS 9.1
Wollesen, Emma . BP 26.8, •BP 26.10, CPP 43.8, •CPP 43.10
Wollschläger, Joachim ..... DS 6.5, DS 20.15, DS 20.27, MA 47.8, O 28.2, O 28.4, O 28.6, O 28.7
Wolny, Juliusz ..... O 41.1, TT 38.1
Wolter, Anja U. B. . MA 3.3, MA 39.19, MA 52.35, TT 4.9, TT 23.1, TT 57.1, TT 57.2, TT 57.3
Wolter, Anja UB ..... TT 11.1
Wolter-Giraud, Anja ..... TT 93.5
Woltering, Steffen ..... CPP 57.1
Wolters, Janik . AKPIK 4.4, AKPIK 5.8
Woltersdorf, Georg ..... DS 20.37, MA 7.13, MA 9.8, MA 27.1, MA 35.3, MA 52.16, MA 59.7, O 14.5, TT 60.3
Wolz, Lukas ..... CPP 44.3, DS 12.3, HL 1.1, HL 12.7
Wolz, Lukas M. .... •MM 4.2, MM 4.3
Wong, Alexander ..... TT 61.12
Wong, Andrew J. .....•O 97.11
Wong, Gerard C. L. ..... BP 8.5
Wong, Jian Cheng .....•O 43.16
Wong, King Cho ..... •MA 43.6
Wong, Megan ..... BP 5.2
Wong, Wang N. ..... TT 22.12
Wong, Wei Wen ..... HL 35.4
Wong, William ..... HL 20.12
Woo, Chul-Ung ... CPP 11.11, DY 17.11, •DY 44.9
Woo, Tae Gyun ..... BP 9.6
Wood, Jonathan ..... AKBP 12.2, AKBP 12.4, AKBP 13.2
Woodcock, Thomas G ..... MA 58.1
Worbs, Andreas .... HL 17.5, MM 11.2
Wörle, Simon ..... DS 11.1, •DS 12.3
Worm, S. ..... BP 27.8, BP 37.2
Worrell, Meghan A. ..... DS 21.3
Worschech, Lukas .. HL 29.5, TT 58.5
Wortmann, Caroline ..... •DD 9.1
Wortmann, Daniel .. MA 16.12, O 37.3, O 50.1, O 71.6, TT 66.6
Wortmann, Martin . CPP 3.4, •DS 6.5, MA 7.63, MA 47.8
Wosnitza, J. ..... MA 18.1, MA 18.4, MA 18.5, MA 23.5, MA 47.7, MA 52.22, MA 52.24, TT 25.6, TT 29.1, TT 30.1, TT 30.4, TT 30.5, TT 35.5, TT 74.5, TT 80.6, TT 93.7, TT 98.1
Wosnitza, Jochen ..... MA 52.27
Wössner, Valentin ..... •BP 12.7
Wowchik, Alexander .....•DY 63.5
Wozniak, Krzysztof ..... CPP 32.3, DY 35.3
Wrachtrup, Joerg .. MA 43.6, TT 92.5
Wrachtrup, Jörg ... •HL 11.1, TT 24.6, QI 13.5, QI 20.1, QI 20.3, QI 20.4, QI 20.6
Wrana, Felix .....•UP 6.4
Wright, Emily ..... QI 2.7
Wrigley, James .... O 40.15, TT 37.15
Wrobel, Nico . AKBP 10.1, •AKBP 10.2, AKBP 12.5
Wrona, Thomas ..... UP 2.3
Wrublewsky, Selina ..... BP 14.41
Wrześniewski, Kacper ..... TT 78.3, •TT 85.8
Wu, Hao ..... MA 36.8
Wu, Jianzhong ..... CPP 21.3
Wu, Jingbo ..... TT 71.2
Wu, Jintong ..... FM 11.17
Wu, Junhui ..... HL 18.7, TT 32.7
Wu, Mengmeng ..... •BP 14.87
Wu, Min ..... BP 37.8
Wu, Weida ..... MA 17.6
Wu, Weikang ..... MA 54.3
Wu, Xianxin ..... TT 39.7
Wu, Y. ..... TT 69.6
Wu, Yao-Ting ..... O 9.11
Wu, Yu-En ..... TT 4.1
Wu, Yufei .....•CPP 46.42
Wu, Zheyu ..... TT 93.17
Wu, Zhiheng .....•BP 32.8, •DY 52.8
Wühl, Friederike .... •O 38.3, O 40.9, TT 37.9
Wulferding, Dirk ..... MA 40.8
Wulff, Peter DD 37.1, DD 39.2, AKC 1.3
Wulfhekel, Wulf •O 1.1, O 12.1, •TT 8.1
Wunderlich, Hannes ..... •BP 14.4
Wunderlich, Jörg .... MA 12.2, O 96.5
Wundrack, Stefan .... O 95.1, TT 96.1
Wünsche, Johannes ..... DD 13.1
Wünschek, Maximilian .....•O 22.4
Wurl, Klemens .....•HL 26.44
Wurm, Gerhard ..... UP 3.2
Wurmehl, Sabine . MA 7.28, MA 7.37, MA 13.1, MA 47.11, MA 54.7, TT 11.1, TT 26.7, TT 92.3, TT 93.5, TT 93.10
Wurmshuber, Michael ..... •MM 32.3
Wurstbauer, Ursula .. DS 21.5, HL 3.6, HL 3.11, HL 13.2, •HL 16.2, HL 20.11, HL 20.17, HL 25.2, HL 36.1, HL 39.2, HL 39.3, HL 39.4, HL 39.6, HL 39.9
Wurster, Stefan ..... MM 24.1
Würthner, Frank ... CPP 17.20, O 31.6, O 96.1
Würthner, Laeschkir .....•BP 10.5, •CPP 18.5, •DY 18.5
Wust, Stephan .... MA 38.7, MA 47.3
Wüthrich, Alwin .....•HL 57.3
Wutke, Dawid ..... HL 24.10
Wuttig, Matthias ... DS 7.4, DS 20.24, DS 20.30, DS 20.31, DS 20.38, DS 20.39, DS 20.40, DS 21.1, FM 11.2, FM 11.7, HL 20.65, O 26.1, O 26.5, O 96.4, O 96.9, O 96.11
Wyart, Claire ..... BP 14.68
wyart, matthieu ..•DY 58.6, •SOE 17.6
Wyderka, Nikolai ....•QI 10.7, QI 15.2, QI 18.8
Wyler, Nicolas ..... O 98.2
Wysmołek, Andrzej HL 26.37, HL 35.7
Xavi, Sharon ..... •CPP 46.65
Xi, Ruijun ..... •TT 14.11, TT 93.2
Xia, Hailiang ..... TT 52.4
Xia, Yonggao ..... CPP 17.32
Xiang, Feifei ..... MA 5.4, TT 7.4
Xiang, Junsen ..... TT 52.4
Xiang, Rong .... AKBP 2.1, •AKBP 2.2, AKBP 2.5
Xiang, Xu ..... MM 19.4
Xiao, Chengcheng ... •O 50.7, O 71.7, TT 66.7
Xiao, Jian .....•DS 20.50
Xiao, Ming ..... FM 18.5
Xiao, Xu ..... QI 6.10
Xiao, Zijie ..... MA 39.1
Xie, Fanqing ..... MM 40.7
Xie, Jiayu .....•CPP 20.1, •DY 23.1
Xie, Qingguang ..... •CPP 33.3
Xie, Ruiwen ..... MA 2.9, MA 2.12, MM 15.3
Xie, Yingjie .....•O 16.1
Xie, Yujie ..... MA 33.4
Xiong, Jie ..... •TT 13.6
Xiong, Liming ....•MM 7.6, •MM 27.2
Xiong, Shilong ..... AKPIK 6.4
Xiong, Shuxian •CPP 25.4, CPP 46.51
Xiong, Zeling ..... MA 59.7
Xu, D. ..... BP 27.8, BP 37.2
Xu, Han-Xiang ..... MA 11.2, TT 21.2, •TT 69.11
Xu, Hongxiang ..... O 83.1
Xu, Rui ... HL 23.1, MA 44.6, MA 49.1, MA 49.5, MA 49.6, TT 76.6
Xu, Tianyi .....•MM 19.42
Xu, Wenqi .....•CPP 54.6
Xu, Xiang .....•MM 11.5, MM 35.6
Xu, Xiaodong ..... MA 43.6, TT 44.4
Xu, Xiaoshan ..... O 60.6
Xu, Xuexin .....•QI 16.2
Xu, Xuqiang ..... CPP 46.57

