# Functional Materials Division
# Fachverband Funktionsmaterialien (FM)

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## Overview of Invited Talks and Sessions

(Lecture halls BEY/0138 and BEY/0E40; Poster P4)

### Invited Talks

| | | | | |
|---|---|---|---|---|
| FM 4.1 | Mon | 15:00–15:30 | BEY/0138 | **(Anti)Ferroelectric HfZrO2: from non volatile memory to energy storage applications** — •Bertrand Vilquin, Gregoire Magagnin, Jordan Bouaziz, Martine Le Berre, Sara Gonzalez, Ingrid Canero Infante, Brice Gautier, Kevin Alhada-Lahbabi, Damien Deleruyelle |
| FM 6.1 | Tue | 9:30–10:00 | BEY/0138 | **Robust Data Generation, Heuristics and Machine Learning for Materials Design** — •Janine George |
| FM 9.1 | Tue | 14:00–14:30 | BEY/0138 | **Thin film combinatorial studies of functional magnetic materials** — •Nora Dempsey |
| FM 12.1 | Wed | 9:30–10:00 | BEY/0138 | **Shedding Light on Polar Topological Textures** — •Salia Cherifi-Hertel |
| FM 17.1 | Thu | 9:30–10:00 | BEY/0138 | **Piled higher, probed deeper: X-ray insights into ferroelectric devices** — •Martina Müller |
| FM 18.1 | Thu | 10:15–10:45 | BEY/0138 | **Stabilizing antiferroelectricity in PbZrO3 thin films using epitaxial tensile strain** — •Vincent Garcia |
| FM 18.2 | Thu | 10:45–11:15 | BEY/0138 | **Strain effects in free-standing membranes of antiferroelectric Lead Zirconate** — •Umair Saeed, Huazhang Zhang, David Pesquera, Philippe Ghosez, Nini Pryds, Jose Santiso, Felip Sandiumenge, Gustau Catalan |
| FM 22.1 | Fri | 9:30–10:00 | BEY/0138 | **Topological thermoelectrics for solid state cooling** — •Yu Pan, Claudia Felser |
| FM 23.1 | Fri | 9:30–10:00 | BEY/0E40 | **Mapping topological textures in compensated magnets with X-rays** — •Claire Donnelly |

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

See SYSD for the full program of the symposium.

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

## Invited Talks of the joint Symposium Beyond Transistors: Material-Based Edge Computing Paradigms (SYBT)

See SYBT for the full program of the symposium.

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

## Sessions

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| FM 1.1–1.5 | Sun | 16:00–18:15 | HSZ/0002 | **Hands-on Tutorial: HyperSpy – Multidimensional data analysis using Python (joint session FM/TUT)** |
| FM 2.1–2.7 | Mon | 9:30–11:30 | BEY/0138 | **Energy Materials** |
| FM 3.1–3.6 | Mon | 9:30–12:00 | POT/0151 | **Focus Session: Novel mechanisms of ferroic switching (joint session MA/FM)** |
| FM 4.1–4.9 | Mon | 15:00–17:45 | BEY/0138 | **Focus Session: (Anti)ferroic states – Non-conventional states I** |
| FM 5.1–5.11 | Mon | 15:00–18:00 | BEY/0E40 | **Focus Session: Holistic structural and safety assessment of battery materials and cells** |
| FM 6.1–6.11 | Tue | 9:30–12:45 | BEY/0138 | **Focus Session: Materials Discovery I – Material informatics** |
| FM 7.1–7.8 | Tue | 9:30–11:45 | BEY/0E40 | **Crystal Defects and Real Structure Physics in Diamond and Functional Materials I** |
| FM 8.1–8.11 | Tue | 9:30–12:30 | POT/0112 | **Multiferroics and Magnetoelectric Coupling (joint session MA/FM)** |
| FM 9.1–9.5 | Tue | 14:00–15:30 | BEY/0138 | **Focus Session: Materials Discovery II – High throughput searches for functional magnetic materials (joint session FM/MA)** |
| FM 10.1–10.5 | Tue | 14:00–15:30 | BEY/0E40 | **Crystal Defects and Real Structure Physics in Diamond and Functional Materials II** |
| FM 11.1–11.38 | Tue | 18:00–20:30 | P4 | **Poster Session Functional Materials** |
| FM 12.1–12.11 | Wed | 9:30–13:00 | BEY/0138 | **German-French Focus Session: Materials Research in Polar Oxides – From Domain Engineering to Photonic and Electronic Devices I** |
| FM 13.1–13.5 | Wed | 10:15–11:30 | SCH/A251 | **Topical Session: Dislocations in Functional Materials I (joint session MM/FM)** |
| FM 14.1–14.4 | Wed | 15:00–16:00 | BEY/0138 | **Focus Session: Materials Research in Polar Oxides – From Domain Engineering to Photonic and Electronic Devices II** |
| FM 15.1–15.3 | Wed | 15:00–15:45 | BEY/0E40 | **Nanoscale Probing of Functional Properties** |
| FM 16.1–16.5 | Wed | 15:45–17:15 | SCH/A251 | **Topical Session: Dislocations in Functional Materials II (joint session MM/FM)** |
| FM 17.1–17.1 | Thu | 9:30–10:00 | BEY/0138 | **Highlighted Talk: Piled higher, probed deeper: X-ray insights into ferroelectric devices (Martina Müller)** |
| FM 18.1–18.8 | Thu | 10:15–12:45 | BEY/0138 | **German-French Focus Session: (Anti)ferroic states – ferroelectrics, ferroelastics and antiferroelectrics II** |
| FM 19.1–19.9 | Thu | 10:15–12:45 | BEY/0E40 | **Advanced Microscopy and Tomography for Functional Materials** |
| FM 20 | Thu | 13:30–17:00 | Infineon | **Excursion and Network-Event at Infineon Dresden AG (joint session FM/HL)** |
| FM 21 | Thu | 18:00–18:45 | BEY/0138 | **Members Assembly** |
| FM 22.1–22.11 | Fri | 9:30–12:45 | BEY/0138 | **Focus Session: Materials Discovery III – New materials and functionalities by general principles** |
| FM 23.1–23.6 | Fri | 9:30–11:30 | BEY/0E40 | **Focus Session: (Anti)ferroic states – Magnetic and magnetoelectric III (joint session FM/MA)** |

## Members' Assembly of the Functional Materials Division

Thursday 18:00–18:45 BEY/0138

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

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

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

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

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

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

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

FM 1.1 Sun 16:00 HSZ/0002

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

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

**Tutorial** FM 1.2 Sun 16:15 HSZ/0002

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

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

**Tutorial** FM 1.3 Sun 16:45 HSZ/0002

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

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

**Tutorial** FM 1.4 Sun 17:15 HSZ/0002

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

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

**Tutorial** FM 1.5 Sun 17:45 HSZ/0002

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

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

# FM 2: Energy Materials

Chair: Anna Grünebohm (Ruhr Universität Bochum, DE)

Time: Monday 9:30–11:30 Location: BEY/0138

FM 2.1 Mon 9:30 BEY/0138

**Fundementals of elctrochemical hydrogen charging of MAX phases and their storage potential** — •Rebeca Miyar, Adam C. Miles, Manoj Prabhakar, Lilian Vogl, Gerhard Dehm, Yug Joshi, Barak Ratzker, and Maria Jazmin Duarte — Max Planck institute for Sustainable Materials, Düsseldorf, Germany

Hydrogen storage remains a central challenge in the transition to renewable energy systems, as current technologies face limitations in scalability, safety, and efficiency. MAX phases, a class of nanolaminated carbides and nitrides composed of an early transition metal, an A-group element, and carbon or nitrogen, are perspective candidates for solid-state hydrogen storage due to their layered structure, which provides potential interstitial trapping sites. Although many theoretical studies discuss their hydrogen trapping behaviour, experimental evidence remains limited and previous work has focused only on gas-phase hydrogenation. Here, we present the first systematic study of electrochemical hydrogen charging and desorption in Ti2AlC and Ti3AlC2, which differ in their metal/ceramic layer ratio. Hydrogen trapping and release were analysed using thermal desorption spectroscopy, Kelvin probe measurements, and electrochemical methods. Two dominant trap types were identified in both materials, with their relative contributions reflecting the layer ratio. These results provide new insight into hydrogen permeation and trapping in MAX phases.

FM 2.2 Mon 9:45 BEY/0138

**Multilayer Na intercalation in bilayer graphene** — •Mahdi Ghorbani-Asl and Arkady V. Krasheninnikov — Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, 01314 Dresden, Germany.

The intercalation of atomic and molecular species into layered materials has emerged as a powerful route for creating novel encapsulated two-dimensional systems with tunable physical properties. Among these, alkali-metal intercalation in graphitic carbon has been widely explored for energy-storage applications. However, sodium (Na) intercalation into bulk graphite is predicted to be energetically unfavorable, making it particularly challenging to realize experimentally. In this work, we combine first-principles calculations with scanning transmission electron microscopy (STEM) to investigate Na intercalation into bilayer graphene. Using DFT simulations, we analyze the energetics and atomic structures of Na intercalants in single-layer and multilayer configurations, and evaluate how charge transfer between graphene and the Na atoms affects their stability. Our simulations reveal that the lowest-energy structure is an fcc trilayer with an A-B-C stacking sequence, whose projected atomic arrangement is fully consistent with the STEM observations. These findings provide new insight into Na intercalation mechanisms and may support the development of future sodium-ion battery technologies.

FM 2.3 Mon 10:00 BEY/0138

**The Role of Lone Pairs in Fast Oxide Ion Conduction in $\mathbf{Bi_{0.8}Pr_{0.2}O_{1.5}}$** — •Marcin Kryński — Warsaw University of Technology

Elucidating the microscopic processes that enable rapid oxide-ion transport is key to advancing solid electrolyte design. In this study, we integrate total neutron scattering with reverse Monte Carlo modelling and ab initio molecular dynamics to dissect the structural and electronic mechanisms underlying a pronounced conductivity increase observed across the order/disorder phase transition. Our results reveal that this transition is driven not by changes in the cation framework, but by a collective reorganization of oxide ions and local coordination environments. Specifically, oxide ions shift from the edges of fluorite-like blocks into the van der Waals gap, where they gain access to extended, predominantly two-dimensional diffusion pathways. Concurrently, $BiO_4$ units undergo a subtle yet systematic reorientation linked to the stereochemical activity of $Bi^{3+}$ lone pairs. Although the local coordination of Bi remains largely preserved, the orientation of these lone pairs evolves in tandem with the redistribution of oxide ions, suggesting a dynamic coupling reminiscent of a paddle-wheel-type mechanism. This interplay between lone-pair-driven asymmetry and anion mobility provides a unified mechanistic picture of how structural flexibility and electronic degrees of freedom cooperate to enhance high-temperature oxide-ion transport. The insights gained here establish general principles for designing fast-ion conductors in systems where active lone pairs play an essential role.

**Coffee break**

FM 2.4 Mon 10:30 BEY/0138

**Metal Poisoning of Nafion Proton Exchange Membrane** — •Souvik Mitra[1], Jialiang Liu[1], Kristina Fröhlich[1], Simone Köcher[1,2], Christoph Scheurer[2,1], and Rüdiger-A. Eichel[1] — [1]IET-1, Forschungszentrum Jülich GmbH, 52425 Jülich, DE — [2]Fritz-Haber-Institute der MPG, 14195 Berlin, DE

Metal-ion contamination of Nafion proton-exchange membranes (PEMs) remains a persistent durability and performance issue in PEM fuel cells. Metal cations originating from insufficiently deionized feed water, coolant leaks, or corrosion of metallic cell components can exchange with protons at the sulfonate groups ($SO_3^-$) of Nafion, thereby reducing proton conductivity and overall cell performance.

In this work, we combine atomistic molecular dynamics simulations with in-plane conductivity measurements to build a consistent picture of how a broad series of mono-, di-, and trivalent cations affect transport in Nafion under comparable conditions. For monovalent ions ($Li^+$, $Na^+$, and $K^+$), our study reveals a reversal of the familiar mobility trend of these cations in the presence of Nafion membrane compared to bulk water, reflecting the competition between ion hydration and specific binding to the $SO_3^-$ groups of Nafion. Our study also shows that, as cation charge increases from +1 to +2 to +3, their mobility drops significantly, correlating with longer residence times at sulfonate sites and increasingly multidentate $SO_3^-$ coordination.

Our study highlights the strengths of simulations in elucidating the atomistic origin of diffusivity trends, but also their challenges in making reasonable physical approximations.

FM 2.5 Mon 10:45 BEY/0138

**Synchrotron X-ray Characterization of Irradiated Ag/PVA Polymer Electrolyte** — Mohamed Salah Soliman Asser and •Mohamed Salah Soliman Asser — Polymer Chemistry Department, National Center for Radiation Research and Technology, Egyptian Atomic Energy Authority, Cairo, Egypt.

Polymer electrolyte membrane thin films were developed and characterized for potential use in electroconductive applications. Polymer composites of polyvinyl alcohol (PVA), sulfuric acid, ethanol, and silver nitrate were prepared using both casting and dip-coating techniques. For the dip-coating method, glass slides were first cleaned by immersion in acetone, rinsed with isopropanol, and dried. The prepared polymer composite solutions were then dip-coated onto the glass substrates. The coated slides were irradiated at three doses: 62 J/cm2 (low), 251 J/cm2 (medium), and 502 J/cm2 (high) using the DXRL beamline. High-resolution X-ray diffraction (HR-XRD) analyses were performed at the Elettra Synchrotron Laboratory, Trieste, Italy, using the MCX beamline at a glancing angle of 1°. The X-rays had an energy of 12 keV ($\lambda = 1.033$ Å). Diffraction patterns were recorded in the $2\theta$ range of 1*80° with a step size of 0.01° and an exposure time of 1 s per step for the Ag*PVA samples.

FM 2.6 Mon 11:00 BEY/0138

**Tailoring Electrochemical Functionality of Transition-Metal Glycerolates for Next-Generation Energy Storage Devices** — •Ali Hyder[1,2], Irlan S Lima[2], Zahid ullah Khan[2], Ayaz Ali Memon[1], and Lucio Angnes[2] — [1]National Centre of Excellence in Analytical Chemistry, University of Sindh, Jamshoro 76080, Pakistan — [2]Departament de Química Fundamental, Institute de Química, University of São Paulo, Av. Prof. Lineu Prestes, 748 * 05508-000, São Paulo, SP, Brazil

Abstract Metal glycerolates are emerging as promising precursors and active materials for electrochemical energy-storage systems due to their tunable coordination chemistry, oxygen-rich structures, and flexible architectures. In this study, transition-metal glycerolates (Mn, Co, Ni, Cu, Fe) were synthesized via a controlled solvothermal method to explore how formation and nanoscale morphology influence electrochemical performance. Structural analyses show that the resulting M*O*C networks form layered or clustered architectures that enhance ion diffusion and electron transport. Used as electrode materials either directly mild thermal treatment the glycerolates exhibit strong pseudo capacitance, improved redox kinetics, and good stability. Metal glycerolytes deliver the highest capacitance due to synergistic redox activity and accessible surfaces. Overall, the results demonstrate the potential of metal glycerolates as low-cost, versatile candidates for advance hybrid energy-storage devices.

FM 2.7 Mon 11:15 BEY/0138

**Thermoelectric properties of In-doped Bi2Te3 crystalline bulk alloys** — •Alaa Adam[1] and E. Ibrahim[2] — [1]Sohag University — [2]Sohag university

Influence of indium doping on the structure, morphology and thermoelectric properties of bulk Bi2Te3 is investigated in the current work. Bi2Te3 and Bi2-xInxTe3 crystalline bulk samples have been fabricated using a simple mono-temperature melting method. Analyses employing X-ray diffraction (XRD) and scanning electron microscopy (SEM) techniques proved the existence of the concerned phases. In addition, morphology and internal structure have been examined via the scanning electron microscopes and the energy dispersive X-ray (EDX) spectroscopy. Thermoelectric properties were determined in a temperature range between 300*700 K. The electrical conductivity ($\sigma$) against the temperature showed metallic-like behavior. Carrier concentration has increased with in-doping. The Seebeck coefficients (S) of the synthesized alloys proved the domination of n-type conduction due to consistently negative S values. The largest Seebeck coefficient was recorded at 203.5 *V/ K which was observed at 700 K for the pristine Bi2Te3 sample. The highest power factor was found at PF = 5.46 mWm-1K-2, obtained for Bi2Te3 at room temperature. Thermal conductivity was measured and studied against temperature elevation. It was found that the thermal conductivity of the In-doped Bi1.98In0.02Te3 alloys are significantly reduced compared with that of the pure Bi2Te3 material.

## FM 3: Focus Session: Novel mechanisms of ferroic switching (joint session MA/FM)

This focus session highlights recent advances in ferroic switching across ferroelectric, multiferroic, ferroaxial and magnetic systems. Topics include topologically protected order-parameter dynamics, ultrafast non-thermal switching, and complex domain-wall phenomena revealed by atomistic modeling, ultrafast optics and advanced imaging. Contributions span machine-learning-based simulations of domain kinetics, optical control of ferroaxial and structural orders, multiferroic multi-cell memory concepts, and theoretically predicted unidirectional domain-wall motion with time-crystal behavior. Together, these works uncover new switching pathways and robust functional mechanisms, offering promising routes toward energy-efficient memory and quantum devices.

Organizer: Andrei Pimenov, andrei.pimenov@tuwien.ac.ac

Time: Monday 9:30–12:00 Location: POT/0151

**Invited Talk** FM 3.1 Mon 9:30 POT/0151

**From ML to Kinetics: Modeling the Switching in Ferroelectric Wurtzites** — •Andrew Rappe, Drew Behrendt, Atanu Samanta, and Von Braun Nascimento — Department of Chemistry, University of Pennsylvania, Philadelphia, PA 19104-6323 USA

We present a series of works, from the development of a new force field (MLFF) for multi-scale simulations of bulk AlN, through application of MLFF to understand the atomistic switching mechanism, to the development of a new kinetic model to uncover how switching changes as a function of experimental conditions.

We train our MLFF to 1000s of DFT calculations, so the underlying calculations are as accurate as DFT with the flexibility in simulation size of classical MD. Powered by the MLFF, we can predict the energies, forces, and phonon dispersions of AlN at dramatically lower cost, thus enabling the study of emergent and long-range effects, such as the frequency-dependent dielectric functions and multiple FE domains.

Applying the AlN MLFF, we uncover the atomistic mechanism of domain wall (DW) migration and domain growth in wurtzites. We find that the critical nucleus is a single broken Al-N bond along the polar axis; this creates a cascade of bond breaking in a single column of atoms due to the stability of the 180° DW in wurtzites. We reveal the switching mechanism of 1D atomic columns propagating from a slow-moving 2D fractal-like DW in the basal plane.

Finally, we develop an analytical extension to the KAI model that accounts for fractal FE domains. To do this, we take the traditional model of circles that can nucleate and grow and add a budding term.

**Invited Talk** FM 3.2 Mon 10:00 POT/0151

**Topological order parameter switching** — •Sergey Artyukhin — Quantum Materials Theory, Genova, Italy

Ferroic orders are widely used to encode information in data storage devices and may provide a beneficial way to circumvent Boltzmann tyranny affecting conventional MOSFET memory [1]. However, information writing involves order parameter switching, facilitated by domain nucleation and motion of domain walls across a disordered material, which leads to energy dissipation. Recently, an alternative order parameter switching paradigm has been introduced, where the ordered state tracking the free energy minimum continuously rotates the order parameter direction as the free energy surface is deformed by an external driving [2]. The process is analogous to Thouless pumping and is topologically protected. A related mechanism allows pumping of topological spin textures in space [3].

[1] S. Manipatruni, D. E. Nikonov, I. A. Young, Nature Physics 14, 338 (2018)

[2] L. Ponet et al., Nature 607, 81-85 (2022)

[3] L. Maranzana et al., arXiv:2502.13083

**Invited Talk** FM 3.3 Mon 10:30 POT/0151

**Optical Control of Ferroaxial Order via Circular Phonon Excitation** — •Zhiyang Zeng[1,2], Michael Först[1], Michael Fechner[1], Dharmalingam Prabhakaran[2], Paolo Radaelli[2], and Andrea Cavalleri[1,2] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Department of Physics, Clarendon Laboratory, University of Oxford, Oxford, United Kingdom

Ferroaxial order is a distinct ferroic order in crystal systems characterized by a rotational texture of electric dipoles. Its unique symmetry prohibits direct coupling to static fields or stress, making conventional control approaches ineffective.

Based on symmetry analysis, we identify a coupling between the ferroaxial order and circularly driven optical phonons, which can be resonantly excited with circularly polarized mid-infrared light. Exploiting this coupling, we experimentally achieve reversible, deterministic switching of the ferroaxial order in the prototype material RbFe(MoO4)2 using single-shot excitation.

This work establishes a new mechanism for manipulating ferroaxial order via light-driven phonons, enabling dynamic control of ferroic properties in complex materials.

**15 min break**

FM 3.4 Mon 11:15 POT/0151

**Coherent Control of Competing Structural Orders in SrTiO3** — •M. Fechner[1], H. Wang[2], M. Foerst[1], G. Orenstein[2], A. Disa[3], M. Trigo[2], and A. Cavalleri[1] — [1]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [2]Stanford Pulse Institute, SLAC National Accelerator Laboratory, Menlo Park, CA, USA — [3]School of Applied & Engineering Physics, Cornell University, Ithaca, NY USA

The interplay between antiferrodistortive (AFD) rotation and polar instability prevents the formation of ferroelectric order in SrTiO3 yet keeps the paraelectric-to-ferroelectric transition on the verge of emerging. Light excitation has been shown to induce metastable ferroelectricity[1], but the response of the AFD order to such optical driving remains unclear. Here we use time-resolved X-ray scattering to track AFD-order dynamics, launched by mid-infrared excitation of the Ti-O stretching vibration, from 10 K to 135 K above the cubic transition. In the tetragonal phase below 110 K, the AFD order transiently increases before the AFD angle is reduced, whereas in the cubic phase rotational fluctuations initially grow before being strongly suppressed[2]. A unified lattice model, incorporating nonlinear coupling of the excited infrared phonon to the AFD mode and to strain, captures both regimes. With a single set of coupling parameters, we reproduce behaviors for both phases, indicating a common underlying mechanism that also constrains explanations for the light-induced ferroelectric state.

[1] T.F., et al. Nova Science 364, 1075 (2019), [2] M. Fechner, et al. NatMat, 23, 363 (2024)

FM 3.5 Mon 11:30 POT/0151

**Multi-cell unit storage based on a multiferroic** — •Maksim Ryzhkov[1], Alexey Shuvaev[1], Maxim Mostovoy[2], Andrei Pimenov[1], Anna Pimenov[1], and Sergey Artyukhin[3] — [1]Institute of Solid State Physics, Vienna University of Technology, Vienna, Austria — [2]Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands — [3]Quantum Materials Theory, Istituto Italiano di Tecnologia, Genova, Italy

Recent advances in multiferroic materials offer promising prospects for next-generation memory and data-processing devices. Previous studies [1,2] have shown that rare-earth manganates $RMn_2O_5$, particularly with R = Gd, are strong candidates for storage applications due to their topologically protected four-state magnetoelectric switching and the efficient electric-field control of this switching.

In this work, we demonstrate that this system enables the realization of a multi-cell storage unit capable of encoding and decoding at least five bits. We show that only two key ingredients are required:
(i) the four-state magnetoelectric switching observed during magnetic-field sweeps, and
(ii) a ferroelectric domain structure in the bulk together with local inhomogeneities (e.g., internal mechanical stresses) that produce a distribution of the spin-flop critical field $H_c$ across different domains.
Thus, the magnetoelectric domains in $GdMn_2O_5$ are not an unwanted bug but an essential feature enabling multi-cell functionality.
[1] L. Ponet, et al., Nature 607, 81-85 (2022)
[2] H. Wang, et al., PRL 134, 016708 (2025)

FM 3.6 Mon 11:45 POT/0151

**E-field induced unidirectional motion of domain wall in a ferromagnet and time crystals** — •Margherita Parodi[1,2], Sergey Artyukhin[1], and Maxim Mostovoy[3] — [1]Quantum Materials Theory, Italian Institute of Technology, Genova, Italy — [2]Physics Department, University of Genova, Italy — [3]Theory of Condensed Matter, Zernike Institute for Advanced Materials, Groningen, The Netherlands

Noncollinear spin textures may break inversion symmetry and induce ferroelectric polarization, giving rise to multiferroicity. Here we study the most basic noncollinear spin texture: a domain wall in a collinear (anti)ferromagnet. The spin chirality of the domain wall is analogous to that in spiral multiferroics and likewise leads to ferroelectric polarization. Here we find that oscillating magnetic and electric fields can drive a unidirectional motion of the magnetic texture, similar to how electrons are transported by the Thouless pump. Furthermore, for certain periods of a driving field, the domain wall demonstrates complex behaviour akin to a time crystal, with the period equal to an integer multiple of the driving periods. The phenomenon arises due to a mismatch between the natural timescale of the domain wall motion and the driving field period.

## FM 4: Focus Session: (Anti)ferroic states – Non-conventional states I

chair: Nives Strkalj (University of Zagreb, HR)

This focus session explores recent advances in understanding and control of (anti)ferroic states. Emphasis will be placed on theoretical modelling, advanced characterization techniques, and the engineering of emergent properties for use in nano-electronic devices. The session aims to bridge fundamental research with emerging device-relevant functionalities, bringing together experimental, and theoretical perspectives on ferroic materials.

Time: Monday 15:00–17:45 Location: BEY/0138

**Invited Talk** FM 4.1 Mon 15:00 BEY/0138

**(Anti)Ferroelectric HfZrO2: from non volatile memory to energy storage applications** — •Bertrand Vilquin[1], Gregoire Magagnin[2], Jordan Bouaziz[3], Martine Le Berre[1], Sara Gonzalez[2], Ingrid Canero Infante[2], Brice Gautier[1], Kevin Alhada-Lahbabi[1], and Damien Deleruyelle[1] — [1]INSA Lyon, Ecole Centrale de Lyon, CNRS, Universite Claude Bernard Lyon 1, CPE Lyon, INL, UMR5270, 69621 Villeurbanne, France — [2]CNRS, INSA Lyon, Ecole Centrale de Lyon, Universite Claude Bernard Lyon 1, CPE Lyon, INL, UMR5270, 69621 Villeurbanne, France — [3]Ecole Centrale de Lyon, INSA Lyon, CNRS, Universite Claude Bernard Lyon 1, CPE Lyon, INL, UMR5270, 69621 Villeurbanne, France

Fluorite-structured HfZrO2 and ZrO2 thin films are promising for both non-volatile memory and energy storage applications. Antiferroelectric (AFE) capacitors were fabricated by PE-ALD and annealed using BEOL-compatible thermal budgets. All devices exhibit AFE double hysteresis loops, with polarization strongly dependent on film thickness and annealing temperature. Phase-field modeling reveals thickness-driven phase transitions enabling low-voltage, high-polarization operation. These characteristics are relevant for future AFE FET. Energy storage performances of linear dielectric (LD), ferroelectric (FE), and AFE films are compared. While FE films show high energy density but large losses, LDs offer high efficiency with low storage density. AFE ZrO2 provides an optimal balance, reaching up to 84 J/cm3 with 75% efficiency. These results position HfZrO2 as a multifunctional platform bridging memory and energy storage technologies.

FM 4.2 Mon 15:30 BEY/0138

**From metal to oxide: Oxygen vacancy evolution in $HfO_2$ controlled by PLD** — •Berk Yildirim[1], Oliver Rehm[1], Philipp Gebauer[1], Marc Neumann[1], Andrei Gloskovskii[3], Christoph Schlueter[3], Lutz Baumgarten[2], Ron Tenne[4], and Martina Müller[1] — [1]FB Physik, U Konstanz — [2]FZ Jülich — [3]DESY, Hamburg — [4]Technion, Haifa, Israel

Hafnium dioxide ($HfO_2$) has emerged as a ferroelectric material for non-volatile memory applications. The ferroelectric phase is linked to the presence and amount of oxygen vacancies (OVs), but their direct experimental observation is challenging. In this work, a combination of in situ soft X-ray and ex situ hard X-ray photoelectron spectroscopy is used to trace the evolution of OVs. To systematically control the oxidation and OV concentration in $HfO_2$, 120 nm films are grown from stoichiometric targets by pulsed laser deposition (PLD) without oxygen supply, but varying the $SrTiO_3$ (001) substrate temperature T. With increasing T, the amount of metallic Hf is systematically reduced, while the oxide fraction increases. The evolution of Hf 4f spectral features is evaluated as the indirect signature of the T-dependent OV concentration through the $Hf^{3+}/Hf^{4+}$ spectral weight. In addition, photoluminescence measurements confirm the presence and T-dependent variation of OVs. In situ RHEED, ex situ AFM and XRD validate T-driven changes in morphology and structure, linking Hf oxidation state, vacancy concentration and film properties. These results demonstrate that T-controlled oxidation enables a systematic control of OVs and helps clarify how defects influence the formation of ferroelectric $HfO_2$.

FM 4.3 Mon 15:45 BEY/0138

**Influence of Different Transition-Metal defect Dipoles on Polarization Rotation in $BaTiO_3$** — •Aldo Raeliarijaona[1], Ronald E. Cohen[2], and Anna Grünebohm[1] — [1]Ruhr-Universität, Bochum,Germany — [2]Carnegie Institution for Science, Washington D.C., U.S.A

Ferroelectric materials are an important class of materials for various technological applications such as non-volatile random-access memory mainly due to spontaneous electric polarization. Key ferroelectric property is the switching mechanism induced by an electric field. However, defect dipoles in ferroelectrics can act like a bias field or restoring forces to rotation of the polarization after an electric field has been applied and then removed. Using first-principles molecular dynamics, we compare polarization rotation induced by defect dipoles, in which divalent transition metal dopants on the perovskite B-site couple with neighboring oxygen vacancies, in the archetypical ferroelectric BaTiO3. We compare the effects of $Cu^{2+}$, $Mn^{2+}$, and $Fe^{2+}$ dopants. We find that copper is much more efficient at enhancing electromechanical coupling or restoring polarization direction, over manganese or iron. We relate this effect of chemistry to the shape and bonding of the transition metal cations.

FM 4.4 Mon 16:00 BEY/0138

**Reentrant relaxor behaviours in Ba(Ti0.85Zr0.15)O3-Bi(Zn2/3Nb1/3)O3** — •Vladimir Shvartsman[1], Eva Kröll[1], Boriana Mihailova[2], Vadzim Haronin[3], Juras Banys[3], and Doru Lupascu[1] — [1]University Duisburg-Essen, Essen, Germany — [2]University of Hamburg, Hamburg, Germany — [3]Vilnius University, Vilnius, Lithuania

Upon decreasing temperature, thermodynamic systems usually transform from a disordered high symmetry phase to a more ordered phase with lower symmetry. However, in some cases an unusual phase sequence is observed, where after this *normal* transition, an ordered system reenters a disordered phase. We observed the reentrant behavior in the relaxor ferroelectrics (1-x)Ba(Ti0.85Zr0.15)O3-xBi(Zn2/3Nb1/3)O3 (x = 0 - 0.15) by analysis of temperature dependences of the dielectric permittivity. Namely, a frequency-independent maximum associated with the ferroelectric phase transition is followed by a frequency-dependent anomaly at lower temperatures, which is typical of relaxors. Raman spectroscopy revealed a competition between polar and antiferrodistortive modes. Softening of the polar mode related to correlated B-cation displacements leads to the ferroelectric phase transition. On the other hand, correlated antiferrodistortive rotations of the oxygen octahedra give rise to nanometer size clusters of antipolary shifted A-site cations distributed within the polar matrix. Slowing down the dynamics of these clusters leads to the low-temperature dielectric anomaly and reentrant relaxor behavior.

FM 4.5 Mon 16:15 BEY/0138

**Time-domain thermoreflectance for monitoring thermal conductivity switching in ferroelectric thin film** — •Wasim Akram[1], Stefan Dilhaire[2], Thomas Maroutian[3], and Guillaume F. Nataf[1] — [1]GREMAN UMR7347, CNRS, Université de Tours, France — [2]CNRS-LOMA/UMR5798, Université de Bordeaux, France — [3]C2N, CNRS, Université Paris-Saclay, France

Ferroelectric materials that exhibit thermal conductivity switching under external stimuli could serve as promising candidates for thermal conductivity switches [1,2]. To integrate these switches into miniaturized devices, nanoscale ferroelectric films are essential. In this work, we aim to study ferroelectric thin films and propose to manipulate their thermal conductivity by applying an electric field. To monitor the thermal conductivity, we employ time-domain thermoreflectance (TDTR). In TDTR, the sample surface is periodically heated with a far-infrared pump laser through a metallic transducer, and the resulting thermoreflectance response is probed using a delayed probe laser. The probe reflectivity change is directly related to the temperature evolution at the sample surface. The analysis relies on multilayer heat-transfer models that incorporate the substrate, film, and transducer. However, modelling is sensitive to several experimental constraints, including non-uniform interface properties and interfacial thermal resistance. Here, we address these challenges by optimizing both data-acquisition and sample-preparation methods. We use a home-made software based on Thermal Quadrupole model to fit the signal received by the photodetector [3]. Additionally, we propose to apply an electric field to ferroelectric films to modulate their domain structures, with the goal of achieving multiple fold switching of thermal conductivity. This approach could pave the way toward a device-compatible ferroelectric thermal conductivity switch. [1] Ihlefeld et al. Nano Letters 15 (3), 1791-1795 (2015). [2] Nataf et al. Nature Reviews Materials 9, 530 (2024). [3] Dilhaire et al. J. Appl. Phys. 110, 114314 (2011).

**Coffee break**

FM 4.6 Mon 16:45 BEY/0138

**Correlated domain and crystallographic orientation mapping in uniaxial ferroelectric polycrystals by interferometric vector piezoresponse force microscopy** — •Ruben Dragland[1], Jan Schultheiss[1], Ivan Ushakov[1], Roger Proksch[2], and Dennis Meier[1,3,4] — [1]NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]Asylum Research an Oxford Instruments Company, Santa Barbara, USA — [3]University of Duisburg-Essen, Duisburg, Germany — [4]Research Alliance Ruhr, Bochum, Germany

Advances in scanning probe microscopy techniques are expanding the possibilities for nanoscale characterization of functional materials, giving new opportunities for correlated studies of their local properties. Here, we apply a recent extension of piezoresponse force microscopy (PFM) for simultaneous mapping of polarization domains and local crystallographic orientation in a uniaxial ferroelectric. By shifting the laser beam position on the cantilever, direction-dependent piezoresponse signals are acquired analogous to classical vector PFM, but without the need to rotate the sample. Using polycrystals of the uniaxial ferroelectric $ErMnO_3$ as a model system, we demonstrate that the reconstructed piezoresponse vectors correlate one-to-one with the crystallographic orientations of the micrometer-sized grains, carrying grain-orientation and domain-related information. We establish a versatile platform for rapid, multimodal characterization of polycrystalline uniaxial ferroelectrics, enabling automated, high-throughput reconstruction of polarization, and grain orientations with nanoscale precision.

FM 4.7 Mon 17:00 BEY/0138

**Optical control of ferroelectric polarization in epitaxial lead titanate thin films** — •Valentine Gillioz, Manfred Fiebig, and Morgan Trassin — ETH Zurich, Switzerland

In this work, we use light as an active tool for remotely and dynamically controlling ferroelectricity in epitaxial $PbTiO_3$-based thin films and heterostructures. The exposure to above-bandgap ultraviolet (UV) light enables the manipulation of charge-screening dynamics via the accumulation of photo-induced charge carriers at the bottom electrode/ferroelectric Schottky interface. A transient light-induced enhancement (or suppression) of spontaneous polarization is observed using second-harmonic generation (SHG) in films with a pristine upward (or downward)-oriented polarization. Here, we explore the impact of $PbTiO_3$ growth conditions on the photoresponse of the films in more depth. Importantly, we show a robust and improved cyclability of the optical modulation of the ferroelectric polarization in films grown at low oxygen partial pressure ($\sim 10^{-2}$mbar) pointing to the role of oxygen vacancies in the light-induced polarization change. In addition, we combine our ability to monitor the polarization dynamics during the thin-film growth process using in-situ SHG with the UV light exposure to balance the depolarizing-field contribution and the light-induced polarizing effect in our heterostructures. We report a strong on/off ratio in the optical manipulation of ferroelectric polarization between a fully depolarized state in dark conditions and a polarized state under UV light exposure. Our work, hence, constitutes a critical step towards all-optical control of ferroelectricity in functional thin films.

FM 4.8 Mon 17:15 BEY/0138

**Ferroelectricity in organic - inorganic TMCM-BCl3 (B=Mn, Fe, Zn) materials** — •Mwanaidi Mauwa Namisi and Anna Grünebohm — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Germany

Ferroelectric materials have switchable polarization in external electric field and play a central role in sensors, memory devices and dielectrics. Although oxide ceramics have been the main focus, they have limited chemical flexibility [1]. In contrast, hybrid organic-inorganic perovskites combine multiple degrees of freedom of both inorganic and organic frameworks enhancing structural versatility [2]. Their phase transition mechanisms and origin of ferroelectricity however remain underrepresented in literature. Here, we investigate the class of TMCM-BCl3 (B=Mn, Fe, Zn) hybrids using DFT methods and discuss these open questions. Furthermore, by B site compositional tuning, we explore the structure-property relations and how the choice of transition metal affects polarization, electronic properties and magnetism.

[1] Y-M You et al., Science 357, 6348 (2017). [2] Ghosh et al., Phys. Rev. Lett. 125, 207601, (2020).

FM 4.9 Mon 17:30 BEY/0138

**Tuning the Properties of the Organic Supramolecular Ferroelectric BTA by Dipole Engineering** — •Sophia Klubertz[1], Florian Behrendt[2], Johannes Brendel[2], and Martijn Kemerink[1] — [1]IMSEAM, Heidelberg University, Germany — [2]Bayreuth University, Germany

Benzene-1,3,5-tricarboxamide (BTA) has become the paramount example of an organic supramolecular ferroelectric. To widen the property space of these compounds, and to gain insight into the underlying structure-property relations, this work examines the impact of a stepwise replacement of BTA's three amide groups by urea groups, as well as of the anchoring point of the dipolar group. We investigate BTA-C6/2 analogues, where one (BUDA), two (BDUA), or three (BTU) amide groups are substituted by urea groups. The compounds were newly synthesized in their C-centered and N-centered versions, regarding the amide connectivity. True ferroelectric behavior was experimentally demonstrated for C- and N-centered BUDA and BDUA through temperature- and time-dependent electrical switching measurements. By investigating remnant polarization values and double structures in the switching currents, we can draw conclusions about the switching behavior of urea groups in comparison to amide groups of either connectivity. Moreover, we find orders-of-magnitude differences in key properties like retention time, which we rationalize through molecular dynamics simulations. Overall, the results show how chemical structure translates into (ferroelectric) properties.