Xu, Yingqian ..... AKPIK 6.4
Xu, Yong ..... TT 95.3
Xu, Yufeng ..... •MM 12.6, MM 22.8
Xu, Z. ..... MA 3.8
Xu, Ze ..... CPP 5.2, •CPP 5.4
Xu, Zhuijun ..... CPP 17.27, CPP 44.3
Xu, Zihan ..... DY 6.10
Xue, Qi-kun ..... TT 29.12, TT 95.3
Xue, Shasha ..... •O 77.7
Xue, Tianhao ..... HL 15.1
Y. Gao, Frank ..... O 49.5
Yada, Keiji ..... TT 98.5
Yadav, Anita ..... •MA 18.3, •TT 30.3
Yadav, C. S. ..... MA 31.5, TT 47.5
Yadav, Khushboo ..... O 9.6
Yadav, Mahesh . •BP 39.6, •CPP 55.6
Yadav, Pooja ..... •BP 27.9, BP 36.5, DY 57.5
Yadav, Rahul ..... •CPP 17.2
Yadav, Sonam ..... DS 21.3
Yadav, Vijay Bahadur ..... •O 10.4, •TT 16.4
Yagmur, Ahmet ..... DS 4.2
Yakhou, Flora ..... MA 33.11
Yakovlev, Dmitri ..... HL 49.3
Yalim, Anja ..... O 7.5, TT 9.5
Yam, Wun Kwan ..... QI 14.7, QI 14.8, •QI 18.2
Yamada, Rinsuke ..... MA 54.1
Yamada, Toyo Kazu ..•O 64.7, O 72.2, TT 67.2
Yamakawa, Kohtaro ..... FM 10.5
Yamakawa, Youichi ..... FM 9.5
Yamamoto, Isamu ..... O 64.5
Yamamoto, Kei ..... MA 9.5, MA 9.10
Yamamoto, Rikako . MA 6.4, MA 7.61, •MA 8.13
Yamamoto, Sh. .... MA 23.5, TT 35.5
Yamamoto, Shingo ..... MA 52.27
Yamashita, Shogo ..... •MA 52.28, MA 52.29
Yamauchi, Kunihiko ..... MA 8.11
Yan, Binghai ..... O 63.11, TT 55.11
Yan, Bixin ..... •FM 23.5
Yan, Hua ..... DY 32.9, TT 45.9
Yan, Mingqi •BP 1.9, •CPP 1.9, •DY 4.9
Yan, Xuzhou ..... DS 16.4
Yan, Yingying ....CPP 4.6, •CPP 16.2, CPP 17.27
Yan, Zewu ..... FM 11.34, FM 18.7
Yanda, Premakumar ..... MM 40.3
Yáñez, Karen ..... BP 26.1, CPP 43.1
Yang, Biaobiao ..... •MM 36.5
Yang, Chia Jung ..... TT 25.1
Yang, Donghai ..... MA 16.9
Yang, Fu ..... O 97.5
Yang, Haiqian ..... BP 27.7
Yang, Hyunsoo ..... MA 6.12
Yang, Ian ..... QI 3.4
Yang, Jiabao . O 42.1, O 70.7, TT 65.7
Yang, Jie ..... TT 69.1
Yang, Jing ..... O 13.3, O 48.1, O 65.7, O 65.9
yang, Jinguang ..... BP 14.13
Yang, Jingzhong ... •HL 31.4, HL 31.4
Yang, Junchun ..... HL 56.1
Yang, Long ..... AKBP 8.8
Yang, Luyi ..... •MA 40.1
Yang, Meng ..... HL 23.8, HL 26.28
Yang, Ming ...•CPP 17.26, CPP 17.29, CPP 17.31, CPP 17.32
Yang, Mingwei •AKPIK 4.4, AKPIK 5.8
Yang, Muyi ..... DS 16.7, DS 20.8
Yang, Qigui ..... FM 11.17
Yang, Qun ..... MA 39.4, •O 9.3
Yang, Rui ..... •MA 7.75, TT 22.22
Yang, Ryan ..... •DS 20.11
Yang, Tao .....•O 95.5, •TT 96.5
Yang, Wei ..... MA 36.12
Yang, Weifeng ..... HL 1.3
Yang, Xiaosheng ..... O 61.1, O 63.9, TT 55.9
Yang, Xingbo ..... BP 10.3, CPP 18.3, DY 18.3
Yang, Yang CPP 3.4, CPP 39.4, O 12.3
Yang, Yiqi ..... •TT 27.2
Yang, Yiwei ..... •SOE 6.3
Yang, Yubo ..... TT 27.2
Yang, Yujia ..... QI 2.6
Yang, Zhao ..... HL 46.1
Yaniv, Omer ..... •MA 40.9
Yao, Fengrui ..... MA 49.2
Yao, Wei ..... O 8.1
Yao, Yugui ..... O 41.4, TT 38.4
Yao, Zhen ..... •CPP 3.4, CPP 39.4
Yaresko, Alexander ..... •MA 11.10, •TT 21.10
Yashwantrao, Priyanka ..... QI 2.1
Yauk, Yale ..... TT 17.8, QI 4.8
Yavilberg, Konstantin ..... QI 11.7
Yazdani, Hossein ..... HL 33.1
Yazdani-Hamid, Meghdad ..•TT 93.9
Yelishala, Sai C. ..... MM 31.2
Yelo-Sarrión, Jesús ..... DY 22.9
Yeltik, Aydan ..... HL 20.1
Yen, Yun •MA 11.7, MA 11.8, MA 38.13, •TT 21.7, TT 21.8
Yershov, Kostiantyn ..... MA 2.11, •MA 20.1
Yettapu, Gurivireddy ..... •HL 52.4
Yevtushynsky, Daniil ..... •O 19.8
Yi, Chang-Hwan .... DY 59.3, TT 99.3
Yi, Changjiang ... DS 20.51, •MM 40.1
Yi, M ..... MA 19.7, TT 31.7
Yi, Minsu ..... •DY 40.2, DY 44.18
Yi, Qinyan ..... •DS 20.52
Yi, Sarah ..... O 56.3
Yifan, Li ..... O 13.5
Yildirim, Berk ..... •FM 4.2, •O 68.3
YILMAZ, Ahmet Hakan .... •FM 19.6, QI 14.12
Yilmaz, Hasan ..... TT 39.6
Yim, Chi Ming ..... •TT 95.1
Yin, C. ..... •MA 3.8
Yin, Hua-Lei ..... HL 31.4
Yin, Rongrong ..... O 34.7
Yin, Sifan ..... •BP 37.11
Yin, Wei-Xiang ..... HL 29.1, TT 58.1
Yin, Yuguo ..... TT 95.3
Yllanes, David ..... •DY 15.5
Yochelis, Shira ....MA 7.66, MA 29.2, TT 46.2
Yogi, Priyanka ..... •TT 23.31, TT 71.1
Yokaichiya, Fabiano ..... TT 57.2
Yokaichiya, Tomoko ..... •DS 14.1
Yokogawa, Gaku ..... O 82.6
Yokota, Hiroko ..... FM 22.8
Yokouchi, Tomoyuki ..... MA 16.6
Yokoyama, Takahiro ..... •CPP 41.1
Yong, Zhihua ..... •DS 20.36
Yoon, Jiho ..... TT 22.2
Yoon, Yeohoon ..... HL 22.3
Yorke, Briony ..... BP 9.6
Yoshida, Hiroyuki ... MA 19.4, O 67.7, O 67.9, •O 82.1, O 82.3, O 82.4, O 82.6, TT 31.4
Yoshida, Suguru ..... FM 22.9
Yoshida, Yasuo ..... O 61.11, •O 64.2
You, Jhih-Shih .... MM 19.24, TT 41.8
You, Mujin ..... •MA 59.9
Youssef, J. B. ..... MA 52.8, MA 59.8
Yu, Boram ..... •BP 14.30
Yu, Chu ..... •MM 19.31
Yu, Guoqiang ..... AKPIK 6.4
Yu, Hongde ..... •MA 36.6, MA 36.7
Yu, Jiabin ..... TT 74.1
Yu, Jisoo ..... O 15.2, O 89.10
Yu, Jusong ..... AKPIK 6.7
Yu, Lebin ..... O 44.7, O 44.9
Yu, Mei ..... QI 14.3, •QI 14.6
Yu, Pengyu ..... BP 37.10
Yu, Sungin ..... BP 9.6
Yu, Tianlun ..... MA 11.8, TT 21.8
Yu, Tonghua ..... •TT 10.7
Yu, Yuan . FM 11.2, FM 11.7, HL 20.65
Yu, Yue ..... •TT 92.1
Yu, Zairan .... •O 55.6, O 81.4, O 88.5
Yuan, Mingyun ..... DS 11.2, HL 11.7, •HL 18.9, •TT 32.9
Yuan, Xiao ..... QI 12.7
Yuan, Yongjie ..... TT 28.7
Yuan, Ziyi ..... FM 18.5
Yücel, Atak Talay ..... QI 12.5
Yücesan, Gündog ..... MA 7.1
Yu-Cheng, Chang ..... TT 97.1
Yüksel, Melih ..... BP 11.11
Yunoki, Seiji ..... QI 5.7
Yurchenko, Sergey ..... •CPP 32.2, •DY 35.2
Yurii, Skourskii ..... TT 94.4
Yuwono, Rio Akbar ..... MM 8.7
Z. Khalid, Muhammad ..... FM 18.8
Zabala, José ..... TT 11.3
Zabila, Yevhen .... MA 49.1, MA 49.6, MA 49.7
Zablotsky, Amir ..... •BP 12.3
Zaburdaev, Vasily ... BP 8.5, BP 14.7, BP 14.9, BP 14.15, BP 14.50, BP 14.61, BP 14.64, BP 14.85, DY 33.3
Zaccarelli, Emanuela ..... CPP 58.5
Zaccone, Alessio ..... MM 41.1
Zachariae, Adrian ..... •BP 8.1
Zacharias, Helmut ..... •CPP 17.11, DS 20.7, O 42.8, O 93.4