## FM 5: Focus Session: Holistic structural and safety assessment of battery materials and cells

chairs: Carlos Ziebert (Karlsruhe Institute of Technology, DE), Philipp Finster (KIT, DE)

The focus session is dedicated to the characterization of microstructure, electrochemical, thermal and safety properties of Lithium-ion and Post-Lithium cells and their individual active and passive materials. This is required to obtain quantitative and reliable data, which are necessary to improve the current understanding in order to design and develop better and safer materials and cells. Potential topics include, but are not limited to electrochemical characterization techniques , thermal characterization techniques, safety testing, development of safer materials and cell designs, thermodynamic modelling of materials, modelling of thermal runaway and propagation.

Time: Monday 15:00–18:00 Location: BEY/0E40

FM 5.1 Mon 15:00 BEY/0E40

**Hot-pressing enhances mechanical strength of PEO solid polymer electrolyte for all-solid-state sodium metal batteries** — •Lanqing Zhao[1,2], Huaping Zhao[1], Feng Liang[2], and Yong Lei[1] — [1]Institut für Physik & IMN MacroNano* (ZIK), Technische Universität Ilmenau, 98693, Ilmenau, Germany — [2]Faculty of Metallurgical and Energy Engineering, Kunming University of Science and Technology, 650093, Kunming, China

A PEO-based composite polymer electrolyte (CPE) was successfully prepared using an emerging solvent-free hot-pressing method, with Na3Zr2Si2PO12 (NZSP) and NaClO4 incorporated to improve ionic conductivity. Benefiting from its good mechanical strength and interfacial contact with the electrodes, the Na||Na3V2(PO4)3@C all-solid-state sodium metal battery (ASSSMB) delivers a high-capacity retention of 97.1% after 100 cycles at 0.5 C and 60 °C. Furthermore, the ASSSMB with an electrolyte thickness of approximately 20 $\mu$m also demonstrates excellent cycling stability. This study provides a promising strategy for designing stable polymer-ceramic composite electrolytes through hot-pressing to realize high-energy-density sodium metal batteries.

FM 5.2 Mon 15:15 BEY/0E40

**Suppressing Li movement in solid-state electrolyte via Cryo EM Workflows: LLZO case study** — •yuqi liu[1], yuwei zhang[1], Jazmin Durate[1], Yug Joshi[1], and Baptiste Gault[2] — [1]Max Planck Institute for Sustainable Materials, 40237 Düsseldorf, Germany — [2]Univ Rouen Normandie, CNRS, INSA Rouen Normandie, Groupe de Physique des Matériaux, UMR 6634, F-76000 Rouen, France

Focused Ion Beam-Scanning Electron Microscopy (FIB-SEM) is widely used to examine solid-state battery materials and prepare site-specific samples for advanced techniques such as Electron Backscatter Diffraction (EBSD), Transmission Electron Microscopy (TEM), and Atom Probe Tomography (APT). However, the electron beam can induce irreversible damage particularly in lithium-containing systems by driving lithium displacement and expulsion, thereby compromising data reliability.

In this work, we investigate how cryogenic conditions mitigate beam-induced damage in LLZO, with an emphasis on lithium expulsion under varying beam parameters. We demonstrate that lithium mobility is significantly suppressed at cryogenic temperatures, leading to a marked reduction in beam-driven lithium redistribution. Based on a comprehensive set of cryogenically prepared EBSD and APT datasets, we show that cryo-enabled workflows are essential for obtaining structurally and chemically artefact-free characterization of LLZO and, more broadly, for reliable analysis of solid-state battery materials.

FM 5.3 Mon 15:30 BEY/0E40

**Synthesizing the Solid-State Electrolyte LLZO via the Mixed-Oxide Route: The Li loss - Reality or Fiction?** — •Daniel Wagner, Torsten E.M. Staab, and Dominik Boras — LCTM/IFB, Julius-Maximilians Universität Würzburg, D-97070 Würzburg, Röntgenring 11

The solid-state electrolyte LLZO is discussed for applications in all solid-state batteries. Undoped and Fe-doped LLZO ($Li_7La_3Zr_2O_{12}$) samples have been synthesized via the mixed-oxide route, i.e. grinding of the educt's powders followed by calcination at 950°C for 6h and a second grinding before pressing into pellets and finally sintering them at 1200°C. The excess Li content and the restrictiveness for atmospheric gas exchange during the synthesis has been varied through usage of lidded crucibles. The samples were characterized by thermogravimetric analysis (TG), mass spectroscopy of its decomposition gas (TG/MS), X-Ray-diffraction (XRD) in reflection geometry and scanning electron microscopy (SEM).The formed phases (cubic and tetragonal) were identified by XRD. The phase fraction showed a clear influence of a varying lithium-excess and/or usage of a restricted gas exchange capability. Lattice defects were investigated by the method of positron annihilation lifetime spectroscopy (PALS). PALS showed clear differences after calcination and at different stages of sintering for both un-doped and Fe-doped samples. One option may be increasingly filled Li-lattice sites after the calcination step or a formation of amorphous Li containing phases. No traces of Li were found in the decomposition gases.

FM 5.4 Mon 15:45 BEY/0E40

**Microstructure of Metal Anodes used in Solid-State Batteries and Strategies for Its Control** — •Till Fuchs — Center for Materials Research & Institute of Experimental Physics I, Justus-Liebig-University Giessen

The microstructure of materials fundamentally dictates their mechanical, electrochemical, and transport properties. Electron backscatter diffraction (EBSD) enables direct microscopic visualization of these microstructural features, providing quantitative insight into crystallographic orientation, grain morphology, and defect structures. This technique has become essential for understanding how processing pathways and operational conditions shape functional materials.

In a series of recent studies on lithium metal, we demonstrated how its microstructure can be visualized and conceptualized in detail, how it evolves depending on electrochemical cycling and charging conditions, and how it can be deliberately modified or controlled through the use of engineered interlayers. These findings highlight the interplay between microstructure and performance, and show how EBSD-guided analysis can inform strategies for guiding the growth morphology of alkali metal anodes during operation.

The principles established in lithium metal research are then extended to a broader class of energy materials, including nickel-rich layered oxides (NCM) and solid electrolytes. These systems exhibit their own characteristic microstructural challenges, from anisotropic degradation to cracking and dendrite formation in solid electrolytes.

FM 5.5 Mon 16:00 BEY/0E40

**Decoding Complex Solid Electrolyte Architectures by an NMR Simulation Approach** — •Javier Valenzuela Reina[1], Vera Barysch[2,3], Simone Köcher[2,1], Josef Granwehr[2,3], and Christoph Scheurer[1,2] — [1]Fritz-Haber-Institute der MPG, Berlin — [2]IET-1, Forschungszentrum Jülich — [3]RWTH Aachen

Advancing next-generation lithium batteries requires a detailed understanding of hybrid electrolytes and the complex organic-ceramic interfaces they contain. Nuclear magnetic resonance (NMR) spectroscopy provides a non-destructive, highly sensitive probe of interfacial structure and ion transport, which however is challenging to interpret unambiguously.

In this work, we combine different NMR experiments with theoretical modeling and high-throughput density-functional theory (DFT) simulations to investigate the structural chemistry of Al-doped lithium lanthanum zirconium oxide (LLZO), a leading hybrid electrolyte candidate. By integrating $^{27}$Al, $^{7}$Li, and $^{1}$H NMR measurements with first-principles calculations and simulated NMR parameters, we resolve key features of the Al-doping mechanism and elucidate both bulk and surface environments within the material.

Our results illustrate how a tightly coupled experimental-computational strategy can reveal interfacial behavior that is otherwise difficult to access, and highlight its promise for guiding the design and optimization of hybrid electrolytes with complex interfaces.

## Coffee break

FM 5.6 Mon 16:30 BEY/0E40

**The Inclusive Investigation of Defect Thermodynamics for Cl-Ion Battery Materials using Grand Canonical Diagrams** — •Johannes Döhn[1] and Axel Gross[1,2] — [1]Institute of Theoretical Chemistry, Ulm University, Germany — [2]Helmholtz Institute Ulm, Germany

In our contribution we use the example of chloride perovskites to discuss the crucial role of defect thermodynamics for electrode and solid electrolyte materials in Cl-ion batteries. In this regard, the energetic relation between the pristine compound, the formation of defects and the conversion into other materials under varying electrochemical conditions is of great importance, though still underexplored.

Here, we suggest an analysis based on grand canonical approaches which is frequently applied using the concepts of ab initio thermodynamics or the computational hydrogen electrode. Grand canonical diagrams contain in a compact form information on the relative stability of the pristine and defective materials as well as potential decomposition products at varying potentials and loadings. Thus they can help to predict whether topotactic or conversion reactions are to be expected during chlorination/dechlorination. Furthermore, relevant properties as the open circuit voltage or the electrochemical stability window can be read off directly from the diagrams.

We demonstrate that this inclusive investigation of all relevant thermodynamic properties presented here enables a comprehensive and intuitive access to the eludication of materials properties which can hardly be gained otherwise.

FM 5.7 Mon 16:45 BEY/0E40

**Polaron Calculations at Scale via a DFT-Based Landau-Pekar Model** — •Daria Ustimchuk, Karsten Reuter, and Christian Carbogno — Fritz-Haber-Institut der MPG, Berlin

Polarons are of ubiquitous importance in material science, be it for charge retention in energy materials or as charge reservoirs in heterogeneous catalysis. While perturbation theory allows for an accurate and efficient assessment of isolated polarons in perfect crystals [1], addressing higher concentrations in complex, disordered compounds typically requires costly hybrid density-functional theory calculations in many, extended supercells. To facilitate such investigations, we here present several strategies to accelerate the required calculations. In line with Landau-Pekar schemes, we model the mechanisms underlying polaron formation at different levels of theory, e.g., using the harmonic approximation or machine-learning potentials for describing lattice distortions and Madelung or Born effective charges for electrostatic screening effects. We discuss the pros & cons of these techniques by carefully benchmarking their accuracy and reliability for polaron formation in MgO and BiVO$_4$. Furthermore, we apply them to lithium titanium oxide (LTO), a prototypical anode material hosting elevated polaron concentrations. We demonstrate how the proposed approaches allow to semi-quantitatively predict the relevant energetics and geometric distortions, and thereby substantially accelerate the exploration of the humongous phase space associated with polaron formation in disordered energy materials.

[1] W.H. Sio *et al.*, Phys. Rev. Lett. **122**, 246403 (2019).

FM 5.8 Mon 17:00 BEY/0E40

**Grain-Boundary-Driven Activity Enabled by Grain Size Engineering in Iron-Air Batteries** — •Adam Cohen Miles[1], Yujun Zhao[1], Yan Ma[1,2], Dierk Raabe[1], and Yug Joshi[1] — [1]Max Planck Institute for Sustainable Materials, Max Planck Str. 1, 40237 Düsseldorf — [2]Department of Materials Science & Engineering, Delft University of Technology, Mekelweg 2, Delft 2628 CD, the Netherlands

Iron-air batteries are gaining renewed attention as cost-effective candidates for long-duration energy storage. While research to date has focused on improving anode performance through surface area enhancement or chemical additives, the role of iron microstructure in dictating electrochemical behavior remains unexplored. Here, we systematically isolate and examine the effect of grain size on the electrochemical activity of high-purity iron anodes by eliminating confounding factors such as porosity, dopants, and additives. The results reveal a strong inverse correlation between grain size and electrochemical performance, with ultrafine-grained anodes exhibiting substantially higher current densities and diffusive contributions than coarser grained counterparts. This enhancement is attributed to the increased grain boundary density, which promotes charge transfer and mitigates surface passivation. These findings represent the first direct demonstration of grain-size-controlled electrochemical activity in iron-air systems and establish microstructural engineering as a powerful design lever for performance optimization.

FM 5.9 Mon 17:15 BEY/0E40

**Bismuth telluride (Bi2Te3) incorporated on 3D-printed carbon electrode for rechargeable aqueous ammonium-ion battery** — •Sunny Nandi[1] and Martin Pumera[2] — [1]NTC, University of West Bohemia in Pilsen, Pilsen, Czech Republic — [2]NTC, University of West Bohemia in Pilsen, Pilsen, Czech Republic

Lithium-ion batteries are leading the battery market but there are ever growing concerns over the sustainability of Li-based batteries due to paucity and escalating cost of Li-resources. Therefore, it become increasingly important to develop a low cost and easily processable novel energy storage technologies in the future. Hence, ammonium-ion battery based on aqueous electrolyte hold great potential owing to their low cost, high safety and excellent electrochemical characteristics. In an effort to develop such NH4+ ion based rechargeable electrochemical cells. Herein, for the first time, we report here the working of a rechargeable aqueous ammonium (NH4+) ion battery by integrating a topological insulator, bismuth telluride (Bi2Te3), onto a 3D printed nanocarbon electrode as anode and copper hexacyanoferrate (CuHCF) as the cathode. Taking advantage of the 3D porous framework and the non-metallic nature of NH4+ ions, the ammonium-ion cell delivers a high energy density of 134.8 Wh kg*1 and a power density of 1800 W kg-1 in 1 M (NH4)2SO4, outperforming previously reported studies. Furthermore, ex-situ characetrization clearly explain the plausible storage mechanism of NH4+ insertion. We show immense promise of the system by recycling and reusing the used 3D printed nanocarbon electrode for next-generation energy storage systems.

FM 5.10 Mon 17:30 BEY/0E40

**Investigation of Degradation Mechanisms in High-Nickel NMC Cathodes for Lithium-Ion Batteries** — •Yosra Dammak — Max Planck Institute for Sustainable Materials, Düsseldorf, Germany

High-nickel layered oxides like NMC955 are attractive cathode materials for lithium-ion batteries. However, their long-term use is often hindered by structural and mechanical degradation during cycling.

This study examined the influence of electrode microstructure and cycling parameters on the performance and degradation of NMC955 cathodes, comparing two average grain sizes: NMC-1.0 (1 micrometer) and NMC-0.5 (0.5 micrometer). The finer-grained NMC-0.5 consistently outperformed NMC-1.0, showing higher specific capacity, better capacity retention, and superior rate capability. Post-mortem analysis indicated that NMC-1.0 suffered from extensive intergranular cracking, while NMC-0.5 particles mostly remained intact. Microstructural analysis (SEM and EBSD) revealed that the coarser NMC-1.0 accumulated higher, heterogeneously distributed strain, especially at the grain boundaries, which promoted fracture. Conversely, the finer NMC-0.5 accommodated strain through more distributed deformation, facilitated by faster grain boundary diffusion. Both grain sizes maintained their layered structure as confirmed by XRD.

In summary, the enhanced electrochemical and microstructural stability of the finer-grained NMC-0.5 is attributed to its ability to manage strain more effectively, contrasting with the strain-induced cracking observed in the coarser NMC-1.0.

FM 5.11 Mon 17:45 BEY/0E40

**Sodium Contamination Impact on Performance of Lithium-Ion Battery Cells** — •Slaheddine Jabri[1], Krum Banov[2], Anita Röstek[3], Wibke Dempwolf[4], Olaf Rienitz[3], Petr Novák[2], Markus Etzkorn[1], and Uta Schlickum[1] — [1]Institute of Applied Physics Mendelsohnstraße 2, 38106 Braunschweig, Germany — [2]Institute of Energy and Process Systems Engineering, Langer Kamp 19b, 38106 Braunschweig, Germany — [3]Physikalisch-Technische Bundesanstalt (PTB), Bundesallee 100, 38116 Braunschweig, Germany. — [4]Institut für Technische Chemie, Hagenring 30, 38106 Braunschweig, Germany

Sodium impurities can enter battery materials through several contamination sources, particularly when NaCl or NaOH are used in the recycling processes. Residual sodium is difficult to eliminate completely, and due to its high solubility, it easily dissolves into the electrolyte, where it may influence the cell performance. In this work, the electrochemical testing of high power NMC881-Graphite cells was studied using LP572 electrolyte containing sodium Na+ impurities with various concentrations. It was found that the discharge capacity decreased drastically and increase of impedance compared to Na+ free electrolyte. The Na+ ion sodium could intercalate between the Graphen layers like Li+ and due to its big ionic radius and higher charge density modify the C-C bonding and lattice parameters. The degradation effects could be found with 3 ppm Na level as impurity in electrolyte.

## FM 6: Focus Session: Materials Discovery I – Material informatics

chairs: Anna E. Böhmer (Ruhr Universität Bochum, DE), Suguru Yoshida (Kyoto University, JP)

Discovering new functional materials is crucial to advance today's technologies, ranging from caloric cooling via catalysis to next-generation energy conversion and storage, such as thermoelectric, ferroelectric, and ionic conductor materials. New materials also form the basis for potential applications in quantum information technologies. This session provides a platform to highlight functional materials discoveries and how they come about. Notably, systematic searches with high-throughput synthesis approaches, as well as predictions from materials informatics, have helped to go beyond serendipitous discoveries in recent years. However, intuition guided by general principles remains an important factor. In this session, we particularly welcome contributions that showcase the discovery of new functional materials with original approaches. Diverse material systems - from well-established to emerging and niche classes across condensed-matter and materials physics - will be featured. Bringing together diverse discoveries in a single session will help delineate general principles and inspire future work.

Time: Tuesday 9:30–12:45 Location: BEY/0138

**Invited Talk** FM 6.1 Tue 9:30 BEY/0138

**Robust Data Generation, Heuristics and Machine Learning for Materials Design** — •Janine George — BAM Berlin, Germany — University of Jena

Machine learning (ML) offers new routes to overcome the limitations of density functional theory (DFT) for advanced materials. We present data-generation strategies and workflows for ML interatomic potentials, including large-scale quantum-chemical bonding analysis.[1,2,3] Incorporating bonding descriptors into ML models enables prediction of phononic properties and validation of correlations between bonding strength, force constants, and thermal conductivity.[3] We introduce autoplex, an automated framework for training ML potentials, supporting general-purpose and phonon-focused workflows.[4] These developments provide a basis for fine-tuning foundation models for thermal transport at reduced cost.[5] For properties such as magnetism or synthesizability, we discuss complementary approaches, comparing ab initio methods with chemical heuristics and experimental data-driven ML models.[6,7] Our work advances scalable, accurate simulations for materials discovery.

References: [1] M. K. Horton, et al. Nat. Mater. 2025, 24, 1522*1532. [2] A. M. Ganose, et al., Digit. Discov. 2025, 4, 1944*1973. [3] A. A. Naik, et al. Sci. Data 2023, 10, 610. [4] Y. Liu, et al. Nat. Commun. 2025, 16, 7666. [5] J. Bustamante, et al. 2025, DOI 10.48550/arXiv.2510.23133. [6] S. Amariamir, et al. Digit. Discov. 2025, 4, 1437*1448. [7] K. Ueltzen, et al. 2025, DOI 10.26434/chemrxiv-2025-xj84d.

FM 6.2 Tue 10:00 BEY/0138

**Data-driven Discovery of 2D Non-van der Waals Materials and Design of Their Heterostructures** — Anastasiia Nihei[1,2], Tom Barnowsky[1,2], and •Rico Friedrich[1,2] — [1]TU Dresden — [2]Helmholtz-Zentrum Dresden-Rossendorf

Two-dimensional (2D) materials and their heterostructures are a platform to realize advanced electronic and magnetic functionalities at the nanoscale. With traditional 2D systems extracted from weakly van der Waals (vdW) bonded bulk layered compounds, the experimental fabrication of semiconducting non-vdW 2D materials obtained from non-layered crystals [1] came as a surprise.

In our recent data-driven investigations [2], we discover several dozens of new candidates exhibiting appealing electronic, optical, and magnetic properties owing to the (magnetic) cations at their active surfaces. The electronic and magnetic properties of these next generation 2D compounds are also demonstrated to be controllable by a surface chemistry approach employing for instance hydrogen passivation [3]. Eventually, their chemically bonded interfaces in non-vdW heterostructures [4] give rise to qualitatively new properties and potential functionalities including hybrid interface bands, strong magnetic coupling, and characteristic strong moiré property variations upon twisting.

[1] A. Puthirath Balan *et al.*, Nat. Nanotechnol. **13**, 602 (2018).
[2] R. Friedrich *et al.*, Nano Lett. **22**, 989 (2022).
[3] T. Barnowsky *et al.*, Nano Lett. **24**, 3974 (2024).
[4] A. Nihei *et al.*, submitted, arXiv:2503.12209 (2025).

FM 6.3 Tue 10:15 BEY/0138

**Exfoliation and Cleavage of Crystals from a Universal Potential** — •Tom Barnowsky[1,2], Carsten Timm[3], and Rico Friedrich[1,2] — [1]Theoretical Chemistry, TU Dresden — [2]Institute of Ion Beam Physics and Materials Research, HZDR — [3]Institute of Theoretical Physics, TU Dresden

Two-dimensional (2D) materials display unique electronic, optical, and mechanical features that differ from their three-dimensional bulk counterparts. Most known 2D materials are derived from layered crystals but recent experiments reveal that even non-layered compounds can give rise to stable so called non-van der Waals (vdW) 2D sheets [1]. Current models, however, provide limited guidance for such materials: existing descriptors and computational approaches are largely tailored to vdW layered systems [2].

We present a computational framework that predicts crystal cleavage and exfoliable 2D sheets directly from arbitrary bulk structures [3]. At its core is a universal interatomic potential enabling rapid, large-scale screening of diverse materials. Two complementary algorithms detect weakly bonded planes and iteratively isolate connected 2D subunits. Applying this approach, we identify several thousand candidate 2D materials from non-layered bulk crystals, opening a systematic route to explore and design new low-dimensional materials with unprecedented chemical and structural diversity.

[1] R. Friedrich *et al.*, Nano Lett. **22**, 989 (2022)
[2] N. Mounet *et al.*, Nat. Nanotechnol. **13**, 246 (2018)
[3] T. Barnowsky, C. Timm, & R. Friedrich, Submitted (2025)

FM 6.4 Tue 10:30 BEY/0138

**Research data management for high-throughput DFT calculations using NOMAD Oasis** — •Vikrant Chaudhary[1,2], Fu Li[2], Yue Zhao[2], Joseph F. Rudzinski[1], Nathan Daelman[1], and Hongbin Zhang[2] — [1]Physics Department and CSMB, Humboldt-Universität zu Berlin, Germany — [2]Institute of Materials Science, Technical University of Darmstadt, Darmstadt, Germany

NOMAD Oasis is an open-source, locally installable version of the central NOMAD software [nomad-lab.eu] [1]. Importantly, it allows users to add custom extensions such as data schemas and workflows. In this work, we showcase two representative cases implemented in our local NOMAD Oasis: (I) high-throughput spin Hall conductivity calculations for 4486 2D materials [2], and (II) medium-throughput bulk-photovoltaic effect in 549 experimentally available two-dimensional hybrid perovskites. In both cases, data generation relies on complex computational workflows involving multiple software packages, including VASP, Wannier90, and WannierBerri. We implement a customized parser for Wannier90, and a locally developed parser for WannierBerri, with the resulting data organized based on NOMAD's built-in workflow functionalities. These examples show how NOMAD Oasis can simplify large-scale computational data management with custom parsers, automated workflows, unrestricted storage and uploads, and enhanced privacy. It also ensures compliance with the FAIR principles, making data Findable, Accessible, Interoperable, and Reusable.

[1] M. Scheidgen et al., JOSS 8, 5388 (2023).
[2] Li, F. et al., arXiv:2509.13204 (2025).

FM 6.5 Tue 10:45 BEY/0138

**Finding interoperable datasets in diverse databases via provenance and similarity analysis** — •Martin Kuban, Alvin Noe Ladines, Thea Denell, Lauri Himanen, Joseph F. Rudzinski, Claudia Draxl, and FAIRmat team — Physics Department and CSMB, Humboldt-Universität zu Berlin, Germany

Collecting data from different sources has the potential to significantly increase the amount of available data for data-driven discovery. However, different producers of data use distinct methods and setups, e.g., approximations and parameters used in computational data, to achieve the best data quality for the properties that are studied in a specific project. Bringing these data together requires to understand the impact of the method and setup on the accuracy and precision of the produced data. In order to do so, two key requirements must be fulfilled: First, the provenance and metadata of each data point need to be recorded. This can be achieved by leveraging the NOMAD infrastructure[1, 2], an ecosystem of parsers, schemas, and workflow tools, to extract rich metadata and provenance information. Second, using this information, similarity metrics can be used to identify data that achieve similar precision besides distinct computational setups[3]. We showcase our approach on different examples using data from NOMAD.

[1] Draxl and Scheffler, MRS Bulletin **9** (2018), 676-682.
[2] Scheidgen *et al.*, Journal of Open Source Software **8** (2023), 5388.
[3] Kuban *et al.*, MRS Bulletin **47** (2022), 991-999.

## Coffee break

FM 6.6 Tue 11:15 BEY/0138

**Search for thermodynamically stable ambient-pressure superconducting hydrides in GNoME database** — Antonio Sanna[1,2], Tiago F. T. Cerqueira[3], Ekin Dogus Cubuk[4], Ion Errea[5,6,7], and •Yue-Wen Fang[6] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]nstitut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [3]CFisUC, Department of Physics, University of Coimbra, Rua Larga, 3004-516 Coimbra, Portugal — [4]Periodic Labs, San Francisco, CA, USA — [5]Fisika Aplikatua Saila, Gipuzkoako Ingeniaritza Eskola, University of the Basque Country (UPV/EHU), Europa Plaza 1, 20018 Donostia/San Sebastián, Spain — [6]Centro de Física de Materiales (CFM-MPC), CSIC-UPV/EHU, Manuel de Lardizabal Pasealekua 5, 20018 Donostia/San Sebastián, Spain — [7]Donostia International Physics Center (DIPC), Manuel de Lardizabal Pasealekua 4, 20018 Donostia/San Sebastián, Spain

There are very few ambient-pressure hydride superconductors in experiment, and their critical temperatures ($T_c$) are typically $< 10$ K. Herein, by combining machine learning techniques with ab initio methods, we have identified 25 cubic thermodynamically stable hydrides with $T_c$ beyond the boiling point of liquid helium (4.2 K) from the GNoME database. These cubic hydrides all crystallize in double-perovskite-like or fluorite-like structures, and most of them demonstrate $T_c$ lower than 10 K. Our study provide more candidates for the study of ambient-pressure superconductivity in the hydrides that can be very likely to be synthesized in experiment despite the low $T_c$.

FM 6.7 Tue 11:30 BEY/0138

**Exploration of high-entropy alloys for key electrochemical reactions: a comparative study for the solid solution systems X-Pd-Pt-Ru (X=Cu, Ir, Ni)** — •Jan Lukas Bürgel[1], Rico Zehl[1], Felix Thelen[1], Ridha Zerdoumi[1,2], Olga A. Krysiak[2], Benedikt Kohnen[1], Ellen Suhr[1], Wolfgang Schuhmann[2], and Alfred Ludwig[1] — [1]Chair for Materials Discovery and Interfaces, Institute for Materials, Faculty of Mechanical Engineering, Ruhr University Bochum, Bochum, Germany — [2]Analytical Chemistry - Center for Electrochemical Sciences (CES), Faculty of Chemistry and Biochemistry, Ruhr University Bochum, Bochum, Germany

Developing new electrocatalysts is essential for green energy technologies such as hydrogen production, fuel cells, and environmental remediation. Compositionally complex solid solutions offer vast opportunities for catalyst discovery due to their tunable surface sites, but exploring their large compositional spaces requires optimised strategies. Using a high-throughput approach, the electrocatalytic activity of the three quaternary systems X-Pd-Pt-Ru (X = Cu, Ir, Ni) was screened for four reactions in alkaline media: oxygen evolution, oxygen reduction, hydrogen evolution, and nitrate reduction reaction. Thin-film materials libraries were synthesised and characterised to identify composition-activity relationships, while also considering relevant information on crystal structure and surface morphology. The resulting multidimensional dataset reveals clear trends, similarities, and distinct activity maxima, demonstrating the effectiveness of this approach for navigating complex multinary systems.

FM 6.8 Tue 11:45 BEY/0138

**Phase formation and stability of transition-metal solid solutions containing volatile elements** — Martin Kostka[1], Luqman Mustafa[1], Jill Fortmann[2], Aurelija Mockute[2], Alan Savan[2], Susanne Kunzmann[3], Anna Grünebohm[3], Alfred Ludwig[2], Andreas Kreyssig[1], and •Anna E. Böhmer[1] — [1]Experimental physics IV, Ruhr University Bochum, 44801 Bochum, Germany — [2]Materials Discovery and Interfaces, Institute for Materials, Ruhr University Bochum, 44801 Bochum, Germany — [3]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr University Bochum, 44801 Bochum, Germany

In the combinatorial synthesis of thin films, multiple elements are simultaneously deposited to achieve well-defined composition gradients and create a materials library. However, including volatile elements directly into the combinatorial synthesis is a challenge. Here, we use instead a two-step synthesis process combining combinatorial cosputtering with a separate ex-situ reaction step with the volatile elements Se and Sb. In particular, we investigate the phase formation and stability of the (Fe,Ni)$Sb_2$ and (Fe,Cr)$Sb_2$ solid solutions in the orthorhombic marcasite structure. Further, we study the (Fe,Co)$Se_2$ solid solution, which is on the brink of transformation from orthorhombic marcasite to cubic pyrite structure. Our preparation route with a separate low-temperature synthesis step permits detailed studies of solid solutions and phase diagrams at well-defined temperatures.

FM 6.9 Tue 12:00 BEY/0138

**AI for Complex Catalytic Systems: C2 Catalysis** — •Haobo Li — Nanyang Technological University, Singapore

AI-driven big data set analysis offers opportunities for theoretical research on systems that combine complex catalyst materials with intricate catalytic reactions. In this study, we explore high-entropy alloys

(HEAs) as potential electrocatalysts for the electrochemical semihydrogenation of acetylene. HEAs provide a variety of surface active sites due to the diverse combination of constituent elements, while the presence of bidentate dicarbon species further complicates surface interactions. By integrating density functional theory computations, geometric optimizer development, and graph neural network-based machine learning predictions, we efficiently compile a comprehensive database of 52,900 adsorption properties for AgAuCuNiPd HEA surfaces. Lasso regression and t-SNE projection reveal the distinct influences of the five metal components on adsorption and reaction properties. Using Cu as a reference, logistic regression assesses the potential for other components to surpass Cu in terms of catalytic activity and selectivity toward ethylene. Our findings suggest that, while HEAs can enhance the reaction, the ternary AgAuCu alloy achieves optimal results, indicating that high entropy is not essential. This research methodology can be extended to other complex catalytic systems, providing valuable insights into catalytic mechanisms and facilitating experimental endeavors.

FM 6.10 Tue 12:15 BEY/0138

**Compositional and Structural Impact on the Hydrogen Evolution Reaction Activity across Noble-Metal-Based Compositionally Complex Solid Solutions Thin Film Libraries** — •Natalia Pukhareva[1], Moonjoo Kim[2], Felix Thelen[1], Geovane Arruda de Oliveria[2], Rico Zehl[1], Wolfgang Schuhmann[2], and Alfred Ludwig[1] — [1]Materials Discovery & Interfaces, Ruhr University Bochum — [2]Analytical Chemistry - Center for Electrochemical Sciences (CES), Ruhr University Bochum

Compositionally complex solid solutions (CCSS) stabilize multielement alloys and allow tuning of surface chemistry for the hydrogen evolution reaction (HER). Three quinary libraries (Ir-Pd-Pt-Rh-Ru, Ag-Au-Pd-Pt-Ru, Ag-Au-Cu-Pd-Pt) were prepared by sputtering and mapped across 342 positions each. Energy-dispersive X-ray spectroscopy (EDX) confirmed smooth composition gradients, and X-ray diffraction (XRD) showed fcc solid solutions with minor hcp fractions in Rh-Ru-rich regions and no detectable phase effect on HER. X-ray photoelectron spectroscopy (XPS) with Gaussian-process regression revealed composition-dependent surface segregation and distinct surface compositions. HER activity, measured by scanning electrochemical cell microscopy (SECCM), followed Ir-Pd-Pt-Rh-Ru > Ag-Au-Pd-Pt-Ru > Ag-Au-Cu-Pd-Pt. In the Ag-containing libraries Pd-rich compositions outperformed Pt-rich ones, and in Ag-Au-Cu-Pd-Pt Ag-rich regions exceeded Cu-rich regions despite Cu's higher intrinsic activity, consistent with segregation limiting surface Pt and Pd and indicating that HER in these CCSS is dominated by multielement interactions.

FM 6.11 Tue 12:30 BEY/0138

**Soft Degradable Magnetic Microcarriers for Encapsulation and Guided Transport of Drugs and 3D Spheroids** — •Lulu Song, Xinne Zhao, Xuan Peng, Željko Janićijević, Lin Guo, Denys Makarov, and Larysa Baraban — Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Soft microrobots hold strong promise for next-generation biomedical applications, including targeted drug delivery, tissue engineering, and minimally invasive therapies. However, their translation remains limited by challenges in scalable fabrication, controlled biodegradation, and insufficient co-encapsulation and transport of diverse cargos. Here, we present degradable hydrogel microcarriers fabricated via droplet-based microfluidics and UV photopolymerization, enabling scalable production with tunable properties. These microcarriers can co-encapsulate therapeutic molecules, superparamagnetic particles, and living cell spheroids, supporting multifunctional delivery strategies. Their motion is precisely actuated under externally applied gradient magnetic fields, allowing guided navigation in microchannels for targeted delivery. Importantly, the microcarriers exhibit programmable degradation under physiological conditions, providing temporary mechanical integrity, controlled release, and safe post-treatment clearance, with complete degradation at 37 °C within several days. Overall, this platform offers a robust and biocompatible soft microrobotic system for targeted therapies, micro-tissue transport, and diagnostic monitoring, representing a promising step toward clinical translation.

## FM 7: Crystal Defects and Real Structure Physics in Diamond and Functional Materials I

chair: Theo Scherer (Karlsruhe Institute of Technoloy, DE)

Time: Tuesday 9:30–11:45 Location: BEY/0E40

FM 7.1 Tue 9:30 BEY/0E40

**Fluorescence lifetime measurements of NV- and NV0 color center ensembles at room temperature and 4K in HPHT, CVD and nanodiamond samples** — •Kai Kühnlenz, Kevin Lauer, Phillip Kellner, Mario Bähr, Andreas T. Winzer, and Thomas Ortlepp — CiS Forschungsinstitut für Mikrosensorik GmbH, Konrad-Zuse-Str. 14, 99099 Erfurt, Deutschland

Nitrogen vacancy (NV) centers in diamond are key solid-state quantum emitters whose photophysical properties depend on their charge state and the surrounding diamond lattice. We analyze diamond samples made of chemical vapor deposition- (CVD), high-pressure-high-temperature- (HPHT) or nanodiamond material by exciting them with a 513nm green laser and detecting the fluorescence light via time resolved photoluminescence (TRPL). This work presents measurements of the fluorescence lifetime of NV-ensembles. Hereby a monochromator is employed to detect 20nm wide spectral bands centered at the NV- phonon sideband (710nm) and the zero-phonon-lines of NV- and NV0 (638nm and 575nm) to differentiate between the charge states. Measurements are performed at both room temperature (293K) and 4K. The influence of varying excitation laser power and of the selected spectral detection window is investigated and compared with established reference values. The measurement approach allows a systematic comparison of NV-diamond materials and provides a baseline for quantitative lifetime-based characterization of NV ensembles.

FM 7.2 Tue 9:45 BEY/0E40

**Diamond windows for microwave application: numerical analyses and characterization by microscope and Raman measurements** — •Gaetano Aiello, Andreas Meier, Theo Scherer, Sabine Schreck, and Dirk Strauss — Karlsruhe Institute of Technology, Institute for Applied Materials, 76021 Karlsruhe, Germany

Electron cyclotron heating and current drive systems in nuclear fusion devices feature optical quality polycrystalline diamond windows for the transmission of microwave beams of 1 to 2 MW power. The windows consist of diamond disks of 1 to 2 mm thickness integrated into a metallic housing. Numerical analyses verify the performance of such windows with respect to temperature and stress limits. In this work, examples of analyses are provided with reference to a Brewster-angle window design featuring a first-of-its-kind manufactured diamond disk with 180 mm diameter. For the first time, instead of a single constant value, the entire map of the loss tangent measured over the disk has been given as input to the analysis. In addition, examples of microscope and Raman investigations of the disks are shown with reference to dark microfeatures and residual stresses generated by the chemical vapour deposition process.

FM 7.3 Tue 10:00 BEY/0E40

**Investigation of irradiation effects in artificial diamond** — •Theo Andreas Scherer and Francesco Mazzocchi — Karlsruhe Institute of Technology KIT-IAM-AWP 76344 Eggenstein-Leopoldshafen

Diamond is used as window material for high power microwave transmission to heat plasmas and to perform diagnostics in nuclear fusion devices like ITER, Wendelstein 7X or ASDEX-UG. In such environments neutron and gamma radiation has a quite important influence on dielectric and thermal properties of diamond. Spectroscopic investigations, like RAMAN, cathode luminescence or EPR can detect all the defects produced by irradiation. Swift heavy ion and neutron irradiation was us to study defect chemistry and physics in diamond (single crystalline and polycrystalline diamond samples). Newest results of this investigation are presented.

FM 7.4 Tue 10:15 BEY/0E40

**EC Heating systems for present and future fusion experiments and power plants** — •Peter Späh — KIT, Institute for Applied Materials, Karlsruhe, Germany

CVD diamond windows are an essential component in Electron Cyclotron (EC) plasma heating and stabilisation systems for nuclear fusion reactors. Beside the characterisation and qualification of CVD diamond disks and the design and analysis of CVD diamond window assemblies, the Institute for Applied Materials (IAM) at Karlsruhe Institute of Technology (KIT) also contributes to concept findings, layout, design and integration of EC heating systems for several fusion experiments and power plant studies.

Experimental fusion devices and future fusion power plants with magnetic confinement require powerful heating systems for plasma core heating, plasma disruption mitigation, breakdown of gas, plasma ramp-up and -down, impurity control and to counteract thermal instabilities. Electron Cyclotron Resonance Heating (ECRH) is one of these heating systems. Microwave beams in the frequency range of 80 to 240 GHz are generated by gyrotrons and subsequently transmitted via waveguides and an antenna into the plasma chamber, where they interact with the electrons.

This talk gives an overview on the design status of the EC heating antennas for the EU DEMO fusion power plant and for the Volumetric Neutron Source (VNS) which is a conceptual study of a beam-driven Tokamak, serving as test-bed for full-sized breeding blanket modules.