Zacharias, Steffen ..... UP 7.5
Zacinskis, Aleksandrs ..... •TT 13.1
Zadoks, Austin ..... •AKPIK 6.7
Zaefferer, Stefan ..... MM 34.5
Zafar, Amina ..... •MM 4.9
Zafari, Shanay ..... BP 7.17, BP 7.18, DY 44.17
Zafra Koch, Sebastian ..... FM 11.33, O 22.2
zaghdoudi, amani ..... •MM 19.23
Zagonel, Luiz F. ..... O 95.6, TT 96.6
Zagrovic, Bojan ..... BP 14.76
Zaharko, Oksana .... MA 3.7, TT 94.3
Zahn, D. ..... MA 27.8
Zahn, D.R.T ..... DS 18.3
Zahn, Daniela ..... MA 7.16
Zahn, Dietrich ..... DS 20.19
Zahn, Dietrich R.T. .... HL 1.4, O 74.9, O 82.5, TT 68.9
Zahn, Manuel .... MA 16.5, •MA 37.9
Zahra, Ali ..... TT 53.6
Zaidi, Fatima Kamal ..... BP 39.1, CPP 55.1
Zaiets, Oleksandr ..... •MA 30.6
Zainab, Zainab ..... •MM 21.6
Zaiser, Michael ..... FM 15.3
Zaitsev, Ignatii ..... HL 38.9
Zajac, Peter ..... HL 26.7, •HL 26.9, HL 26.12
Zajusch, Sarah ..... O 38.6
Zakharov, Vladimir A .O 63.6, TT 55.6
Zalom, Peter ..... TT 85.8
Zaluzhnyy, Ivan .... CPP 48.1, •HL 4.1
Zámbó, Dániel ..... DS 6.4
Zamborlini, Giovanni .. O 61.1, O 69.6, O 83.6
Zamora, Santiago ..... QI 12.6
Zander, Tom ..... DY 9.8
Zandieh, Amirali ..... •BP 14.62
Zangi, Ronen ..... CPP 13.4
Zanker, Sebastian ..... MA 6.8
Zannier, Valentina ..... HL 20.34
Zapata, Nicolas ... TT 22.12, TT 43.6, QI 11.2, QI 11.4, QI 11.5
Zarand, Gergely ... DY 46.10, TT 17.7, TT 41.9, TT 75.10, QI 4.7, •QI 21.9
Zare Pour, Mohammad Amin HL 12.4, HL 26.11
Zarei, Mina ..... SOE 8.4
Zaremba, N. ..... TT 5.9
Zarini, Omid ..... AKBP 10.1
Zarzuela, Ricardo .. MA 2.5, MA 7.53, MA 47.6
Zaumseil, Jana ..... CPP 46.57
Zaunick, Alexander ..... HL 35.5
Zavatta, Alessandro ..... QI 18.1
Zaw, Lin Htoo ..... QI 15.8
Zayko, Sergey ..... MA 27.3
Zech, Paul BP 7.3, BP 14.34, BP 26.6, CPP 43.6
Zecha, Marius ..... UP 3.5
Zechel, Cliona ..... DD 27.3
Zechel, Paul ..... CPP 38.5
Zechlau, Sabrina ..... UP 7.4
Zechner, Christoph ..... BP 12.9
Zeer, Mahmoud .. •MA 51.7, •TT 88.7
Zeeshan, S. ..... BP 27.8, BP 37.2
Zehl, Rico ..... FM 6.7, FM 6.10
Zehner, Jonas ..... MA 57.6
Zeier, Robert ..... QI 10.1, QI 15.1
Zeil, Karl ..... AKBP 5.4, AKBP 6.1, AKBP 6.3, AKBP 7.5, AKBP 8.8
Zeilerbauer, Matthias ..... O 6.6
Zeilinger, Sophie •CPP 23.6, •DY 24.6
Zeininger, Johannes ..... O 85.6
Zeissberger, Matthias .... CPP 46.65
Zeitler, Julian ..... •O 89.5
Zelenka, Moritz ..... O 87.5
Zelenskiy, Andrey CPP 20.2, DY 23.2, •DY 33.6
Zelent, Mateusz ..... •MA 16.11
Zeljkovic, Ilija ..... MA 33.12
Zeller, Genrich ..... •DS 21.10
Zeller, Hanna ..... •TT 82.5
Zeller-Pulmhoff, Berit ..... BP 33.9
Zelsmann, Mark ..... O 74.6, TT 68.6
Zeman, Martin ..... •MA 39.6
Zena, Yared ..... HL 56.4, HL 56.5
Zena, Yared G. ..... HL 55.7
Zeng, Bo-Yue ..... •DS 20.46
Zeng, Xianzhe ..... TT 73.2
Zeng, Zhiyang ..... •MA 4.3
Zengin, Berk FM 11.23, O 44.3, O 44.9
Zeni Cunha, Laura ..... •FM 11.25
Zeppenfeld, Peter ..... DS 21.6, O 4.7
Zerdoumi, Hamza . MA 2.9, •MA 2.12
Zerdoumi, Ridha ..... FM 6.7
Zerefos, Christos ..... UP 3.3, UP 5.2
Zerial, Marino ..... BP 27.3
Zerson, Mario ..... BP 7.3, •BP 14.34, BP 26.6, CPP 43.6
Zerulla, Benedikt ..... DS 21.2
Zettergren, H. ..... TT 22.31
Zeuner, Maurice ..... •AKBP 8.7
Zeuschner, Steffen-P. ..... MA 38.9
Zewdie, Tsedenia ..... DS 9.3
Zgadzaj, Rafal ..... AKBP 10.1
Zhai, Yufeng ...•CPP 15.1, CPP 17.42, CPP 25.4, CPP 46.24
Zhakina, Elina ....MA 6.12, MA 42.11, •MM 40.2, TT 40.1
Zhang, Cheng ..... HL 15.2, O 96.1
Zhang, Chenhui ..... MA 6.12
Zhang, D. ..... TT 69.6
Zhang, Deqing ..... CPP 17.11
Zhang, Ding ..... TT 29.12
Zhang, Dongliang ..... •BP 10.3, •CPP 18.3, •DY 18.3
Zhang, Dongxin ....FM 18.6, TT 69.4, TT 69.5
Zhang, Guo-Xu ..... •O 4.4
Zhang, Hanxu ..... MA 57.1
Zhang, Heda ..... DS 20.51
Zhang, Heng ..... HL 39.8
Zhang, Hongbin .... FM 6.4, •MA 2.9, MA 2.12, MA 8.7, MA 17.1, MA 33.7, MM 13.1, MM 13.2, MM 15.3
Zhang, Hou ..... •MM 19.19
Zhang, Huai ..... MM 21.1
Zhang, Huaide ..... •HL 33.4
Zhang, Huazhang ..... FM 18.2
Zhang, Jiawen .. MM 23.1, •MM 23.2
Zhang, Jiinsheng ..... CPP 44.3
Zhang, Jinsheng CPP 12.4, CPP 44.5
Zhang, Jixi ..... O 34.4
Zhang, Jixing ..... QI 13.5, QI 20.1
Zhang, Jiyao ..... MM 17.1, •MM 21.5
Zhang, Juan ..... •HL 23.5
Zhang, Junyi ..... TT 85.1
Zhang, Kai ..... BP 7.10
Zhang, Kan ..... MM 7.5
Zhang, Ling ..... TT 57.7
Zhang, Lulu ..... •O 39.4
Zhang, Qinghua ..... TT 29.12
Zhang, Ran ..... •AKPIK 6.4
Zhang, Rui ..... •MM 7.5
Zhang, Shaoming ..... MM 9.3
Zhang, Shengming ..... O 45.4
Zhang, Shihao ..... MM 20.1
Zhang, Shiwei ..... TT 27.2
Zhang, Shu ..... MA 40.4
Zhang, Shuai ..... •TT 29.6, TT 52.4
Zhang, Tiantian ..... MA 33.4
Zhang, Tianyi ... CPP 22.3, CPP 25.5
Zhang, Wei ..... MM 31.2
Zhang, Wenhao ..... MM 11.4
Zhang, Xi ..... MM 11.5, MM 19.4, MM 35.6
Zhang, Xianmin ..... MA 27.1
Zhang, Xiao ..... HL 29.1, TT 58.1
Zhang, Xin ..... MA 23.1, TT 35.1
Zhang, Xin H. H. ..... TT 23.28
Zhang, Xue ..... O 99.4
Zhang, Xuejing ..... •TT 3.4, TT 13.5, TT 56.7
Zhang, Y ..... MA 19.7, TT 31.7
Zhang, Yang DS 20.51, TT 3.1, TT 44.2
zhang, yi ..... •O 63.7, •TT 55.7
zhang, yifan ..... •BP 14.88
Zhang, Yiqi ..... •O 77.2
Zhang, Yiteng .. •DS 20.21, HL 20.45, HL 20.50, HL 20.51, HL 55.10
Zhang, Yu ..... O 66.8, O 76.5
Zhang, Yuan ..... HL 4.7
Zhang, Yuan-Shan ..... TT 49.3
Zhang, Yufan ..... •MM 25.5
Zhang, Yuhao ..... •AKPIK 2.1
Zhang, Yuna ..... BP 21.5
Zhang, Yuqi ..... O 41.4, TT 38.4
zhang, yuwei ..... FM 5.2
Zhang, Yuyang ..... •O 28.8
Zhang, Zhijia ..... •MA 30.4
Zhang, Zichun ..... TT 95.3
Zhang, Ziyan ..... •MM 19.16
Zhao, Bo ..... •MA 8.7, MA 33.7
Zhao, Dongming .. •TT 4.10, TT 93.15
Zhao, Fangzhou ..... •HL 35.2
Zhao, Huan ..... O 48.1
Zhao, Huaping ..... CPP 4.5, FM 5.1, MM 4.8

zhao, jinchen ..... DY 19.3
Zhao, Jingtian ..... FM 12.9
Zhao, Kan ..... MA 37.9
Zhao, Khan ..... MA 23.2, TT 35.2
Zhao, Lanqing ..... •FM 5.1
Zhao, Lingxiao ..... O 63.2, TT 55.2
Zhao, Meng ..... FM 15.1
Zhao, Pai ..... DS 20.10
Zhao, Pengfei ..... O 45.4
Zhao, Qiang ..... CPP 28.1, DY 29.1
Zhao, Shiheng .. •CPP 20.6, •DY 23.6
Zhao, Shuo ..... •MM 31.5
Zhao, Suocheng ..... •QI 17.3
Zhao, Tonghan ..... HL 4.5
Zhao, Weisheng ..... O 64.9
Zhao, Xinne ..... FM 6.11
Zhao, Xizhu ..... •DY 7.5
Zhao, Yijun ..... •CPP 46.26
Zhao, Yuchen .... •MA 6.12, MA 7.36, TT 40.1
Zhao, Yue ..... FM 6.4
Zhao, Yujun ..... FM 5.8, MM 11.1, •MM 34.5, MM 39.6
Zhao, Zhe ..... QI 13.5
Zhao, Zhiying ..... TT 23.14
Zharnikov, Michael . •O 45.2, •O 46.11
Zheng, Boyang ..... O 33.3
Zheng, Feifei ... CPP 31.4, CPP 46.12
Zheng, Fengshan ..... MA 16.9
Zheng, Hao . O 77.7, TT 14.11, TT 85.1, TT 93.2
Zheng, Jueting ..... TT 90.6
Zheng, Mingqian ..... O 41.4, TT 38.4
Zheng, Tianle .... CPP 4.6, CPP 17.32
Zheng, Xian ..... HL 20.51, •HL 26.30
Zheng, Yating .... •BP 36.9, CPP 11.7, DY 17.7, •DY 57.9
Zheng, Zejie ..... AKPIK 6.4
Zherebtsov, Sergey ..... HL 8.4
Zherlitsyn, S. ..... MA 23.5, TT 25.6, TT 35.5
Zherlitsyn, Sergei .... MA 2.6, MA 9.1, MA 23.4, TT 35.4
Zhia, Yufeng ..... CPP 58.2
Zhiang, Zhihao ..... O 95.11, TT 96.11
Zhong, Bo-Yi ..... •O 55.7
Zhong, Qigang ... O 3.1, O 8.4, O 58.1
Zhong, Xiu ..... •O 97.5
Zhong, Yu-Jie ..... HL 20.55
Zhou, Benjamin ..... O 84.9, TT 84.9
Zhou, Chao ..... DY 45.4, SOE 14.4
Zhou, D. ..... TT 80.6
Zhou, Daniel .... •BP 10.9, •CPP 18.9, •DY 18.9
Zhou, Di ..... TT 80.8
Zhou, Hangyu ..... O 64.9
Zhou, Jin-Jian .. O 7.2, O 41.4, TT 9.2, TT 38.4
Zhou, Jinyi ..... •O 81.7
Zhou, Jungui .... CPP 15.1, CPP 17.15
Zhou, Kai ..... BP 11.5
Zhou, Leqi ..... •QI 14.26
Zhou, Ping .... O 59.5, O 71.1, O 71.18, TT 48.5, TT 66.1, TT 66.18
Zhou, Qi ..... CPP 23.2, CPP 23.4, DY 24.2, DY 24.4
Zhou, Rui ..... TT 69.1
Zhou, S. ..... MA 3.8
Zhou, Shengqiang HL 17.5, HL 20.22, HL 56.1, •MA 43.1
Zhou, Shiyu ..... MA 16.3
Zhou, Shuyun ..... •SYFC 1.3
Zhou, Xin ..... HL 15.4
Zhou, Xinyu ..... TT 29.12, TT 95.3
Zhou, XuanKai ..... QI 20.3, •QI 20.4
Zhou, Xuyang ..... MM 15.4
Zhou, Yishui MA 5.8, MA 47.10, O 2.2, TT 7.8
Zhou, Yuan ..... SYBS 1.5
Zhou, Yuean ..... •MA 55.2
Zhou, Zheng ..... TT 2.11
Zhu, Changqing ..... TT 41.2
Zhu, Chenglian ..... HL 20.49
Zhu, D. ..... MA 25.6
Zhu, Diling ..... HL 8.6
Zhu, J-X ..... MA 19.7, TT 31.7
Zhu, Kai ..... HL 46.1
Zhu, Ruidan ..... •HL 26.55
Zhu, Senyin ..... •MA 57.1
Zhu, Xiangzhou ..... •HL 8.2, MM 9.5
Zhu, Yinghao ..... •MA 7.6, MA 47.10
Zhu, Yu ..... MA 54.3
Zhu, Yuanran ..... DY 6.10
Zhu, Yunxuan ..... MM 31.2
Zhuang, Zhaotong ..... TT 52.4
Zhugayevych, Andriy ..... •CPP 53.3
Zhumagulov, Yaroslav ..... MA 35.9, TT 60.9
Zhuromskyy, Paul ..... DS 20.24
Zibrov, Mikhail ..... MM 7.7
Zick, Isabell .... •CPP 19.3, CPP 46.1, •DY 20.3
Zid, Amina ..... •HL 38.11
Ziebert, Falko ..... BP 1.4, BP 12.7, BP 14.21, BP 30.3, CPP 1.4, CPP 11.4, CPP 47.3, CPP 49.4, DY 4.4, DY 17.4, DY 44.5, DY 49.6
Ziefuß, Anna ..... MA 50.5
Ziefuss, Anna ..... MA 13.7
Ziegele, Lutz ..... TT 22.32
Zieger, Luise ..... BP 37.8
Ziegler, Andreas ..... O 94.5
Ziegler, Christiane .... O 61.7, O 83.10
Ziegler, Jonas ..... HL 3.7
Ziegler, Mario ..... TT 93.6
Ziegler, Melanie ..... TT 28.8
Ziegler, Tim ..... AKBP 5.4
Ziehmer, Markus ..... MM 30.3
Zielinski, Przemyslaw ..... MA 23.1, TT 35.1
Ziener, Ulrich ..... TT 92.4
Zier, Maximilian ..... •AKPIK 4.3
Zier, Tobias ..... •MM 37.3
Zierenberg, Johannes ..... DY 15.2
Zierold, Robert .... BP 26.8, BP 26.10, CPP 43.8, CPP 43.10, DS 16.3, •DS 20.10, FM 11.26, FM 11.29, O 71.19, TT 66.19, AKBP 9.2
Zieske, Katja .... •BP 26.9, •CPP 43.9
Ziethen, Noah ... •BP 10.8, •CPP 18.8, DY 15.7, •DY 18.8
Zihlmann, Simon ..... QI 2.10
Zijderveld, Johanna ..... •TT 74.8
Zilker, Bianca ..... UP 6.2
Ziller, Steffen ..... DS 20.28
Zimmer, David Noel ..... •BP 4.2
Zimmer, Joanne CPP 26.4, CPP 46.11, •CPP 49.5
Zimmer, Patrick ..... •BP 7.54
Zimmermann, Leonard K.S. . •HL 11.6
Zimmermann, Paul ..... CPP 48.1
Zimmermann, Richard ..... HL 55.11
Zimmermann, Sebastian .... •DS 4.3
Zimmermann, T. ..... AKBP 1.1
Zimmermann, Wolfram ..... BP 7.43
Zinchenko, Vadim ..... UP 5.4
Zinke, Gregor ..... MA 54.8, •O 14.2, O 40.16, TT 37.16
Ziolkowski, Franziska ..... •MA 38.11, MA 38.12
Zippo, Emanuele •BP 29.6, •CPP 45.6
Zirkelbach, Johannes ..... AKBP 8.7
Zisiadis, Konstantin ..... •CPP 12.2
Žitko, Rok ..... TT 22.6
Zitong, Liu ..... CPP 17.11
Zitzmann, Jasmin ..... HL 12.2
Zobač, Ondřej ..... MM 8.10
Zobel, Hendik ..... •AKPIK 3.3
Zoellner, Marvin Hartwig .... HL 38.9
Zojer, Egbert ... MM 19.36, MM 22.5, MM 31.4
Zojer, Karin ..... •CPP 6.4
Zok, Tomasz ..... BP 14.54
Zollinger, Julien ..... MM 21.1
Zöllner, J. ..... HL 17.7
Zöllner, Johann ..... •HL 17.3
Zollner, Klaus ..... DS 12.2
Zöllner, M. ..... HL 17.7
Zollner, Stefan ..... •DS 21.3, DS 21.7
Zolthoff, Philipp ..... •BP 14.22
Zoltner, Kassandra ..... O 8.7, O 31.5, O 35.4, •O 35.5
Žonda, Martin ..... TT 85.3
Zong, Han ..... TT 29.11
Zopf, Michael ... DS 20.21, HL 20.45, HL 20.49, HL 20.50, HL 20.51, HL 26.30, HL 31.4, HL 55.10
Zou, Ji ..... TT 74.12
Zou, Ke ..... DS 6.2
Zozoulenko, Igor ..... HL 53.6
Zscharschuch, Jens HL 18.4, HL 47.3, TT 32.4
Zschech, Ehrenfried ..... CPP 16.4
Zscherp, Mario F. .. HL 26.3, HL 42.2, HL 45.3
Zschetzsche, Lilith ..... QI 1.1, •QI 1.2
Zschornak, Matthias ..... FM 12.8, FM 23.6
Zu, Fengshuo ..... HL 4.7
Zucal, Giulio ..... •DY 15.9
Zugayevych, Andriy ..... CPP 57.2
Žukauskaite, Agne ..... MA 52.11
Zullo, Ludovica ... DS 12.4, •HL 24.10, TT 49.4
Zundel, Fabian ..... BP 9.1
Zuñiga-Puelles, Esteban ..... FM 9.3, •MM 19.46
Zuo, Guangzheng ..... CPP 37.2
Zuo, Ruixin ..... HL 1.3
Zuo, Shengnan ..... HL 4.7
zur Horst, Laura ..... O 77.4
Zurbriggen, David ..... O 44.15
Zverev, Vladimir ..... •DY 44.22
Zvezdin, Anatoly ..... MA 30.3
Zvyagin, Sergei .... MA 19.6, TT 31.6, TT 98.1
Zvyagin, Sergey ..... TT 94.6
Zwedie, Tsedenia ..... DS 8.1
Zweng, Ludwig ..... TT 51.7, •TT 53.3
Zwicker, David ..... BP 7.6, BP 14.84, BP 14.87, BP 14.95, BP 29.2, BP 32.1, BP 32.2, CPP 10.4, CPP 45.2, DY 16.4, DY 33.2, •DY 33.4, DY 49.2, DY 52.1, DY 52.2
Zwicknagl, G. ..... TT 25.6
Zwicknagl, Gertrud ..... HL 17.6
Zyczkowski, Karol ..... QI 9.4
Zykov, Vladimir ..... DY 22.1
Zysman-Colman, Eli ..... CPP 17.17
Zyuzin, Alexander ..... TT 83.4