**coffee break**

FM 7.5 Tue 10:45 BEY/0E40

**Application of Raman and Photoluminescence Spectroscopy to MgO-C Refractories** — •Julia Richter[1], Felix Drechsler[1], Till Stadtmüller[2], Cameliu Himcinschi[1], Christos Aneziris[2], and Jens Kortus[1] — [1]Technische Universität Bergakademie Freiberg - Institut für Theoretische Physik, Leipziger Straße 23, 09599 Freiberg, Germany — [2]Technische Universität Bergakademie Freiberg - Institut für Keramik, Feuerfest und Verbundwerkstoffe, Agricolastraße 17, 09599 Freiberg, Germany

By applying Raman and photoluminescence (PL) spectroscopy in the visible and near-infrared range to MgO, magnesia-carbon (MgO-C) refractory bricks - partially produced from recycled magnesia - are examined in hardened and coked state, and compared with nominally pure MgO powder as a reference. Two sharp, high-intensity PL signals (699 nm and 871 nm), each accompanied by symmetrical sidebands, are investigated by varying the excitation wavelength (532, 633, and 785 nm). The 699 nm PL feature observed for both brick and reference arises from $Cr^{3+}$ impurities within the MgO lattices, whereas the 871 nm signal, associated with $V^{2+}$, appears only in the brick-derived MgO. To elucidate the origin of the symmetrical sidebands, temperature-dependent spectroscopic measurements from 100 to 295 K are performed, monitoring the intensity ratio of the higher-energy (anti-Stokes) and lower-energy (Stokes) sidebands. The results confirm phonon participation in both the $MgO:Cr^{3+}$ and $MgO:V^{2+}$ emission processes. Together, these findings connect fundamental defect physics with practical considerations in refractory material science.

FM 7.6 Tue 11:00 BEY/0E40

**Creation of Color Centers in Magnesium Fluoride Single Crystals by Irradiation with MeV Heavy Ions** — •Ayman El-Said — Physics Department and Interdisciplinary Research Center for Advanced Materials, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia

The irradiation of ionic halide single crystals with MeV heavy ions can lead to the creation of various types of color centers [1]. Here, MgF2 single crystals were irradiated with MeV heavy ions of different energies and fluence [2]. UV-Vis spectroscopic measurements demonstrate the existence of F1-, F2-, and F3-centers due to ion irradiation. The type, concentration and creation efficiency of the observed color centers are studied in terms of ion fluence and energy loss. The results are not only of high importance for understanding the creation mechanism of the induced color centers but also for the degradation of optical materials in high-altitude and space environments.

Acknowledgements: Parts of this research were carried out at the Ion Beam Center at the Helmholtz-Zentrum Dresden-Rossendorf e. V., a member of the Helmholtz Association. Ayman S. El-Said acknowledges the support by KFUPM, Saudi Arabia (Project: ISP24236).

[1] K. Schwartz, C. Trautmann, A.S. El-Said, R. Neumann, M. Toulemonde, W. Knolle, Phys. Rev. B 70, 184104 (2004). [2] A.S. El-Said, Rad. Phys. and Chem. 227, 112369 (2025).

FM 7.7 Tue 11:15 BEY/0E40

**Oxygen vacancies in vanadium dioxide: A DFT+$V$ study** — •Oskar Leibnitz[1,2], Peter Mlkvik[1], Nicola A. Spaldin[1], and Claude Ederer[1] — [1]Materials Theory, Department of Materials, ETH Zurich, Switzerland — [2]Present address: Multifunctional Ferroic Materials, Department of Materials, ETH Zurich, Switzerland

We present a density-functional theory study of the effects of oxygen vacancies on the structural and electronic properties of vanadium dioxide ($VO_2$). Our motivation is the reported suppression of the metal-insulator transition by oxygen vacancies and the lack of a clear consensus on its origin. We use the DFT+$V$ method with a static intersite vanadium-vanadium interaction term, $V$, to calculate the properties of the oxygen-deficient metallic rutile and insulating monoclinic M1 phases of $VO_2$ on the same footing. We find that oxygen vacancies induce local distortions in the M1 phase, but do not destroy the dimerization usually associated with the insulating behavior. In spite of this, we find that the M1 phase becomes metallic as a result of the partial filling of the conduction band due to a rigid-band-like doping effect.

FM 7.8 Tue 11:30 BEY/0E40

**Distortion tensor around dislocations in GaN studied by electron backscatter diffraction and cathodoluminescence spectroscopy** — •Domenik Spallek, Vladimir Kaganer, Oliver Brandt, Thomas Auzelle, and Jonas Lähnemann — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

The effect of elastic distortion in the vicinity of a threading dislocation (TD) in GaN on its luminescence has been shown previously [1]. However, quantifying this distortion and its components remains a challenge. Therefore, we investigate individual TDs by correlated high-resolution electron backscatter diffraction (HR-EBSD) and cathodoluminescence (CL) spectroscopy. The sample is a high-purity, homoepitaxial GaN layer grown by molecular beam epitaxy with a low TD density.

A cross-correlation analysis with the software CrossCourt from BLG Vantage is used to determine the spatially-resolved components of the distortion tensor from the HR-EBSD results [2]. Signatures of the TDs are resolved in the elastic strain and rotation components. Through reference measurements, we explore the resolution limit of this analysis and its dependence on the material and measurement conditions. Hyperspectral CL maps show a reduced intensity as well as a shifted emission wavelength around the TD. With additional modeling of the distortion around a TD, these correlated measurements are related to the Burger's vector of the dislocation, determining its type.

[1] Kaganer *et al.*, Phys. Rev. Appl. **12**, 054038 (2019).

[2] Wilkinson *et al.*, Ultramicroscopy **106**, 307 (2006).

# FM 8: Multiferroics and Magnetoelectric Coupling (joint session MA/FM)

Time: Tuesday 9:30–12:30 Location: POT/0112

FM 8.1 Tue 9:30 POT/0112

**Electric polarization driven by non-collinear spin alignment: first principles calculations** — •Sergiy Mankovsky[1,3], Svitlana Polesya[1], Jan Minar[2], Hongbin Zhang[3], and Hubert Ebert[1] — [1]Ludwig Maximilian University of Munich, Munich, DE — [2]University of West Bohemia, Pilsen, CZ — [3]TU Darmstadt, Darmstadt, DE

We present an approach for first principles investigations of the spin driven electric polarization in type II multiferroics. We propose a parametrization of the polarization with the parameters calculated using the multiple scattering Green function (KKR-GF) formalism. On this basis, the induced electric polarization of a unit cell can be represented in terms of three-site parameters. Those antisymmetric with respect to a spin permutation can be seen as an ab-initio based counter-part to the phenomenological parameters used in the inverse-DMI model. Beyond to this, our new approach gives direct access to the element- and site-resolved electric polarization. To demonstrate the capability of the approach, we consider several examples, for which the magneto-electric effect is observed either as a consequence of an applied magnetic field ($Cr_2O_3$), or as a result of a phase transition to a spin-spiral magnetic state ($MnI_2$ and $AgCrO_2$).

FM 8.2 Tue 9:45 POT/0112

**Competition Between Multiferroic and Magnetic Soliton Lattice States in DyFeO3** — •Nikita Andriushin[1], Stanislav Nikitin[2], Oystein Fjellvag[1,3], Ekaterina Pomjakushina[2], Alexandra Turrini[2], Sergey Artyukhin[4], Christof Schneider[2], and Maxim Mostovoy[5] — [1]TU Dresden, Germany — [2]PSI, Switzerland — [3]IFE, Norway — [4]IIT, Italy — [5]University of Groningen, The Netherlands

Simultaneous breaking of time-reversal and inversion symmetries in multiferroics couples ferroelectricity to magnetism and produces unusual phenomena relevant for next-generation electronics. A notable case is $DyFeO_3$, which under magnetic fields shows a giant linear magnetoelectric response and a large spontaneous polarization arising from coexisting Fe and Dy orders. Using high-resolution neutron diffraction, we demonstrate that at zero field $DyFeO_3$ hosts an incommensurate magnetic soliton lattice formed by spatially ordered Dy domain walls with an average size of 231(8) Å. Long-range interactions between these walls are mediated by magnons in the Fe subsystem, analogous to a Yukawa force. An applied magnetic field destroys the incommensurate order, restores the linear magnetoelectric response, and stabilizes the ferroelectric state. The magnetic domain walls carry electric charge, and the soliton array dimerizes when both electric and magnetic fields are applied. Simulations using experimental parameters indicate that competition between ferroelectric and incommensurate states can be effectively tuned by an electric field.

FM 8.3 Tue 10:00 POT/0112

**Magnetoelectric coupling in antiferromagnetic $BiCoO_3$** — •Veronica Goian[1], Fedir Borodavka[1], Petr Proschek[2], Maxim Savinov[1], Christelle Kadlec[1], Hong Dong Nguyen[1], Andrei A. Belik[3], and Stanislav Kamba[1] — [1]Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic — [2]Department of Condensed Matter Physics, Charles University, Prague Czech Republic — [3]National Institute for Materials Science: Tsukuba, Ibaraki, Japan

$BiCoO_3$ is a potential multiferroic material with a C-type antiferromagnetic phase transition at $T_N$=470 K and a hypothetical ferroelectric phase transition around 1000 K (the sample decomposes at around 470 °C).[1] First-principles calculations predict an unusually strong antimagnetoelectric coupling in $BiCoO_3$.[2] However, no experimental measurements have been reported in the literature to determine the magnetoelectric coupling or related structural properties. This is mainly because $BiCoO_3$ requires high-pressure and high-temperature sintering. We have measured the dielectric permittivity, ferroelectric hysteresis loops, and Raman, THz, and IR spectra to probe the ferroelectric behavior. In addition, we found that $BiCoO_3$ exhibits well-measurable non-linear magnetoelectric coupling.

[1] Oka et al., J. Am. Chem. Soc., 132, 9438-9443 (2010)

[2] Braun et al., Phys. Rev. B, 110, 144442(2024)

FM 8.4 Tue 10:15 POT/0112

**Investigation of the piezomagnetic effect in $CaBaCo_4O_7$** — •Jyotiranjan Rout[1], Yusuke Tokunaga[2], Yasujiro Taguchi[2], Yoshinori Tokura[2], Bernd Büchner[1,3], and Vilmos Kocsis[1] — [1]IFW-Dresden — [2]RIKEN, CEMS, Japan — [3]TU-Dresden

In a magnetoelectric material the electric and magnetic responses are intertwined and cross control via the application of external magnetic and electric field are enabled. Ferroelectric polarization implies a special distortion of the lattice where dipolar moment related to the separation of the positive and negative ions are not compensated within the unit cell. Therefore we immediately can imagine the intricate and complicated connection between the magnetoelectric and magnetoelastic properties of a multiferroic.

The Swedenborgite $CaBaCo_4O_7$ exhibits a polar structure, which is accompanied by a ferrimagnetic order at $T_C$=62 K and a record large change in the ferroelectric polarization. Correspondingly, former magnetoelastic measurements have indeed confirmed the presence of a giant magnetoelastic distortion close to $T_C$; However, less is known about the magnetoelastic anisotropies.

Here, we report a detailed study of the magnetoelastic anisotropy, completing the connection between magnetoelasticity and magnetoelectricity in this material family. We also report on an unusual feature of the piezomagnetic effect, which suggests the importance of the orbitals in the piezomagnetoelectric effects.

FM 8.5 Tue 10:30 POT/0112

**Multiferroic altermagnetism and magneto-orbital excitations in monolayer VCl3** — •Luigi Camerano[1,2], Adolfo Otero Fumega[3], Alessandro Stroppa[2], Jose Lado[3], and Gianni Profeta[1,2] — [1]University of L'aquila, 67100 L'Aquila, Italy — [2]CNR-SPIN L'Aquila, 67100 L'Aquila, Italy — [3]Aalto University, 02150 Espoo, Finland

Van der Waals monolayers featuring magnetic states provide fundamental building blocks for artificial quantum matter. In this contribution I will present the emergence of a symmetry broken multiferroic ground state featuring magneto-orbital excitations and nematic d-wave altermagnetism in monolayer VCl3 [1-4]. All these physics arises from a pure electronic symmetry breaking ultimately stabilizing an antiferro-orbital order ground state showing the emergence of an electronic polarization. Recent experimental evidence report signatures of symmetry breakings and ferroelectricity combined with 2D magnetism, establishing monolayer VCl3 as a novel 2D multiferroic driven by orbital ordering.

References

1. Mastrippolito D., Camerano L. et al. Phys. Rev. B 108,045126 (2023)
2. Camerano, L. et al. 2D Mater. 11, 025027 (2024)
3. Camerano, L. et al. Nano Lett. 25, 4825,4831 (2025)
4. Camerano, L. et al. npj 2D Mater Appl 9, 75 (2025)

FM 8.6 Tue 10:45 POT/0112

**Electric control of antiferromagnetic states in an insulator** — •Somnath Ghara[1], Maximilian Winkler[1], Sebastian Schmid[1,2], Lilian Prodan[1], Korbinian Geirhos[1], Vladimir Tsurkan[1,3], Wenbo Ge[4], Weida Wu[4], András Halbritter[2], Stephan Krohns[1], and István Kézsmárki[1] — [1]EP5, Institute of Physics, University of Augsburg, Germany — [2]Department of Physics, Budapest University of Technology and Economics, Hungary — [3]Institute of Applied Physics, Moldova State University, Republic of Moldova — [4]Department of Physics and Astronomy, Rutgers University, USA

Electric control of antiferromagnetic (AFM) order is highly desirable for the development of ultrafast and energy-efficient spintronic devices. In this talk, I will show that the strong linear magnetoelectric coupling in the collinear AFM insulator $Co_3O_4$ enables full isothermal control of AFM order by electric fields deep within its AFM phase, i.e. the Néel vector can be either reversed instantaneously or rotated smoothly. Importantly, we found that even in macroscopic volumes of $Co_3O_4$, the non-volatile switching between time-reversed AFM states occurs on timescales as short as a few tens of nanoseconds. These observations suggest that the quasi-cubic AFM insulators, such as $Co_3O_4$, provide an ideal platform for ultrafast manipulation of microscopic AFM domains and may lead to the realization of antiferromagnet-based spintronic devices.

Ref: S. Ghara et al., Phys. Rev. Lett. 135, 126704 (2025).

**15 min break**

FM 8.7 Tue 11:15 POT/0112

**Optical detection of magnetic order in SmFe3(BO3)4** — •Bálint Beke[1], Bence Szász[1], I. A. Gudim[2], L. N. Bezmaternykh[2], Dávid Szaller[1], and Sándor Bordács[1] — [1]Budapest University of Technology and Economics, Budapest, Hungary — [2]Krasnoyarsk, Russia

The chiral crystal structure of $SmFe_3(BO_3)_4$ hosts an easy-plane antiferromagnetic phase below 32 K. Due to the broken inversion, the magnetic order induces electric polarization in this compound, but this polarization averages out to zero when domains are randomly oriented in the ab plane. We studied the 4f-4f excitations of $Sm^{3+}$ ions using polarization resolved magneto-optical spectroscopy. Low magnetic fields, <2 T give rise to linear dichroism that we associate with the rearrangement of antiferromagnetic domains. In finite fields, we could determine the polarization selection rules in a state where the orientation of the antiferromagnetic domains is well defined. Moreover, we detected non-reciprocal absorption of light, which is a finite frequency fingerprint of the optical magnetoelectric effect.

FM 8.8 Tue 11:30 POT/0112

**A high-temperature multiferroic** $Tb_2(MoO_4)_3$ — •Shimon Tajima, Hidetoshi Masuda, Yoichi Nii, Shojiro Kimura, and Yoshinori Onose — Institute for Materials Research, Tohoku University, Sendai, Japan

We demonstrated magnetic control of ferroelectric polarization at 432 K in ferroelectric and ferroelastic $Tb_2(MoO_4)_3$, in which the polarity of ferroelectric polarization is coupled to the orthorhombic strain below the transition temperature 432 K.

The paramagnetic but strongly magnetoelastic $Tb^{3+}$ magnetic moments enable the magnetic control of ferroelectric and ferroelastic domains; the ferroelectric polarization is controlled depending on whether the magnetic field is applied along [110] or $[1\bar{1}0]$.

FM 8.9 Tue 11:45 POT/0112

**Towards topological switching in multiferroics** — •Alessandro Granero and Sergey Artyukhin — Italian Institute of Technology (IIT), Genova, Italy

Magnetoelectric switching in GdMn2O5 [1] is the first known example of topological ferroic switching, where magnetic field sweeps across the spin-reorientation transition induce incremental 90° spin rotations described by a topological winding number. While the behavior has been rationalized with a microscopic model, symmetry conditions and minimal model ingredients that enable this behavior are poorly understood. Here we use a symmetry-based Landau theory approach and demonstrate that a toy model with two frustrated antiferromagnetic subsystems and a low-symmetry anisotropy captures the topological switching behavior. The model reveals how sweeps of the driving field move the free-energy minimum continuously in spin-orientation space, in contrast to conventional ferroelectric switching that relies on fixed *P minima and domain-wall nucleation. Multiple switching pathways enabled by the simultaneous presence of E and H fields are summarized by a "switching diagram" [2], linking regions of the H and E field amplitudes to distinct sequences of magnetoelectric transitions. Small parameter variations near diagram boundaries redirect the system along different routes. The results establish a minimal model for topological switching in GdMn2O5 and guide the search for topological switching phenomena in other materials. [1] L. Ponet, et al.: Nature 607, 81-85 (2022) [2] M. Ryzhkov, A. Granero et al.: Communication Materials, in press

FM 8.10 Tue 12:00 POT/0112

**Observation of antiferromagnetic domains by low-temperature photoluminescence microscopy** — •Bence Szász — Physics Department, Budapest University of Technology and Economics, Budapest, Hungary

The optical oscillator strengths of crystal-field transitions in magnetoelectric antiferromagnets can serve as specific signatures of the underlying magnetic order. In this work, I investigate the feasibility of identifying magnetic domains using a low-temperature optical photoluminescence microscopy system.

FM 8.11 Tue 12:15 POT/0112

**Spectroscopy of coupled magnetic and electric resonances** — •Dávid Szaller[1,2], Artem M Kuzmenko[3], Alexander A Mukhin[3], Alexey Shuvaev[2], and Andrei Pimenov[2] — [1]HUN-REN-BME Condensed Matter Physics Research Group, and Department of Physics, Institute of Physics, Budapest University of Technology and Economics, Muegyetem rkp. 3., H-1111 Budapest, Hungary — [2]Institute of Solid State Physics, TU Wien, 1040 Vienna, Austria — [3]Moscow, Russia

Controllable non-reciprocal propagation of light is an intensively investigated field of optics, with studies motivated both by fundamental questions and possible telecommunication applications. So far, polarization-independent, switchable one-way transparency has been demonstrated at certain resonances of multiferroic crystals at cryogenic temperatures and in high magnetic fields, limiting the practical implementation. As an alternative approach, we present one-way transparency of an artificial layered structure consisting of split-ring metamaterial and magnetic substrate layers interacting in the dynamic regime [1]. Our quasi-optical experiments in the GHz frequency range show that this unique combination breaks time and space inversion symmetries in external magnetic field. The ease of tuning the dynamic response and the controllable one-way transparency make this approach promising for real-world applications.

[1] A. M. Kuzmenko et al., Phys. Rev. B 112, 134434 (2025).