Index of Exhibitors Dresden 2026

Exhibition venue:

Technische Universität Dresden, Campus Südvorstadt, 01069 Dresden

- Tent A — Bergstraße 64
- Tent C — Mommsenstraße (opposite of 'Alte Mensa')

Exhibition opening hours:

Tuesday, 10 March	09:30 — 18:00
Wednesday, 11 March	09:30 — 18:00
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Action Park Estate, London, W3 7QE, United Kingdom

Magnet systems.

CryoVac GmbH & Co. KG Tent A A85

Langbaurghstraße 13, 53842 Troisdorf

Helium-, Bad- und Verdampferkryostate, Temperaturmess- und Regelgeräte.

ctd.qmat Exzellenzcluster Tent A A78

01062 Dresden

Quantum Alliance.

D.I.S. Germany GmbH Tent A A56

Lohmener Straße 13 d, 01796 Pirna

Electron and Ion Beam Technology | Ultra-High Precision Manufacturing.

Deutsche Forschungsgemeinschaft (DFG) Tent A A49

53170 Bonn

Information und Beratung zu den Förderprogrammen der DFG.

DFG Cluster of Excellence — Physics of Life (PoL) Tent C C19

Arnoldstraße 18, 01307 Dresden

PoL is an international research center at TU Dresden combing physics, biology, and computer science to explore the physical laws behind the organization of life into molecules, cells, and tissues.

Dr. Eberl MBE-Komponenten GmbH Tent A A70

Josef-Beyerle-Straße 18/1, 71263 Weil der Stadt

MBE systems for III/V, IV/VI, oxide and SiGe semiconductors, effusion cells and sublimation sources, electron beam evaporators and customized vacuum components.

Edwards GmbH Tent A A61

Philipp-Hauck-Straße 2, 85622 Feldkirchen

Vakuumsysteme und Vakuumpumpen.

Entropy GmbH Tent A A75

Gmunder Straße 37 a, 81379 München

Entropy GmbH is a cryostat manufacturer based in Munich, Germany. The product range offers various types of closed-cycle cryostats for the temperature range of Kelvin and Millikelvin.

Excelitas Deutschland GmbH Tent A A36

Hans-Riedl-Straße 9, 85622 Feldkirchen (München)

Excelitas ist ein führender Anbieter von fortschrittlichen, lebensbereichernden Technologien und beliefert internationale Marktführer in den Bereichen Life Sciences, Advanced Industrial, Halbleiter der nächsten Generation und Avionik.

FAIRmat c/o Humboldt-Universität zu Berlin Tent A A50

Zum Großen Windkanal 2, 12489 Berlin

FAIRe Dateninfrastruktur für die Physik der kondensierten Materie und die Chemische Physik von Stoffen.

FEMTO Messtechnik GmbH Tent A A22

Klosterstraße 64, 10179 Berlin

Rauscharme Signalverstärker, Kompakte Lock-In Verstärkermodule, Empfindliche Photoreceiver.

Fermiologics Tent A A25

George-Bähr-Straße 20, 01069 Dresden

ARPES analyzers, cryomanipulators, complete systems.

Ferrotec Europe GmbH Tent C C23

Seerosenstraße 1, 72669 Unterensingen

Ferrotec provides customers with manufacturing products and materials for semiconductor, electronics and high-power applications. EB-PVD equipment, Peltier modules and cooling units will be displayed.

Forschungszentrum Jülich GmbH Tent A A82

Wilhelm-Jonen-Straße, 52425 Jülich

The ER-C provides industry and academia access to advanced electron microscopy, state-of-the-art TEMs, and professional scientific support.

Goodfellow GmbH Tent A A53

Postfach 13 43, 61213 Bad Nauheim

Materialien in kleinen Mengen für Entwicklung und Forschung.

GVL Cryoengineering Dr. George V. Lecomte GmbH Tent A A80

Aachener Straße 89, 52223 Stolberg

Mischkryostate, kryotechnisches Zubehör.

Hamamatsu Photonics Deutschland GmbH Tent A A79

Arzbergerstraße 10, 82211 Herrsching

HAMAMATSU PHOTONICS Deutschland GmbH; our capabilities are rooted in photonics technology including optics, electronics, mechanics and software.

Helmholtz-Zentrum Dresden-Rossendorf e. V. (HZDRI) Hochfeld-Magnetlabor Dresden (HLD) Tent A A26

Bautzner Landstraße 400, 01328 Dresden

Tensormeter, Tiefsttemperatur-Probenhalter ROTAX, Portable Pulsed Micro Magnetometer PPMM, Terahertz-Antenne.