## FM 9: Focus Session: Materials Discovery II – High throughput searches for functional magnetic materials (joint session FM/MA)

chairs: Jan Schultheiß (Norwegian University of Science and Technology, NO), Hiroki Taniguchi (Nagoya University, JP)

Discovering new functional materials is crucial to advance today's technologies, ranging from caloric cooling via catalysis to next-generation energy conversion and storage, such as thermoelectric, ferroelectric, and ionic conductor materials. New materials also form the basis for potential applications in quantum information technologies. This session provides a platform to highlight functional materials discoveries and how they come about. Notably, systematic searches with high-throughput synthesis approaches, as well as predictions from materials informatics, have helped to go beyond serendipitous discoveries in recent years. However, intuition guided by general principles remains an important factor. In this session, we particularly welcome contributions that showcase the discovery of new functional materials with original approaches. Diverse material systems - from well-established to emerging and niche classes across condensed-matter and materials physics - will be featured. Bringing together diverse discoveries in a single session will help delineate general principles and inspire future work.

Time: Tuesday 14:00–15:30 Location: BEY/0138

**Invited Talk** FM 9.1 Tue 14:00 BEY/0138

**Thin film combinatorial studies of functional magnetic mate-**

**rials** — •Nora Dempsey — Institut NEEL, CNRS/UGA, Grenoble, France

Combinatorial studies based on the preparation and characterisation of compositionally graded thin films are being used for the screening and optimization of a range of functional materials [1]. When combined with Machine Learning (ML), such high-throughput film-based studies hold much potential to guide data driven design of new materials [2,3]. In this talk I will outline our work at Institut Néel on high throughput fabrication and characterisation of functional magnetic materials as well as our recent developments concerning data handling and analysis. I will then show examples from on-going studies of the effect of composition and fabrication conditions on both structural and magnetic properties of hard magnetic and magnetocaloric materials. I will finish up by briefly outlining preliminary results from ML-driven data analysis for the accelerated development of functional magnetic materials with reduced dependence on critical elements, carried out in the framework of various collaborations. [1] ML Green et al., J. Appl. Phys. 113 (2013) 231101 [2] A.G. Kusne et al. Sci. Rep. 4 (2014) 6367 [3] A. Ludwig, npj Comput. Mater. 5 (2019) 70

FM 9.2 Tue 14:30 BEY/0138

**Potentially magnetic platinum oxides obtained by computationally guided high-pressure synthesis** — •Yasuhito Kobayashi[1], Akitoshi Nakano[2], Shunsuke Kitou[3], Tomasz Klimczuk[4], Hidefumi Takahashi[1,5], and Shintaro Ishiwata[1,5] — [1]Division of Materials Physics, The University of Osaka, Japan — [2]Department of Physics, Nagoya University, Japan — [3]Department of Advanced Materials Science, The University of Tokyo, Japan — [4]Advanced Materials Center, Gdansk University of Technology, Poland — [5]Institute for Open and Transdisciplinary Research Initiatives, The University of Osaka, Japan

The exploration of Pt-based oxides has remained significantly limited, primarily due to the high chemical inertness of platinum and the typically nonmagnetic $d^6$ or $d^8$ electronic configurations. Here, we report the discovery of a new layered homologous series of Pt-based ternary oxides, Na(PtO$_2$)$_{2n+1}$ ($n$ = 1, 2), synthesized through a combination of highly oxidizing high-pressure techniques and density functional theory (DFT) calculations. This series features unprecedented layered structural motifs composed of rutile-based PtO$_6$ octahedra and one-dimensional PtO$_4$ square-planar chains, distinct from the perovskite-based Ruddlesden-Popper oxides. We discuss the possibility that this layered homologous series represents the first realization of a magnetic Mott insulator within Pt-based oxides, where NaPt$_3$O$_6$ ($n$ = 1) exhibits localized spin behavior with an effective spin $S = 1/2$, likely arising from the unusual $d^7$ electronic configuration of square-planar Pt$^{3+}$ along with one-dimensional antiferromagnetic interactions.

FM 9.3 Tue 14:45 BEY/0138

**Magnetism and electrical and thermal transport in the natural Fe$_{1-x}$Mn$_x$WO$_4$ ($x$=0.2) mineral from Potosí, Bolivia** — •Skachko Dmytro[1], Bohdan Kundys[2], Volodymyr Levytskyi[1], Esteban Zuñiga-Puelles[1], Andreas Leithe-Jasper[3], and Roman Gumeniuk[1] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg, 09596 Freiberg, Germany — [2]Université de Strasbourg, CNRS, Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504, Strasbourg F-67000, France — [3]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany

The natural ferberite single crystal of Fe$_{0.8}$Mn$_{0.2}$WO$_4$ composition with the monoclinic NiWO$_4$-type structure ($P2/c$) [$a$ = 4.74751(6) Å, $b$ = 5.71335(7) Å, $c$ = 4.96847(5) Å, $\beta$ = 90.15(1)°] reveals multiple magnetic transitions at $T_{\mathrm{N1}} = 67(1)$ K, $T_{\mathrm{N2}} = 28(3)$ K, $T_{\mathrm{N1}}^{c_p} = 66(1)$ K and $T_{\mathrm{N2}}^{c_p} = 8(1)$ K. The reduced magnetic entropy of $\approx R\ln3$ observed near $T_{\mathrm{N1}}$ indicates the simplified $LS$-coupling scheme to fail in the description of complex magnetic behavior of the studied ferberite. The temperature dependence of electrical resistivity [$\rho(T)$] shows a semiconducting exponential decay saturating at $\approx$ 300 K. The activation energy of the decay is found to be ≈310 meV. Temperature dependence of thermal conductivity [$\kappa(T)$] is characterized by a well defined maximum at ≈68 K, which is described by the Debye-Callaway model, pointing to the dominance of phonon scattering on defects and *umklapp* processes. Despite revealing relatively low $\kappa(T)$ and high Seebeck coefficient Fe$_{0.8}$Mn$_{0.2}$WO$_4$ is rather poor thermoelectric material because of enhanced $\rho(T)$.

FM 9.4 Tue 15:00 BEY/0138

**Ab initio-based phase diagrams for compositionally complex ThMn12-type alloys** — •Sourabh Kumar[1], Semih Ener[2], and Tilmann Hickel[1] — [1]Bundesanstalt für Materialforschung und -prüfung, 12489 Berlin — [2]Technische Universität Darmstadt, 64289 Darmstadt

The structural and chemical stability of rare-earth-based transition-metal (such as Nb, Ce, and Sm) alloys is critical in determining the performance of modern hard magnets (HMs), particularly their coercivity and thermal robustness. This study examines the intrinsic phase competition in (Sm/Ce)-(Fe/Co)-Ti systems, focusing on how Ti additions influence the thermodynamic stability of high-temperature HMs. Two compositional pathways were examined: one dominated by Sm/Ce-Fe/Co binary chemistry and the other influenced by (Sm/Ce)-(Fe/Co)-Ti ternary interactions. We employed ab initio calculations to investigate the finite-temperature stability of ordered, disordered, and metastable phases, thereby guiding experiments. Based on the computed energetics, we analyzed how Ti incorporation alters local bonding environments and stabilizes magnetically desirable motifs. Furthermore, we constructed an ab initio phase diagram to reveal the interplay between rare-earth metals and transition metals across a broad temperature range. We have revealed that Ti addition promotes the formation of a more robust Sm-rich phase by strengthening the local Sm-Fe-Ti matrix. This stabilization enhances alloy coercivity and provides insights into the thermodynamic and chemical factors driving phase evolution, enabling the design of better permanent HMs.

FM 9.5 Tue 15:15 BEY/0138

**Molecular orbital degeneracy lifting in NbSeI** — •Keita Kojima[1], Hayato Takano[1], Youichi Yamakawa[2], Shunsuke Kitou[3], Ryutaro Okuma[1], and Yoshihiko Okamoto[1] — [1]Institute for Solid State Physics, University of Tokyo, Kashiwa 277-8581, Japan — [2]Department of Physics, Nagoya University, Nagoya 464-8602, Japan — [3]Department of Advanced Materials Science, University of Tokyo, Kashiwa 277-8581, Japan

The breathing pyrochlore lattice, composed of alternating small and large tetrahedra, hosts molecular orbitals within the smaller tetrahedra that strongly influences its physical properties. Such molecular-orbital and frustration-driven effects have led to diverse electronic states in related compounds. We investigated NbSeI, a MoSBr-type material with a particularly large breathing distortion whose physical properties remain unexplored despite previous synthesis reports. We synthesized single crystals and conducted x-ray diffraction, physical property measurements, and first-principles calculations. While the calculations predict metallic flat bands originating from Nb 4d orbitals, magnetic and transport measurements reveal a nonmagnetic insulating state below 300 K. NbSeI also undergoes a structural transition at Ts = 106 K. Our structural studies demonstrate local atomic displacements above Ts and a trimer-like molecular transformation below Ts. Our results show that the combination of strong breathing distortion and flat-band*derived electronic structure stabilizes molecular-orbital degrees of freedom, advancing orbital physics beyond single-ion descriptions toward cluster-based electronic phenomena.

# FM 10: Crystal Defects and Real Structure Physics in Diamond and Functional Materials II

chair: Theo Scherer (Karlsruhe Institute of Technoloy, DE)

Time: Tuesday 14:00–15:30 Location: BEY/0E40

FM 10.1 Tue 14:00 BEY/0E40

**Identification of defects in iron molybdate catalysts via first principles calculations** — •Young-Joon Song and Roser Valentí — Institut für Theoretische Physik, Goethe-Universität, 60438, Frankfurt am Main, Germany

Iron molybdate ($Fe_2(MoO_4)_3$) is well known as a commercial catalyst for oxidative dehydrogenation. Recently, L. Schumacher et al. reported an experimental reduction in Raman intensity at 782 $cm^{-1}$ during catalytic processes. The authors attribute this decrease to oxygen migration from the bulk to the surface during the reaction, in contrast to the conventional understanding that oxygen atoms are supplied only near the surface. To identify the types of defects responsible for the observed reduction in Raman intensity, we performed DFT electronic and phononic structure calculations for $Fe_2(MoO_4)_3$. Our findings reveal that optical phonon modes involving oxygen dominate the spectrum at around 790 $cm^{-1}$, with a small contribution from Mo, corresponding to asymmetric $MoO_4$ stretching modes. In the Raman calculations, a major peak appears at 789.68 $cm^{-1}$ with a small shoulder-like feature and a minor peak at 972.05 $cm^{-1}$, consistent with the experimental observations. By selectively freezing specific phonon modes, we introduced an effective method to incorporate defect effects into Raman calculations without explicitly creating oxygen vacancies. Using this approach, we found that oxygen vacancies play a dominant role in the reduction of Raman intensity. Finally, we discuss the relaxed structure containing explicit oxygen vacancies. This research was supported by the German Research Foundation for funding through CRC 1487.

FM 10.2 Tue 14:15 BEY/0E40

**Exsolution of metal nanoparticles by control of point defects** — •Andreas Rosnes[1], Bo Jiang[2], Holger von Wenckstern[1], Øystein Prytz[1], and Jonathan Polfus[2] — [1]Department of Physics, Centre for Materials Science and Nanotechnology, University of Oslo, PO Box 1048 Blindern, NO NO-0316 Oslo, Norway — [2]Department of Chemistry, Centre for Materials Science and Nanotechnology, University of Oslo, PO Box 1033 Blindern, NO-0315 Oslo, Norway

Exsolution involves redox precipitation of metal nanoparticles from metal oxides, resulting in materials that exhibit excellent electrocatalytic properties and hold great promise for novel types of nanoscale heterostructures. However, a coherent understanding of the phenomenon is lacking. Here, exsolution is described by three point defect equations involving the reduction of the host oxide, reduction and exsolution of the transition metal, and annihilation of host unit cells. Guided by their predictions, significantly enhanced exsolution in terms of molar amount, rate, and nucleation density is shown by acceptor substitution to the system $La_{0.2}Ca_{0.7}Ti_{0.95}Cu_{0.05}O_{3-\delta}$ through atomic scale imaging and in situ X-ray diffraction and spectroscopy. It is demonstrated that the oxygen stoichiometry of the parent oxide increases upon exsolution despite oxygen loss in the reducing environment. Furthermore, strain in both the host oxide and the exsolved metal can constitute an additional thermodynamic barrier for exsolution beyond the availability of the required point defects.

FM 10.3 Tue 14:30 BEY/0E40

**Machine-Learning Potentials Reveal Defect Segregation at Grain Boundaries in Lithium Solid Electrolytes** — •Waldemar Kaiser[1], Hyunwon Chu[2], Jennifer L.M. Rupp[1,2], and David A. Egger[1] — [1]TUM School of Natural Sciences, Technical University of Munich — [2]Department of Materials Science and Engineering, Massachusetts Institute of Technology

Grain boundaries (GB) play a central role in ionic and electronic transport in polycrystalline solid electrolytes [1, 2], yet their local defect chemistry remains difficult to resolve. Their structural complexity and chemical heterogeneity introduce a wide distribution of possible defect configurations that are computationally demanding to characterize with first-principles methods. As a result, the origins of variations of ionic and electronic transport often remain unclear.

Here, machine-learning potentials (MLPs) are applied to representative $\Sigma5$ and $\Sigma3$ GB structures to investigate ionic defects in lithium lanthanum zirconate (LLZO). The MLPs enable the systematic and efficient mapping of lithium- and oxygen-vacancy formation energies, revealing reductions of up to 1 eV within GB cores relative to bulk sites. Structural analysis further identifies locally Zr-deficient coordination environments as preferred incorporation sites for lithium vacancies, and experiments show that Ta-doping fills these bottlenecks and enhances the material's stability.

[1] B. Gao et al., Adv. Energy Mater. 12, 2102151, 2021 [2] Y. Zhu et al., Nat. Rev. Mater. 6, 313-331, 2021

**coffee break**

FM 10.4 Tue 15:00 BEY/0E40

**2 - Dimensional hybrid perovskite as a promising semiconductor for large area electronics** — •Tomasz Marszalek, Shuanglong Wang, Zhitian Ling, Denis Andrienko, Hai Wang, Paul W.M. Blom, and Wojciech Pisula — Max Planck Institute for Polymer Research, Mainz, Germany

Two-dimensional (2D) perovskites with bulky spacer cations are promising candidates for field-effect transistors due to the suppressed ion movement caused by large size insulating ligands. However, the relationship between the chemical nature of organic cations and film morphology, crystallinity, molecular organisation and charge carrier transport in 2D layered perovskites is not yet fully understood, which significantly limits the development of 2D perovskite FETs.

This report presents a distinct odd-even effect in 2D Sn-based perovskite semiconductors for the first time, incorporating monovalent phenylalkylammonium-based organic cations with alkyl side chains of different lengths containing either an odd or an even number of carbon atoms. An odd-even oscillation of charge carrier transport was revealed using optically pumped terahertz spectroscopy and transistor devices. By combining density functional theory calculations with simulated grazing-incidence wide-angle X-ray scattering, we demonstrate that organic ligands featuring odd carbon atoms exhibit a disordered crystal lattice and tilted inorganic octahedra. This results in a larger effective mass and inferior charge mobilities compared to perovskites with an even number of carbon atoms in the organic cations. (J. Am. Chem. Soc. 2024, 146, 19128, Mater. Horiz., 2024,11, 1177)

FM 10.5 Tue 15:15 BEY/0E40

**On the origin of the strange metal Hall effect in BaFe2(As1-xPx)2** — •Augusto Ghiotto[1], Darian Hall[1], Yuanqi Lyu[1], Kohtaro Yamakawa[1], John Singleton[2], and James Analytis[1] — [1]University of California, Berkeley, USA — [2]National High Magnetic Field Laboratory's Pulsed Field Facility at Los Alamos, USA

BaFe2(As1-xPx)2 is an unconventional superconductor in which the antiferromagnetic, nematic and structural order is suppressed by isovalent P substitution, leading to a quantum critical point at $x = 0.31$. It has been shown that the Hall effect of the overdoped series contains an anomalous contribution arising from the correlations within the strange metal, whose behavior emanates from a quantum critical point and, in the zero-temperature limit, decays together with the superconducting critical temperature. Here, we present new data on the underdoped series taken at pulsed high magnetic fields. To achieve a large signal to noise ratio and an accurate measurement of the Hall coefficient, we microstructured the crystals into well-defined Hall bars. In this talk, we will draw parallels between the Hall effect in the ordered state and in the strange metal.

# FM 11: Poster Session Functional Materials

chairs: Jan Schultheiß (NTNU, NO), Anna Grünebohm (Ruhr Universität Bochum, DE)

Time: Tuesday 18:00–20:30 Location: P4

FM 11.1 Tue 18:00 P4

**Structural and Optical Characterization of FeGaInS* Layered Crystals** — •Zeynab Addayeva and Mustafa Muradov — Baku State University, Baku , Azerbaijan

FeGaInS4 layered crystals were synthesized using the Bridgman technique, and their crystal structure was investigated via powder X-ray diffraction (XRD). FeGaInS4 is a quaternary complex metal chalcogenide that belongs to the class of layered, quartz-like A-B-C-X4 type compounds. The material crystallizes in the rhombohedral system and adopts the R3m (No. 160) space group, according to the International Union of Crystallography (IUCr) classification. The refined lattice parameters (a = b = 5.406 Å, c = 10.708 Å) confirm the presence of a highly symmetric and anisotropic layered crystal structure. Within the structure, Fe, Ga, and In atoms occupy different coordination environments and form tetrahedral bonds with sulfur (S) anions, resulting in a complex three-dimensional network. These bonding interactions directly influence the material's electronic structure and related functional properties, including electrical conductivity, optical absorption, dielectric response, and thermal stability. Due to its anisotropic layered architecture, FeGaInS4 exhibits natural cleavage along specific crystallographic directions. This property renders it suitable for exfoliation into few-layer or monolayer nanosheets, making it a promising candidate for the fabrication of two-dimensional (2D) materials and high-performance composite systems. The optical band gap of FeGaInS4 is approximately 1.46 eV.

FM 11.2 Tue 18:00 P4

**An Atom Probe Tomography Study of the Bond Breaking Behavior of Transition Metal Chalogenides** — •Sophia Schreinemacher[1], Jan Köttgen[1], Elias Hildebrnad[1], Felix Hoff[1], Christian Stenz[1], Vicky Hasse[3], Yuan Yu[1], and Matthias Wuttig[1,2] — [1]I. Institute of Physics (IA), RWTH Aachen University, Germany — [2]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany — [3]Max Planck Institute for Chemical Physics of Solids 01187 Dresden, Germany

Chemical bonds are a vital subject in materials science, as they are one of the central factors that define the properties of a material. Transition metal chalcogenides are a group of materials characterized by the bonding between the chalcogenide p-orbitals and the metal d-orbitals, which exhibit unique electronic, optical, and magnetic properties. The main bonding indicator in this study is the probability of multiple events (PME) obtained during atom probe tomography (APT) acquisition.

The results show a medium PME (40-60%), highlighting the unique bond-breaking behavior that transition metal chalcogenides display during APT evaporation. In a plot of the PME against the electrical conductivity, the studied materials cluster at the border between the metavalent and covalent materials. These findings expose a clear connection between transition metal chalcogenides, their d- and p-orbital interaction, and their bonding characteristics, thereby broadening our understanding of metavalent materials.