HORIBA Jobin Yvon GmbH Tent A A09

Hans-Mess-Straße 6, 61440 Oberursel

Ihr Partner für instrumentelle Analytik und innovative Spektroskopie.

Hositrad Deutschland Tent A A10

Lindnergasse 2, 93047 Regensburg

CF, KF, ISO, UHV-Vakuumbauteile, Elektrische Durchführungen, Membranbalgen, Special Products.

Hübner Photonics Tent A A67

Heinrich-Hertz-Straße 2, 34123 Kassel

Lasers

ICEoxford Tent C C11

Avenue 4, Station Lane, Witney, Oxon, OX28 4BN, United Kingdom

High Performance Cryogenic Systems.

Incienta Technologie GmbH Tent A A14

Pommernstraße 22, 63110 Rodgau-Weiskirchen

Closed Cycle Cryostats, Helium Flow Cryostats, Cryogenic Probe Stations, Piezo- & Ferro-electric Test Systems, UHV Components, Thin Film Deposition, Hot-plates, Wire Bonder, Die Bonder.

ISEG Spezialelektronik GmbH Tent A A55

Bautzner Landstraße 23, 01454 Radeberg / Rossendorf

Hochspannungsversorgungen, Hochspannungsnetzgeräte, HV-DC/DC- Konverter.

JUST VACUUM GmbH Tent A A31

Daimlerstraße 17, 66849 Landstuhl

Vakuumtechnik

Kleindiek Nanotechnik GmbH Tent A A60

Aspenhaustraße 25, 72770 Reutlingen

Nanoprobing und Nanomanipulation in SEM, FIB-SEM, UHV.

Korvus Technology Ltd. Kings Grove Tent A A84

Kings Grove, Maidenhead SL6 4DP, United Kingdom

Highly Modular PVD System for Depositing Thin Films.

Kurt J. Lesker Company GmbH Tent C C10

Fritz-Schreiter-Straße 18, 01259 Dresden

Kurt J. Lesker Company provides high-quality vacuum equipment and services for LEDs, optics, electronics, coatings, R&D, and advanced vacuum solutions worldwide.

Leybold GmbH Tent C C17

Bonner Straße 498, 50968 Köln

Vakuumpumpen

magnitude GmbH Tent A A13

Bahnhofstraße 21, 85737 Ismaning

Our product portfolio combines proven SC magnet technology with modern design optimization, offering both standard configurations and tailor-made solutions for demanding experimental needs.

MaTeck — Material-Technologie & Kristalle GmbH Tent A A40

Im Langenbroich 20, 52428 Jülich

Einkristalle, Sputtertargets, Substrate, hochreine Materialien, Isotope, Halbleiterkristalle.

Menlo Systems GmbH Tent A A02

Bunsenstraße 5, 82152 Martinsried

Frequency Combs, Quantum Systems, Ultrastable Lasers, FS Lasers, THz Systems.

Munich Quantum Valley Tent A A71

Leopoldstraße 244, 80807 München

Munich Quantum Valley promotes quantum science and quantum technologies in Bavaria and offers various research positions, especially in connection to quantum computing.

NanoMagnetics Instruments Ltd. Suite 290 Tent A A28

266 Banbury Road, Oxford OX2 7DL, United Kingdom

NanoMagnetics Instruments, Producer of Scanning Hall Probe Microscope and Atomic Force Microscope.

nanoscore tech GmbH Tent A A48

Zum Greifenstein 5, 65594 Runkel

European distributor for Unisoku instruments.

Nanosurf GmbH Tent A A43

Rheinstraße 5, 63225 Langen

Atomic Force Microscopes, AFM, Scanning Probe Microscopes, SPM, Rasterkraftmikroskope.

Onnes Technologies B.V. Tent A A72

Kenauweg 21, 2331 BA Leiden, Niederlande

mK SPM, EC-STM, Cryogenic Nanopositioners, Cryogenic Vibration Isolation.

Park Systems Europe GmbH Tent A A21+A33

Schildkrötstraße 15, 68199 Mannheim

Atomic Force Microscopy, Imaging Spectroscopic, Ellipsometry, Anti Vibration Isolation.

Pfeiffer Vacuum GmbH Tent A A19+A20

Berliner Straße 43, 35614 Asslar

With our product portfolio, we offer solutions for all vacuum applications. We are not only driven by highest quality standards. It is our vision to be the most sustainable and fastest growing market player to drive technology for a sustainable future.

PINK GmbH Vakuumtechnik Tent A A17

Gyula-Horn-Straße 20, 97877 Wertheim

Vakuum- und UHV-Kammern, Beschleunigerkomponenten, vakuumtechnische Anlagen und Systeme, Manipulatoren.

PREVAC Sp. z o.o. Tent A A08

Raciborska 61, 44-362 Rogow, Poland

PREVAC develops and delivers advanced HV and UHV vacuum systems, components and research equipment designed for scientific applications and high-technology industries.

pureions GmbH Tent A A34

Zeppelinstraße 16, 82205 Gilching

Mass selected ion beam deposition systems for STM, AFM and components. Electrospray (ESI), clusters, ion guides, mass spectrometers, quadrupoles, ion traps, Paul traps, digital square wave RF supplies.

Qlibri GmbH Tent A A18

Karlsplatz 3, 80335 München

Ultra-sensitive absorption microscopes for hyperspectral imaging, fiber-based micromirrors, and quantum optics platforms at ambient and cryogenic temperatures.

Qnity SAS Tent A A05

42 bis rue Théodore de Banville, 91120 Palaiseau, France

Quantum hardware

Quano Technologies Limited Tent A A58

Unit 1017-8, 10/F, Bldg. 19W, 19 Science Park West Avenue, HK Science Park, Pak Shek Kok, NT, HONGKONG

Quano.X (horizontal stage), Quano.Z (vertical stage), Quano.R (rotational stage), Quano.XYZ (three-axes stage), Specialty fasteners, Nuts, Sapphire Crystals, Control Electronics.

QuantaMap Tent A A46

Robert Boyleweg 4, 2333CG Leiden, Niederlande

SQUID-AFM microscopes for material science and quantum devices.

Quantum Design GmbH Tent A A03+A04

Breitwieserweg 9, 64319 Pfungstadt

Quantum Design will exhibit systems and components for magnetometry, cryogenic, electric measurements, spectroscopy and material science.

Quantum Design Oxford Tent A A11

Tubney Woods, Abingdon, Oxon OX13 5QX, United Kingdom

Quantum Design Oxford (previously Oxford Instruments NanoScience) provides leading solutions in low temperature measurement for materials physics and quantum technologies, with open-architecture superconducting magnet measurement systems and Cryofree® dilution refrigerators.

Qzabre Tent A A15

Neunbrunnenstrasse 50, 8050 Zurich, Schweiz

We offer high-precision scientific instruments: NV scanning tips with unprecedented sensitivity, quantum scanning microscopes for nanoscale magnetometry and a hands-on educational kit for teaching.

Raith GmbH Tent C C09

Konrad-Adenauer-Allee 8, 44263 Dortmund

Elektronenstrahl-Lithography, Ionenstrahl-Lithography, Nano-Engineering, CAD-Navigation.

Rohde & Schwarz GmbH Tent A A23+A24

Mühldorfstrasse 15 81671 München

Munich based Rohde & Schwarz is striving for a safer and connected world with its Test & Measurement, Technology Systems and Networks & Cybersecurity Divisions, pushing technical boundaries.

SAES Getters S.p.A. Tent A A62

Viale Italia, 77, 20020 Lainate (Milan), Italy

UHV NEG-Pumpen, Alkalimetall-Dispenser, Hochvakuumpumpen, Getter.

Schaefer Technologie GmbH Tent A A27

Robert-Bosch-Straße 31, 63225 Langen

Scanning Probe Microscopy (UHV, Cryo, Ambient, Liquid), NV-vacancy Magnetometer, High-Resolution Capacitance Bridge

Schäfter + Kirchhoff GmbH Optics, Metrology and Photonics Tent A A35

Kieler Straße 212, 22525 Hamburg

Polarization-maintaning fiber optic components including laser beam coupler, fiber collimators, fiber cables, polarization analyzers and fiber port clusters.

Scienta Omicron GmbH Tent A A16

Limburger Straße 75, 65232 Taunusstein

Surface Science Tools, Electron Spectroscopy, SPM and MBE.

SEKELS GmbH Tent A A83

Dieselstraße 6, 61239 Ober-Mörlen

Magnetwerkstoffe, Magnetische Abschirmungen, Magnetsysteme, Induktive Bauelemente, Magnetische Messtechnik.

SENTECH Instruments GmbH Tent A A68

Schwarzschildstraße 2, 12489 Berlin

Plasma-Prozess-Technologie (Anlagen für RIE / ALE / PECVD / ALD) & Dünnschichtmesstechnik (Messgeräte auf Basis Reflektometrie / Ellipsometrie).

SI Scientific Instruments GmbH Tent C C07

Römerstraße 67, 82205 Gilching

Rekonfigurierbare Messtechnik, Lock-In Verstärker, Gas- & Vakuummesstechnik, Mikropositionierer mit Piezoträgheitsantrieb & Schrittmotor, Piezo- & Schrittmotorsteuerungen.

Silent Waves Tent A A63

69-73 Rue Félix Esclangon, 38000 Grenoble, France

Superconducting ultra-low noise amplifiers.

SmarAct GmbH Tent A A38

Schütte-Lanz-Straße 9, 26135 Oldenburg

High precision positioning and metrology solutions.

SPECS Surface Nano Analysis GmbH Tent A A41+A42

Voltastraße 5, 13355 Berlin

Photoelectron Spectroscopy (ESCA/XPS,HAXPES), Scanning Probe Microscopy (SPM), Angel-resolved Photoemission Spectroscopy (ARPES), Momentum Microscopy (MM), Electron Microscopy (LEEM/PEEM).

Springer-Verlag GmbH Tent A A44

Europaplatz 3, 69115 Heidelberg

Springer ist ein weltweit führender Wissenschaftsverlag, der wissenschaftliche Bücher und Zeitschriften für Forschende an Universitäten, Forschungseinrichtungen und Unter nehmen anbietet.

Staib Instrumente GmbH Tent A A54

Hagenaustraße 22, 85416 Langenbach

RHEED, TorrRHEED, in-situ AugerProbe, AUGER, AES, XPS, UPS, EELS, electron sources, ion sources.

STS Elionix Tent C C13

118 Cedar Street Wellesley Hills, MA 02481, USA

Electron Beam Lithography Systems

Sumitomo (SHI) Cryogenics of Europe GmbH Tent A A12

Daimlerweg 5 a, 64293 Darmstadt

Cryocoolers: @4K: GMJT (9watt); RDK-101D(L); RDE-412D4; RDK-415D2; RDE-418D4; RP-062B2(S); RP-082B2(S); RP-182B2S @10K: CH-204; CH-210 @20K: RDK-500B2 @77K: CH-110; CH-160D2; New compressor: E77A.

Surface Concept GmbH Tent A A51+A52

Am Sägewerk 23 a, 55124 Mainz

Detector Technics, Momentum Microscopes, Cameras, Fast Time-Resolving Electronics.

SweepMe! GmbH Tent A A74

Bienertstraße 18, 01187 Dresden

SweepMe! automatisiert Messungen mit einer modularen Softwareplattform. Geräte verschiedener Hersteller einfach integrieren und komplexe Abläufe ohne Programmierkenntnisse erstellen.

Technische Universität München Forschungs-Neutronenquelle Tent A A45

Lichtenbergstraße 1, 85747 Garching

As a cooperation between TU München, Forschungszentrum Jülich, and Helmholtz-Zentrum hereon, the Heinz Maier-Leibnitz Zentrum is a user facility for cutting-edge research with neutrons and positrons.

THORLABS GmbH Tent A A06+A07

Münchner Weg 1, 85232 Bergkirchen

Optische & optomechanische Komponenten, Test & Measurement Systeme, optische Tische und Vibrationskontrolle, Nanopositionierungen, Lichtquellen sowie Imaging, Mikroskopie und Life Science Komponenten.

TransMIT GmbH Tent A A76

Kerkrader Straße 3, 35394 Gießen

Pulse Tube Cryocoolers and Cryocooler Systems.

Wiley-VCH GmbH — Jobbörse Tent A A86

Boschstraße 12, 69469 Weinheim

Präsenz-Jobbörse von Dienstag, den 10. März bis Donnerstag, den 12. März 2026.

Wiley-VCH GmbH Tent A A87

Boschstraße 12, 69469 Weinheim

Verlag, Fachzeitschriften, Fachbücher.

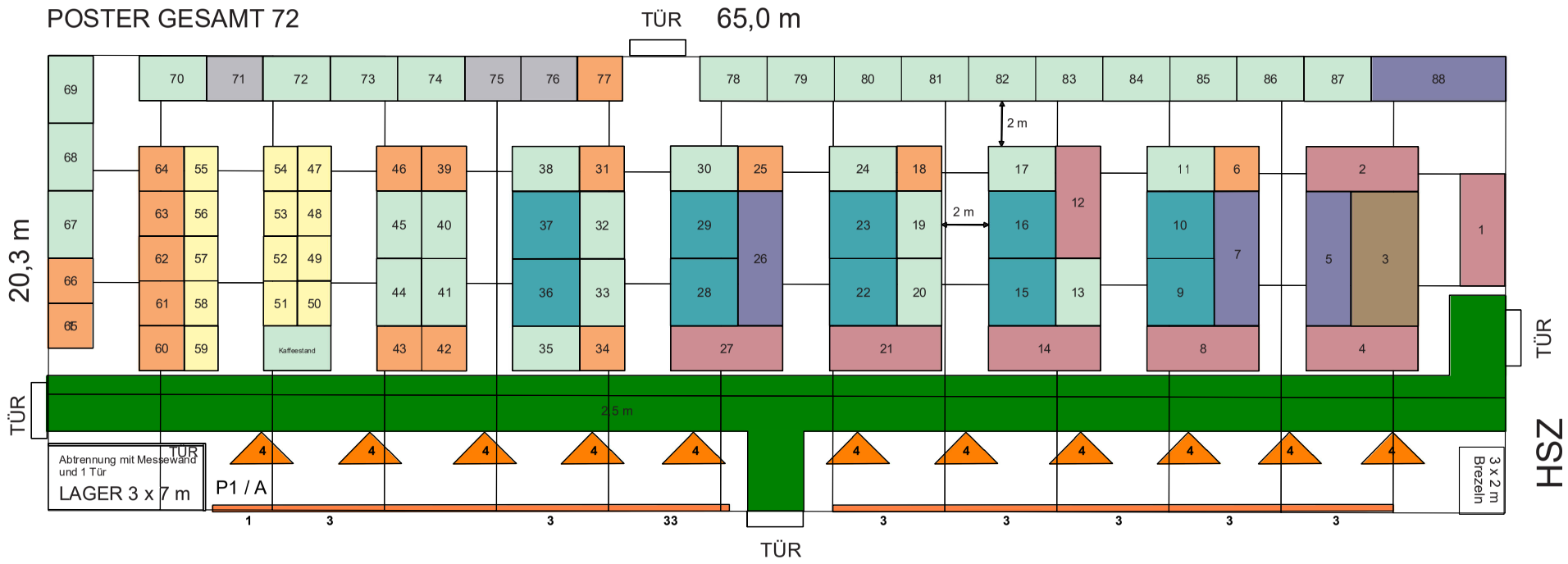
Zurich Instruments Germany GmbH Tent A A23+A24

Mühldorfstraße 15, 81671 München

Test & Measurement, Lock-in Amplifiers, Impedance Analysis, Quantum Computing Control System, Quantum Sensing.

Exhibition / Poster Map TENT A

Stand: 08.12.2025



Betonauflastung

3 x 2 m Brezeln

4 Posterflächen_ soweit möglich alle als Innenraum-Nutzung für Ablage

1	Stand 3m² 2 x 1,5 m
2	Stand 4m² 2 x 2 m
3	Stand 5m² 2,5 x 2 m
4	Stand 6m² 3 x 2 m
5	Stand 9m² 3 x 3 m
6	Stand 10m² 5 x 2 m
7	Stand 12m² 6 x 2 m
8	Stand 18m² 6 x 3 m