FM 11.3 Tue 18:00 P4

**Epitaxial Growth and Optimization of LiNbO3 Thin Films on LiTaO3 and Al2O3 by Pulsed Laser Deposition Using Machine Learning** — •Hyeyeon Cho, Milena Petkovic, Steffen Ganshow, and Jutta Schwarzkopf — Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, 12489 Berlin, Germany

Lithium niobate (LiNbO3) thin films are widely used in electro-optical and electro-acoustic devices due to their excellent ferroelectric, piezoelectric, and nonlinear optical properties, offering broader bandwidths at higher frequencies and reduced operational voltages compared to bulk materials. The development of high-quality, phase-pure, and smooth LiNbO3 films is essential for achieving superior device performance. Pulsed Laser Deposition (PLD) offers precise control over growth parameters, enabling the fabrication of epitaxial LiNbO3 layers with tunable structural properties. In our work, we investigated the epitaxial growth of LiNbO3 thin films on LiTaO3 and Al2O3 substrates using PLD. The influence of various PLD growth conditions and substrate materials was systematically investigated with regard to phase formation and structural ordering by x-ray diffraction and surface roughness by atomic force microscopy. Furthermore, a four-step machine learning workflow, including Artificial Neural Network (ANN) and Random Forest (RF) models, was employed to analyze the nonlinear relationships between PLD parameters and structural film properties. This combined experimental and computational approach accelerates development and provides deeper insight into LiNbO3 thin film growth for advanced photonic and optoelectronic applications.

FM 11.4 Tue 18:00 P4

**Ferroelectricity in spin-liquid candidate TbInO$_3$** — •Andrea Tobiassen[1], Elvia Chavez[1], Jiali He[1], Dennis Meier[1,2], and Jan Schultheiss[1] — [1]NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]University of Duisburg-Essen, Duisburg, Germany

Hexagonal rare-earth oxides exhibit a variety of intriguing physical phenomena, ranging from rich magnetism to improper ferroelectricity. Among them, TbInO$_3$ has recently been proposed as a spin-liquid candidate, where magnetic frustration suppresses long-range magnetic order at low temperatures. The ferroelectric properties of TbInO$_3$ remain largely unexplored.

In this work, we synthesize TbInO$_3$ polycrystals via a solid-state route. Phase purity is confirmed by X-ray diffraction (XRD), while Scanning Electron Microscopy (SEM) and Piezoresponse Force Microscopy (PFM) reveal a pronounced domain contrast, evidencing a topological ferroelectric domain structure typical for hexagonal oxides. High-temperature XRD indicates a Curie temperature ($T_C$) of approximately 1630 K, corresponding to the polar $P6_3cm$ to nonpolar $P6_3/mmc$ phase transition. Understanding the ferroelectricity in TbInO$_3$ provides a foundation for engineering its domain structure and exploring potential magnetoelectric coupling effects.

FM 11.5 Tue 18:00 P4

**Localized High-Concentration High-Entropy Electrolytes for Superior Lithium Metal Anodes via Solvation Cluster Regulation** — •Haixuan Luo and Peter Müller-Buschbaum — TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany

The practical deployment of high-energy-density lithium metal batteries (LMBs) is severely hindered by the thermodynamic instability of the lithium metal anode, which precipitates dendritic growth and poor Coulombic efficiency. Although localized high-concentration electrolytes (LHCEs) have emerged as a promising solution, optimizing their cluster configurations to maximize interfacial durability remains a challenge. Herein, we propose a groundbreaking localized high-concentration high-entropy electrolyte (LHCHEE) strategy that leverages the high-entropy effect to tailor solvation structures at the molecular level. Our systematic investigation reveals that the introduced configurational entropy promotes the formation of uniform, anion-rich solvation clusters while suppressing solvent decomposition. This unique solvation environment facilitates the construction of a robust, inorganic-dominated solid electrolyte interphase (SEI) on the lithium metal. Consequently, the LHCHEE enables exceptional stability, while Li||Cu cells demonstrate significantly improved Coulombic efficiency. Furthermore, full cells paired with high-voltage cathodes exhibit remarkable capacity retention. This work not only demonstrates the superiority of LHCHEEs but also establishes entropy engineering as a critical dimension for designing advanced electrolyte systems.

FM 11.6 Tue 18:00 P4

**Ferroelectric switching at edge dislocations in BaTiO$_3$ modelled at the atomic scale** — •Himal Wijekoon[1,2], Pierre Hirel[3], and Anna Grünebohm[1,2] — [1]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) and Center for Interface-Dominated High Performance Materials (ZGH), Ruhr-University Bochum, Universitätsstr 150, 44801 Bochum, Germany — [2]Faculty of Physics and Astronomy, Ruhr-University Bochum, Universitätsstr 150, 44801 Bochum, Germany — [3]Univ. Lille, CNRS, INRAE, Centrale Lille, UMR 8207 - UMET - Unité Matériaux et Transformations, F-59000 Lille, France

Domain nucleation and switching largely govern the functional properties of ferroelectric perovskites. Consequently, one can utilize defects to tailor domain switching and thereby tune the functional properties of these materials. While previous studies have mainly focused on switching in pristine pervoskite materials, the influence of defects, particularly dislocations, on domain nucleation and switching remains insufficiently understood. Using molecular static simulations, we show that $\langle 100\rangle$ edge dislocations cores in barium titanate can serve as domain nucleation sites. By applying an external electric field in three different orientations relative to the Burgers vector and dislocation line, we show how domain nucleation and subsequent growth occurs in dislocations-induced strain variations. Our simulations reveal that the coupling between electric field and polarization is strongest when the field is applied parallel to the Burgers vector.

FM 11.7 Tue 18:00 P4

**Topology and Bonding: A bonding-based approach to topological insulators via Atom Probe Tomography** — •Elias Hildebrand[1], Jan Köttgen[2], Yuan Yu[1], and Matthias Wuttig[1,2] — [1]I. Institute of Physics (IA), RWTH Aachen University, Germany — [2]Peter Grünberg Institute - JARA-Institute Energy Efficient Information Technology (PGI-10), Jülich, Germany

Ever since the discovery of the quantum Hall effect, interest in topological phases of matter has steadily increased. Initially attributed to spin-orbit coupling, the underlying guiding principle causing these topological phases of matter has been a topic of ongoing discussion.

Here, we want to propose a bonding-based approach to explain nontrivial topological states. The experimental foundation for this connection is established through Atom Probe Tomography (APT). While APT is primarily employed for microstructural analysis, it has recently been proposed as a tool capable of identifying different bonding mechanisms.

Within this method, most topologically nontrivial materials also exhibit distinct bond-breaking behaviour corresponding to their characteristic bonding mechanisms. Here, different materials are investigated regarding their topological nature and behaviour in the APT.

Consequently, APT can be established as an experimental method for identifying topological phases of matter and as an empirical argument highlighting the significance of bonding in understanding the fundamental principles governing topological materials.

FM 11.8 Tue 18:00 P4

**Strain-driven phonon instabilities in BaSnO3** — •Benyao Sun and Anna Grünebohm — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum, Germany

The perovskite BaSnO3(BSO) has attracted extensive research interest due to its favorable properties, including non-toxicity, high thermal stability, and distinctive electronic characteristics. However, bulk BSO is generally non-ferroelectric, limiting its applications. Fortunately, strain engineering can induce ferroelectricity by tuning the perovskite structure. For example, strain-induced tetragonality leads to a large dipole moment and, consequently, to a high polarization in strained ferroelectrics [1]. BSO exhibits ferroelectric polarization under applied epitaxial strain [2]. Strain-induced ferroelectricity in BSO has been studied, but phonon-spectrum analyses under sustained strain remain limited. In our work, we carry out a systematic study of the phonon instabilities of BSO under compressive strain. We calculate the critical compressive strain at which soft modes appear in the phonon dispersion of BSO, analyze the contributions of the polar mode and the antiferrodistortive mode to the ferroelectricity as well as the couplings between different soft modes, and also discuss the effect of an external electric field on these soft modes.

[1] Zeches,R.J.et al.Science 2009, 326,977-980.

[2] Zhang,Y.et al.Phys.Chem.Chem.Phys.2017,19, 26047-26055.

FM 11.9 Tue 18:00 P4

**Virtual Characterization Lab: A Python Toolkit for Material Characterization from Molecular Dynamics** — •Vahid Jamebozorgi[1,2] and Christian Schröder[1,2] — [1]HSBI, Bielefeld, Germany — [2]Bielefeld University, Bielefeld, Germany

Material discovery using traditional experimental methods is a slow and costly process, often limited by the sampling process, characterization condition constraints, and the requirement for expensive equipment. While computational tools have transformed materials research by accelerating the investigation of material properties, a significant gap remains in connecting high-fidelity simulations with established experimental characterization techniques. We present the Virtual Characterization Lab (VCL), a unified, open-source Python toolkit designed to bridge this gap. The VCL streamlines the entire workflow from molecular dynamics simulations, enabling researchers to generate and analyze key characterization data, such as X-ray Diffraction (XRD), Selected Area Electron Diffraction (SAED), and Vibrational Density of States (VDOS), all within a single, intuitive environment. By integrating every step from initial structure preparation to final data visualization, the VCL accelerates materials discovery by making virtual characterization more efficient, accessible, and directly comparable to experimental results.

FM 11.10 Tue 18:00 P4

**Structural Factors Governing Stability and Electronic Transport in Future Neuromorphic Memristor Technologies** — •Wiktoria Szopa[1,2,3], Marcin Krynski[1], Attila Cangi[2,3], and Piotr Wisniewski[4] — [1]Faculty of Physics, Warsaw University of Technology, 00-662 Warsaw, Poland — [2]Center for Advanced Systems Understanding, 02826 Görlitz, Germany — [3]Helmholtz-Zentrum Dresden-Rossendorf, 01328 Dresden, Germany — [4]Centre for Advanced Materials and Technologies CEZAMAT, Warsaw University of Technology, 02-822 Warsaw, Poland

With the rapid rise of artificial intelligence, the demand for technologies that enable its development and application is high, as AI is now widely used across science, industry, and everyday life. Neuromorphic materials may offer a promising solution to the increasingly complex hardware requirements posed by next-generation, high-throughput AI.

Silicon-oxide-based memristors may operate as adjustable weights within hardware neural networks, enabling more efficient, neuromorphic computation. The electronic component contains two electrodes separated by a thin amorphous silicon oxide layer, within which charge transport occurs through filamentary silicon chains that form conductive pathways.

In this project, we investigate how the local atomic structure influences electronic transport. To this end, we generated hundreds of memristor models and identified their most stable configurations, with high structural robustness and defined conduction pathways by using a combination of DFT calculations and machine learning modeling.

FM 11.11 Tue 18:00 P4

**Computational modelling of phonon, elastic, and electronic properties of layered quantum crystalline materials** — •Zoya Eremenko[1], Yuri Savin[2], and Vladimir M. Fomin[1] — [1]IFW Dresden, Germany — [2]O.Ya. Usikov Institute for Radiophysics and Electronics, National Academy of Sciences of Ukraine, Kharkiv, Ukraine

We present a comparative computational study of the phonon, elastic, and electronic properties of several crystalline quantum materials NbSe$_2$, FeSe, MoS$_2$, and BSCCO using density functional theory (DFT) and COMSOL Multiphysics. For each material, we analyze the primitive-cell geometry, symmetry, the resulting vibrational and mechanical responses extracted from both the first-principles calculations and the available experimental references. Layered transition-metal dichalcogenides NbSe$_2$, and MoS$_2$, show significantly anisotropic elastic responses, consistent with their quasi-2D bonding. MoS$_2$ shows elastic constants aligned with experimental values. Properties of the tetragonal iron-based chalcogenide FeSe are modelled using its primitive cell and the electronic band structure. By leveraging elastic constants obtained from the available experimental and theoretical studies, the BSCCO phonon frequencies are calculated with COMSOL Multiphysics. The close agreement between our simulated phonon frequencies and the experimental data for BSCCO validates our multiscale approach, providing a solid foundation for future studies of the electron-phonon interactions and structural effects in complex quantum materials. We thank Dr. Golam Haider for providing us with the experimental data for verification of the simulated Raman frequencies.

FM 11.12 Tue 18:00 P4

**First-Principles Modeling and ESR Identification of an Intrinsic Radical Spin Center in UiO-66-NH$_2$ Metal-Organic Framework** — •Timur Biktagirov[1], Anastasiia Kultaeva[2], Daniel Klose[3], Eugenio Otal[4], and Wolf Gero Schmidt[1] — [1]Physics Department, University of Paderborn, 33098 Paderborn, Germany — [2]Experimental Physics 6, Julius-Maximilian University of Würzburg, 97074 Würzburg, Germany — [3]ETH Zurich, 8093 Zurich, Switzerland — [4]Institute for Aqua Regeneration (ARG), Shinshu University, 4-17-1 Wakasato, Nagano 380-8553, Japan

Metal-organic frameworks (MOFs) are emerging as tunable platforms for sensing, photocatalysis, and energy conversion, where charge transfer, spin interactions, and defect states play key roles. Here, we identify and characterize a native NH· radical defect intrinsic to the aminoterephthalate linker in UiO-66-NH$_2$ MOF. Combining density functional theory (DFT) modeling with multi-frequency electron spin resonance (ESR) spectroscopy, we elucidate the radical's electronic structure, spin density distribution, formation pathway, and spin-coherence properties. Our findings reveal the radical's exceptional stability and highlight its relevance for both photocatalytic charge separation and quantum-enhanced sensing in MOFs.

FM 11.13 Tue 18:00 P4

**Efficient Discovery of Intermediate-Temperature Proton Conductors via Ion Exchange Strategy with Machine Learning Potential** — •Yun An, Karsten Reuter, and Christoph Scheurer — Fritz Haber Institute of the Max Planck Society, 14195 Berlin, Germany

Proton-conducting solid-oxide fuel cells (H-SOFCs) are promising for direct ammonia-fed SOFC applications, as they eliminate NO$_x$ emissions compared to conventional oxide-ion-conducting solid-oxide fuel cells. However, current proton-conducting electrolytes operate at high temperatures and suffer from leakage currents. Known suitable materials remain rare, calling for systematic investigations into novel proton conductor classes. We present a framework that combines machine-learning techniques with high-throughput computation to screen and design efficient proton conductors at intermediate temperatures. Through an ion-exchange strategy applied to known alkaline-ion conductor classes, we identify a database of potential proton-conducting materials. Machine learning molecular dynamics simulations are employed to assess stability and diffusion barriers, enabling the selection of top-performing candidates. The screened proton conductors contain cations that span from monovalent to pentavalent, including Rb$^+$, Ba$^{2+}$, Ca$^{2+}$, B$^{3+}$, Zr$^{4+}$, and Nb$^{5+}$, and predominantly feature SO$_4{}^{2-}$ and PO$_4{}^{3-}$ polyanion groups. Proton transport in these materials follows the Grotthuss mechanism. The strength of hydrogen bonds increases after ion-exchange engineering, thereby enhancing proton transfer.

FM 11.14 Tue 18:00 P4

**Dual Strategy Engineering of Zn4Sb3: Indium Doping and ZnO Coating for High zT** — •Abhishek Pandey[1], Amin Bahrami[2], and Kornelius Nielsch[3] — [1]Leibniz Institute for Solid State and Materials Research, Helmholtzstraße 20, Dresden 01069, Germany — [2]Leibniz Institute for Solid State and Materials Research, Helmholtzstraße 20, Dresden 01069, Germany — [3]Leibniz Institute for Solid State and Materials Research, Helmholtzstraße 20, Dresden 01069, Germany

Zn4Sb3 is one of the promising thermoelectric materials due to its very low thermal conductivity and favorable electronic properties for high TE performance. However, its practical application to TE device is limited by structural instability and Zinc-ion migration, which lead to the formation of zinc whiskers and degradation of TE performance. In this work, a dual-strategy approach has been adopted to enhance and stabilize Zn4Sb3, (1) Indium doping, and (2) ZnO surface coating of powder. Indium substitution within the Zn4Sb3 lattice is shown to increase the figure of merit (zT). In parallel the bulk modification, ZnO coating on Zn4Sb3 particles acts as a diffusion barrier that mitigates zinc migration and whisker formation, which improves the structural robustness during prolonged thermal cycling.

FM 11.15 Tue 18:00 P4

**Towards Quantification of Convergent Beam Electron Diffraction Patterns** — •Jimmy Steinweh[1], Daniel Wolf[1], and Axel Lubk[1,2] — [1]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [2]Institute of Solid State and Materials Physics, TU Dresden, Germany

Convergent beam electron diffraction (CBED) is a transmission electron microscopy (TEM) method, that utilizes a convergent electron beam to investigate the symmetry of crystalline samples at the nanoscale. A method for quantifying discrete rotational and mirror symmetries in CBED patterns is presented, involving a quantification algorithm for both simulated and experimental CBED patterns. This approach is used to investigate the influence of probe shifts, beam tilts, and thermal lattice vibrations on the symmetry of simulated CBED patterns of silicon to identify crystal structure related asymmetries. It is found that for a semi-convergence angle of $\alpha = 1.7\,\mathrm{mrad}$, the asymmetry introduced by probe shifts is barely detectable in simulations, whereas beam tilt effects are significant at beam tilt angles as low as 0.1 mrad. Consequently, precise alignment of the beam in zone axis is crucial. We find furthermore that consideration of lattice vibrations within the frozen lattice approximation also slightly breaks the symmetry and discuss the origin of this effect. These results aim to establish a foundation for further development of CBED as a quantitative tool for probing crystal symmetries at the nanoscale.

FM 11.16 Tue 18:00 P4

**Correlated Imaging of Thermal Conductivity and Ferroelectric Domains in PbTiO$_3$ Using Scanning Probe Microscopy** — •Ciara Ward, Lindsey Lynch, and Raymond McQuaid — Queen's University Belfast, Belfast, UK

Perovskite ferroelectrics are an attractive platform for realising thermal conductivity switching through voltage configuration of domain microstructure. Reported mechanisms involve thermal conductivity modulation through structural re-orientation (anisotropy) [1,2] or phonon scattering by domain wall defects [3-5], both of which can be controlled through sample geometry and applied fields. Heat flow measurements and thermoreflectance investigations have quantitatively benchmarked thermal switching ratios but, in some cases, a lack of direct thermal mapping introduces ambiguity as to the relative role played by the two mechanisms. We are using Scanning Thermal Microscopy to explicitly map the local thermal conductance in samples of archetypal ferroelectric PbTiO$_3$ to clarify the underlying mechanisms that enable modulation of thermal transport. In tandem, we are using domain engineering and electric-field poling techniques to demonstrate the maximum achievable contrast in thermal conductance in this system.

[1] J. Seijas-Bellido *et al. Appl. Phys. Lett.* 115, 192903 (2019). [2] L. Féger *et al. Phys. Rev. Mater.* 8, 094403 (2024). [3] Ihlefeld *et al. Nano Lett.* 15, 1791 (2015). [4] E. Langenberg *et al. Nano Lett.* 19, 7901 (2019). [5] R. Belrhiti-Nejjar *et al. Adv. Sci.* 12, e06931(2025).

FM 11.17 Tue 18:00 P4

**Impurity-Driven Vacancy Evolution in Irradiated Tungsten Revealed by Positron Annihilation Spectroscopy and Multiscale Modeling** — •Zhiwei Hu[1,2], Qigui Yang[3], Jintong Wu[4], François Jomard[5], Thomas Jourdan[6], and Marie-France Barthe[2] — [1]HZDR, Dresden, Germany — [2]CEMHTI-CNRS, Orléans, France — [3]KTH, Stockholm, Sweden — [4]University of Helsinki, Finland — [5]GEMAC; Versailles; France — [6]CEA,Gif-sur-Yvette, France

Thermonuclear fusion demands plasma-facing materials that withstand extreme heat and irradiation. Tungsten, selected for ITER, develops microstructural evolution. Predicting defects behavior is therefore crucial. Using Positron Annihilation Spectroscopy, TEM, atomistic modeling, and DFT, irradiation-induced defects were examined. A new PAS data-inversion method using quadratic programming and two-component DFT was created. This method reconstructs full vacancy-cluster distributions from PAS data. Results show small vacancy clusters dominate after high-temperature irradiation. These clusters remain invisible to TEM yet strongly affect microstructure. Room-temperature electron irradiation showed reduced pure vacancy fractions. Unexpected positron traps were observed. SIMS and DFT identified these traps as oxygen-vacancy complexes. Cluster-dynamics simulations confirmed oxygen interacts with Frenkel pairs. Such interactions significantly modify defect evolution. Comparative irradiations of varying-purity tungsten were performed, PAS and TEM together revealed impurity effects.