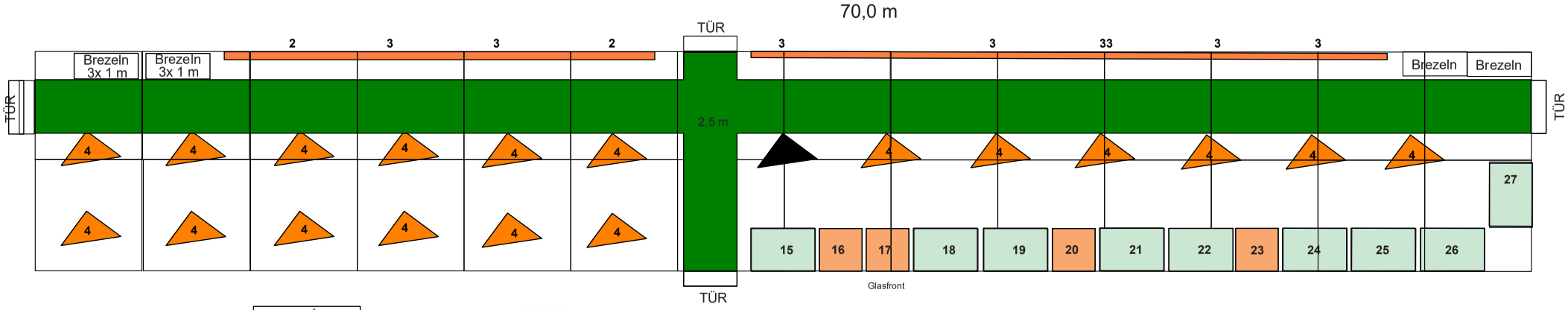
WEIßBACH VERANSTALTUNGSSERVICE

1010

Exhibition / Poster Map TENT C

Stand:05.01.2026

POSTER GESAMT 100



4 Posterflächen_
soweit möglich alle als
Innenraum-Nutzung
für Ablage

Stand 4m²
2 x 2 m

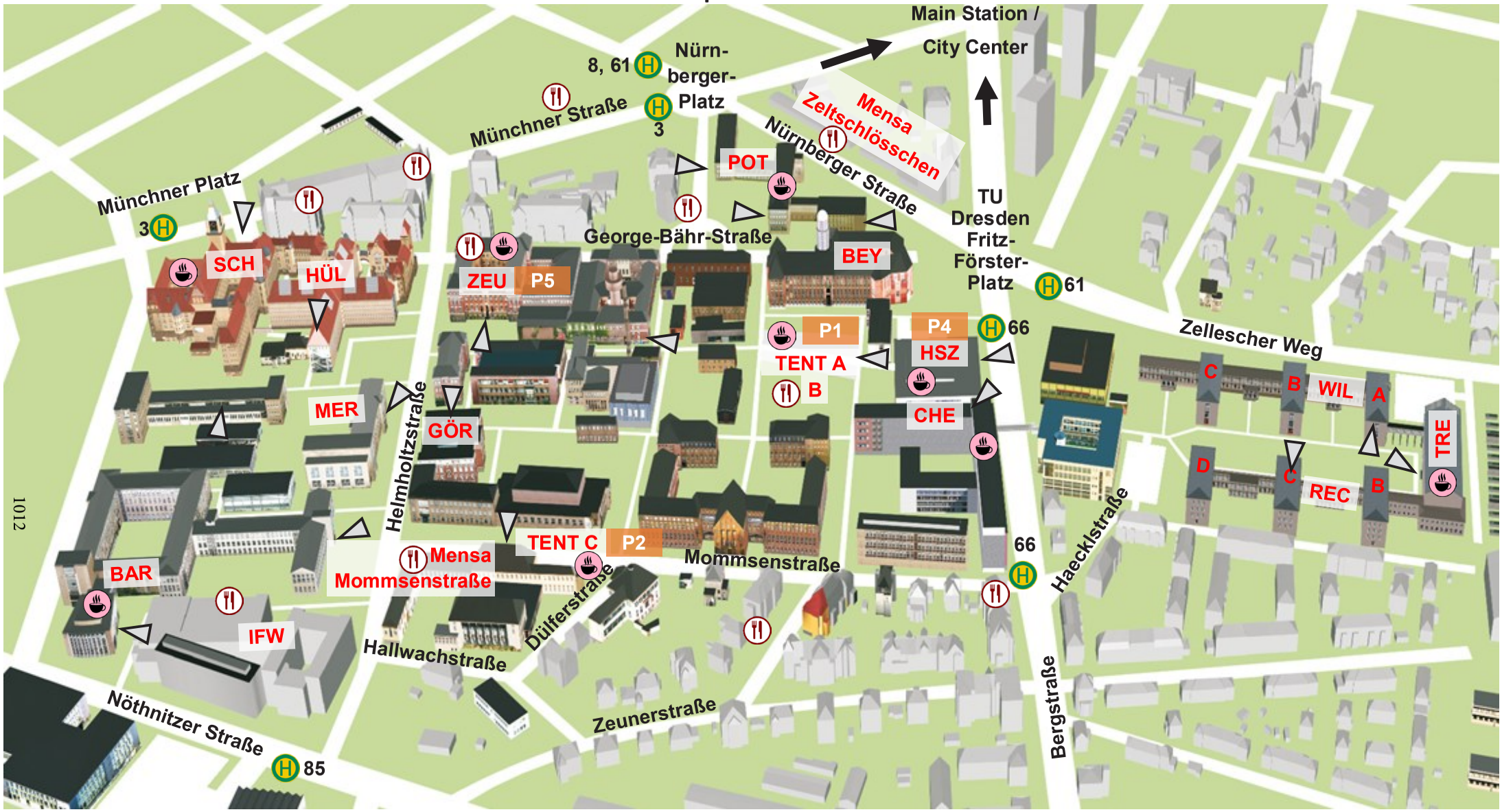
Stand 6m²
3 x 2 m

3 x 2 m
Brezeln

MENSA

WEIßBACH
VERANSTALTUNGSSERVICE

Map SKM 2026



HSZ Lecture hall name (abbreviation)
https.//navigator.tu-dresden.de

Entrance

Coffee

Mensa, Snacks

Tram or bus stop with number

BAR	Barkhausen-Bau
BEY	Beyer-Bau
CHE	Chemiegebäude
GÖR	Görges-Bau
HSZ	Hörsaalzentrum (Lecture Hall Center), Conference office, Plenary talks, Symposia, Tutorials, Einstein Slam, Evening talk, Job market, Coffee station, P4
HÜL	Hülsse-Bau
MER	Merkel-Bau
POT	Gerhard-Potthoff-Bau
REC	Recknagel-Bau
SCH	Georg-Schumann-Bau
TRE	Trefftz-Bau
Tent A, B, C	Poster P1, P2 Exhibition & Coffee, Snacks
WIL	Willers-Bau
ZEU	Zeuner-Bau, P5

Timetable

Start	Sunday, March 8	Monday, March 9	Tuesday, March 10	Wednesday, March 11	Thursday, March 12	Friday, March 13
08:15						
08:30		Plenary Talk (HSZ/AUDI)	Plenary Talk (HSZ/AUDI)	Plenary Talk (HSZ/AUDI)	Plenary Talk (HSZ/AUDI)	Plenary Talk (HSZ/AUDI)
08:45						
09:00						
09:15						
09:30		SYFC (HSZ/AUDI)	SYBS (HSZ/AUDI)	SYBT (HSZ/AUDI)	SYAI (HSZ/AUDI)	SYQF (HSZ/AUDI)
09:45		SKM Diss. Prize Symp. (SYSD) (HSZ/0002)				
10:00						
10:15						
10:30						
10:45		Sessions of Divisions	Sessions of Divisions	Sessions of Divisions	Sessions of Divisions	Sessions of Divisions
11:00						
11:15						
11:30						
11:45						
12:00						
12:15						
12:30						
12:45						
13:00		Disc. Lunch (HSZ/AUDI)	Disc. Lunch (HSZ/AUDI)	Disc. Lunch (HSZ/AUDI)	Prize Talks (HSZ/0002, HSZ/0003)	
13:15		Prize Talk (HSZ/0002)	Prize Talks (HSZ/0002 HSZ/0004)	Prize Talk (HSZ/0003)	Lunch Talk (HSZ/0004)	Closing Talk (HSZ/0002)
13:30		Lunch Talk (HSZ/0004)	DFG - Lunch (HSZ/0003)	Lunch Talk (HSZ/0002)		
13:45						
14:00		Plenary Talks (HSZ/AUDI + HSZ/0002)		Plenary Talks (HSZ/AUDI + HSZ/0002)	Plenary Talks (HSZ/AUDI + HSZ/0002)	
14:15			Sessions of Divisions			
14:30						
14:45						
15:00	Registration	SYSC (HSZ/AUDI)	Special Plenary Session with Award Ceremony and Ceremonial Talk (HSZ/AUDI)	SYGF (HSZ/AUDI)	SYTP (HSZ/AUDI)	
15:15						
15:30						
15:45						
16:00	Tutorials (HSZ/0002, HSZ/0003, HSZ/0004 BEY/0137, TRE/PHYS TRE/MATH)					
16:15						
16:30						
16:45						
17:00			Poster of Divisions	Sessions / Poster of Divisions	Sessions / Poster of Divisions	
17:15						
17:30						
17:45						
18:00					Members' Assemblies of the Divisions	
18:15						
18:30	Welcome Evening (Alte Mensa)					
18:45						
19:00				Public Evening Talk (HSZ/AUDI)	Members' Assembly (HSZ/AUDI) and Postdeadline Session of the Surface Science Division (Alte Mensa)	
19:15						
19:30						
19:45						
20:00		EinsteinSlam (HSZ/AUDI)				
20:15						
20:30						
20:45						
21:00						
21:15						
21:30						
21:45						