FM 11.18 Tue 18:00 P4

**Phase Transitions and Ferroic Properties in Organic*Inorganic Hybrid Halide TMCM-Mn*-*Fe*Cl* Crystals** — •Chithra Kandappanthodi, Boris Slautin, Sobhan M Fathabad, Daniil Lewin, Doru Lupascu, and Vladimir Shvartsman — University of Duisburg-Essen

Organic*inorganic hybrid halides have garnered significant attention in materials science due to their eco-friendly, cost-effective synthesis, and outstanding optoelectronic properties. We report the properties of Fe-substituted trimethyl chloromethyl ammonium manganese trichloride TMCM-Mn1-xFexCl3 single crystals. The samples were obtained via the solvent evaporation seed assisted crystal growth method. Temperature-dependent X-ray diffraction and differential scanning calorimetry measurements confirm a sequence of structural phase transitions: from a monoclinic P121 phase at 302 K to monoclinic Cc, and subsequently to a hexagonal P6*/mmc phase at 408K for the pure TMCM-MnCl3 sample. Dielectric permittivity measurements indicate the improper ferroelectric transition at 408 K. Piezoresponse force microscopy further identifies well-defined ferroelastic domains at room temperature, which vanish upon heating above 304 K, as also observed using polarized light microscopy. Fe-substituted TMCM*Mn***Fe*Cl* samples exhibit a new intermediate phase transition near 328 K. UV*vis absorption spectra also demonstrate that increasing Fe content tunes the electronic bandgap. This comprehensive characterizations highlights TMCM-MnCl3, and TMCM-Mn1-xFexCl3 as a promising candidate for multifunctional applications.

FM 11.19 Tue 18:00 P4

**Polymorph Stability and Mo Substitution in WO$_3$** — •HIran Kankanamge[1], Susanne Susanne[2,1,3], and Anna Grünebohm[1] — [1]Scale-bridging simulations of functional composites, Interdisciplinary Centre For Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Universitätsstr. 150, 44801 Bochum, Germany — [2]Applied Quantum Materials, Institute for Energy and Materials Processes (EMPI), Faculty of Engineering, University of Duisburg*Essen, Forsthausweg 2, 47057 Duisburg, Germany — [3]Research Center Future Energy Materials and Systems (RC FEMS), University of Duisburg*Essen, Forsthausweg 2, 47057 Duisburg, Germany

Mixed molybdenum-tungsten oxides offer tunable electrochromic and catalytic properties [1]. Pure WO$_3$ exhibits several polymorphs separated by only a few meV·atom$^{-1}$ [2], leaving the structural trends in Mo$_x$W$_{1-x}$O$_3$ insufficiently resolved. As a baseline for substitution, we use first-principles calculations to reassess the stability of the main WO$_3$ polymorphs and recover the characteristic low-energy grouping of the $\beta$, $\gamma$, and $\varepsilon$ phases.

Building on these optimized structures, the focus of this work is to introduce molybdenum across all phases and trace how composition modifies the energy landscape, octahedral tilting, and relative phase preferences. The resulting trends are compared with experimental observations on mixed Mo-W oxides [1] to evaluate their consistency and refine the microscopic picture of phase competition within the Mo-W-O system.

[1] H.-J. Lunk and H. Hartl, ChemTexts 9, 5 (2023).
[2] H. Hamdi et al., Phys. Rev. B 94, 245124 (2016).

FM 11.20 Tue 18:00 P4

**Mechanistic Origin of Charge Separation and Enhanced Photocatalytic Activity in D-$\pi$-A-Functionalized UiO-66-NH$_2$ MOFs** — •Anastasiia Kultaeva[1], Timur Biktagirov[2], Volodymyr Vasylkovskyi[1], Andreas Sperlich[1], Eugenio Otal[3], Wolf Gero Schmidt[2], and Vladimir Dyakonov[1] — [1]Experimental Physics 6, University of Würzburg, 97074 Würzburg, Germany — [2]Physics Department, Paderborn University, D-33098 Paderborn, Germany — [3]Institute for Aqua Regeneration, Shinshu University, Nagano 380-8553, Japan

Donor-$\pi$-acceptor (D-$\pi$-A) functionalization of MOF linkers offers a promising route to enhance visible-light photocatalysis, yet the underlying photophysical mechanisms remain insufficiently resolved. Here we investigate UiO-66-NH$_2$ modified via diazo coupling with anisole, diphenylamine (DPA), and N,N-dimethylaniline (NNDMA) dyes. Optical measurements and first-principles calculations show that all donor groups introduce new occupied states near the valence-band edge, enabling dye-to-framework charge transfer and red-shifted absorption. EPR and transient photoluminescence reveal that anisole uniquely promotes efficient intersystem crossing to a long-lived triplet charge-transfer state, whereas bulkier donors such as DPA and NNDMA can also generate defect-associated traps that enhance recombination. These results clarify how donor structure dictates electronic-state formation, triplet pathways, and defect behavior, providing mechanistic guidelines for tailoring charge dynamics and photocatalytic activity in D-$\pi$-A-modified MOFs.

FM 11.21 Tue 18:00 P4

**Isovalent exchange of Al, Mg and Zr in strontium hexagallate ($SrGa_{12}O_{19}$)** — •Finn Bietz[1], Christian Rhode[2], and Simone Sanna[1,3] — [1]Institut für Theoretische Physik, Justus-Liebig-Universität Gießen, Gießen 35392, Germany — [2]Leibniz Institut für Kristallzüchtung, Max Born Straße 2, 12489 Berlin — [3]Center for Materials Research (ZfM), Justus Liebig University Gießen, Gießen 35392, Germany

Strontium hexagallate (SrGa$_{12}$O$_{19}$) can be used as a substrate for the growth of barium hexaferrite (BaFe$_{12}$O$_{19}$), a ferrimagnetic and a quantum paraelectric material. The lattice parameters of SrGa$_{12}$O$_{19}$ can be adjusted by substitution of Ga by Al or Mg and Zr, respectively, for the lattice-matched growth and strain engineering of (BaFe$_{12}$O$_{19}$) thin films. Unfortunately, a microscopic picture of the doping mechanisms, as well as of their effect on the lattice parameters, is still missing. In this contribution, we report on first-principles calculations performed to determine the lattice site of Al, Mg and Zr atoms in the SrGa$_{12}$O$_{19}$ structure, and support corresponding experiments performed at the IKZ in Berlin. Thereby the defect formation energies of Al, Mg and Zr atoms incorporated in the dilute limit at different lattice sites were calculated within density functional theory (DFT). The atomistic models reveal that Mg populates the so called Ga$^{(3)}$ position, Al prefers the Ga$^{(1)}$ site, but also populates the Ga$^{(4)}$ and Ga$^{(5)}$ sites, and that the Zr is incorporated at the Ga$^{(4)}$ site. A substitution at the Sr site is energetically unfavorable for all dopants, instead. The calculated formation energies are in good agreement with the experimental results.

FM 11.22 Tue 18:00 P4

**Ferroelectric domain shapes in LiNbO3 and LiTaO3 from a revised Ising model** — •Jonas Paul[1], Leonard Verhoff[2], and Simone Sanna[1] — [1]Justus-Liebig-Universität Giessen, Giessen, Germany — [2]Technische Universität Wien, Wien, Austria

Lithium niobate (LN) and lithium tantalate (LT) are both ferroelectric materials whose domains can be influenced by external electric fields. While both crystallize within the same symmetry group (R3c), congruent LN and LT form different domain shapes as experimentally observed [1]. DFT calculations could explain the domain shapes of LN and LT via calculations of the domain wall energy [2], however, knowledge about build-up of domain shapes in mixed lithium niobate-tantalate (LNT) mixed crystals is still lacking.

In this contribution, we demonstrate that the domain build-up in LNT can be modeled with a modified Ising model and performed Monte Carlo and Greedy calculations to simulate the domain growth. We show that an additional interaction term in the Ising model determines the characteristic domain shape. Furthermore, we employ Greedy simulations for different parameters, obtaining a phase diagram for the domain shape transition. In consequence, we predict domain shapes for LN, LT, and LNT mixed crystals.

[1] D. A. Scrymgeour et al., Phys. Rev. B 71, 184110 (2005)
[2] D. Lee et al., Aplied Physics Letter 98, 092903 (2011)

FM 11.23 Tue 18:00 P4

**Reversible nanoscale patterning of WTe$_2$ with a scanning tunneling microscope** — •Kevin Hauser[1,2], Danyang Liu[1], Berk Zengin[1], Jens Oppliger[1], Samuel Mañas-Valero[4], Catherine Witteveen[5], Fabian O. von Rohr[5], Jennifer E. Hoffman[2,3], and Fabian D. Natterer[1] — [1]Department of Physics, University of Zurich, Switzerland — [2]Department of Physics, Harvard University, Cambridge MA, USA — [3]School of Engineering & Applied Sciences, Harvard University, Cambridge MA, USA — [4]Instituto de Ciencia Molecular, Universitat de València, Spain — [5]Department of Quantum Matter Physics, University of Geneva, Switzerland

Manipulating the lattice structure of quantum materials that host ferroelectric or Weyl semimetal phases provides a route to control these states on nanometer length scales. Prior experiments on the type-II Weyl semimetal candidate WTe$_2$ have demonstrated ferroelectric switching on micrometer length scales and transient control of the predicted topological phase via ultrafast excitations. However, both approaches lack the ability to induce persistent, localized distortions on the nanometer scale. In this contribution, we use current pulses applied by a scanning tunneling microscope (STM) to write, move, and erase nanoscale lattice distortions on WTe$_2$. The resulting lattice distortions consist of picometer-scale in-plane and out-of-plane atomic displacements, accompanied by changes in the local density of states. The in-plane shifts are on the same order of magnitude as expected for ferroelectric switching. These results demonstrate local, reversible control of the lattice structure of WTe$_2$ on nanometer length scales.

FM 11.24 Tue 18:00 P4

**Phase and microstructure evolution of $SnO_x$:Ta thin films as a function of the oxygen partial pressure during deposition** — Cecilia Bauden[1], Lukas Prager[1], Frans Munnik[1], Fabian Ganss[1], Harish Parala[2], Anjana Devi[2], Carlos Romero-Muniz[3], Ramon Escobar-Galindo[3], and •Matthias Krause[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]IFW Dresden, Dresden, Germany — [3]Universidad de Sevilla, Sevilla, Spain

Recent research on $SnO_2$-based TCOs has focused on Ta-doped $SnO_2$ (TTO), since it surpasses $In_2O_3$:Sn and ZnO:Al in thermal stability under vacuum and in air [1, 2]. This work presents a Raman spectroscopy and XRD study on the phase and microstructure evolution of $SnO_x$:Ta thin films as a function of the oxygen partial pressure during thin film deposition by reactive DC magnetron sputtering. At low $O_2$ flow rates a phase structure comprising metallic $\beta$-Sn, SnO and $Sn_3O_4$ without incorporated Ta is found. Higher $O_2$ flow rates yield the formation of the rutile structure of $SnO_2$:Ta, where Ta replaces Sn as $Ta_{Sn}$ and transfers free charge carriers into the Sn 5s* conduction band [3]. A resistivity minimum of 1.3 x $10^{-3}$ Ω cm, a maximum mobility 16 $cm^2$ $(Vs)^{-1}$, and a distinct reflectivity edge in the NIR were found for the films with the best transport properties.

[1] F. Lungwitz et al., SolMat 196, 84-93 (2019); [2] M. Krause et al., J. Mat. Chem. A 11, 17686-17698 (2023); [3] M. Krause et al., J. Mat. Chem. A 13, 15128-15139 (2025).

FM 11.25 Tue 18:00 P4

**Controlled synthesis of the magnetic topological insulator $MnSb_2Te_4$ with variable Curie temperature** — •Laura Zeni Cunha[1], Laura T. Corredor[2,3], Anja U.B. Wolter[4], and Anna Isaeva[1,2,3] — [1]University of Amsterdam, The Netherlands — [2]TU Dortmund University, Germany — [3]Research Center Future Energy Materials and Systems, Germany — [4]Leibniz IFW Dresden, Germany

Magnetic topological materials $(MnX_2Te_4)(X_2Te_3)_n$ are promising candidates for spintronic and energy-efficient technologies.[1] $MnSb_2Te_4$ features tunable Mn content that enables optimization of the magnetic ground state and ordering temperature[2-4] - key requirements for potential applications. However, synthetic control over Mn stoichiometry remains to be fully harnessed. This work presents a controlled, rapid, and reproducible synthesis route to phase-pure $MnSb_2Te_4$ by using an optimized tellurium precursor. I investigate by powder XRD, EDX/SEM, and DC magnetization studies how varied synthetic parameters impact its structural and magnetic properties. I observe an increased stability range of ferrimagnetic $MnSb_2Te_4$ compared with Ref. [2], and demonstrate a clear correlation between synthesis conditions and the Tc, spanning more than 10 K across the samples. This insight into synthesis-structure-property relationship advance our goal of a topological ferromagnet with higher Tc, moving toward the quantum anomalous Hall effect at practical temperatures.

[1] Nat. Sci. Rev. 11 (2024), nwad282; [2] Phys. Rev. X 11 (2021), 021033; [3] Mater. Today Phys. 38 (2023), 101265; [4] Chem. Mater. 37 (2025), 1446-1456.

FM 11.26 Tue 18:00 P4

**Simulation-based optimization of gain characteristics for 3D-nanoprinted microchannel plates** — •Kamila Murat, Kristian Deneke, Robert Zierold, Stefanie Haugg, and Robert H. Blick — Universität Hamburg, Hamburg, Germany

Microchannel plates (MCPs) are essential components for signal amplification. However, accurately modeling the complex electron multiplication processes represents one of the most demanding challenges.

Direct laser writing (DLW) techniques enable enhanced design freedom that extends beyond conventional glass-drawn MCPs, allowing the fabrication of structures with diverse materials and complex geometries. Since experimentally iterating such printed structures is both time-consuming and costly, numerical methods become crucial for development.

However, existing theoretical descriptions of electron multiplication remain incomplete and probabilistic, which presents a significant challenge for accurate simulations. To address this, we employ a finite-element-based simulation framework in COMSOL Multiphysics to model the electrostatic fields and electron transport in a 480 $\mu$m-long, 12 $\mu$m-diameter MCP channel biased at 1000 V. Within this configuration we investigate how geometry, bias voltage, and incidence energy influence electron trajectories and the total gain. To model the underlying electron avalanche mechanism driven by secondary electron emission (SEE), different theoretical models are evaluated to analyze the material-dependent SEE parameters. The resulting workflow establishes a scalable basis for extensions of the model.

FM 11.27 Tue 18:00 P4

**Polarons in $LiNb_{1-x}Ta_xO_3$ solid solutions on both sides of the Curie temperature** — •Christa Fink-Bauer and Simone Sanna — Institute for Theoretical Physics, Justus-Liebig-University, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

Polaronic defects in LN, LT and their solid solutions $LiNb_{1-x}Ta_xO_3$ are important to understand their (electrical) conductivity. We do not only model these defects in the low-temperature ferroelectric phase, which is of great interest due to its spontaneous polarization leading to special properties as piezoelectricity, photoelasticity or nonlinear optical response, but also model the high-temprature paraelectric phase, which is stable above the Curie temperature and is of relevance for high-temperature applications. We calculate defect levels in the electronic band gap to extract activation energies for electronic transport. In addition, we calculate formation energies in pure LN and LT and their solid solutions, all from first principles using density-functional theory as implemented in VASP [1, 2]. [1] G. Kresse, J. Furthmüller, Computational Materials Science 6, 15 (1996). [2] G. Kresse, J. Furthmüller, Phys. Rev. B 54, 11169 (1996).

FM 11.28 Tue 18:00 P4

**Local nanoscale probing of electron spins using NV centers in diamond** — •Sergei Trofimov[1], Christos Thessalonikios[1], Victor Deinhart[2,3], Alexander Spyrantis[2], Lucas Tsunaki[1], Kseniia Volkova[1], Katja Höflich[2], and Boris Naydenov[1] — [1]Berlin Joint EPR Laboratory and Department Spins in Energy Conversion and Quantum Information Science (ASPIN), Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany — [2]Leibniz-Institut für Höchstfrequenztechnik, Ferdinand-Braun-Institut (FBH), Berlin, Germany — [3]Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy, Berlin, Germany

Substitutional nitrogen atoms in a diamond crystal (P1 centers) are crucial for creation of nitrogen-vacancy (NV) centers. However, P1's electron spin generates paramagnetic noise that degrades the NV's performance by shortening its coherence time. Bulk characterization methods of nitrogen concentration based on optical absorption or electron paramagnetic resonance often overlook local variations in the nitrogen content. In this work, we use a helium ion microscope to fabricate nanoscale NV center ensembles at predefined sites with a nanoscale resolution in a diamond crystal containing low concentrations of nitrogen. We then utilize these NV-based probes to measure the local P1 concentration on the level of 230 ppb using the double electron-electron resonance (DEER) technique. Moreover, by comparing the DEER spectra with numerical simulations, we determined the concentration of other unknown paramagnetic defects created during the ion implantation to be up to 15 ppb depending on the implantation dose.

FM 11.29 Tue 18:00 P4

**Plug-and-play modification of a scanning electron microscope with a secondary electron yield detector** — •Kristian Deneke[1], Stefanie Haugg[1], Isabel González Díaz-Palacio[2], Marc Wenskat[1,3], Wolfgang Hillert[2], Bent Andersen[1], Robert Zierold[1], and Robert Blick[1,3] — [1]Center for Hybrid Nanostructures, University of Hamburg, Germany — [2]Institute of Experimental Physics, University of Hamburg, Germany — [3]Deutsches Elektron-Synchrotron (DESY), Hamburg, Germany

Secondary electrons are already detected and used to achieve image contrast in a scanning electron microscope (SEM). However, measuring the secondary electron yield (SEY) requires a detector configuration that goes beyond the standard features of an SEM. The SEY is an important figure of merit for many different applications and research fields such as electron multipliers, vacuum cavities, and spacecrafts. Therefore, we present a plug-and-play configuration that allows an existing SEM to be modified with an SEY detector. This detector unit enables SEY measurements of conductive and insulating thin films in a pulsed operation mode. Furthermore, planar thin films can be examined not only at normal incidence, but also at an angle of inclination of the primary electrons, allowing for angular-dependent SEY characterization. Finally, the integration of our detector unit within an SEM enables the recording of a 2D SEY map, visualizing structural variations of patterned substrates. This detector setup could increase accessibility of SEY measurements and pave the way to improvements of applications and new measurement techniques.

FM 11.30 Tue 18:00 P4

**A high-temperature optical spectroscopy study of congruent $LiTaO_3$** — •Ludmila Eisner[1], Angélique Hoffmann[2], Ani Manucharyan[2], Sebastian Inckemann[2], Yuriy Suhak[1], Steffen Ganschow[2], Holger Fritze[1], and Klaus.-D. Becker[3] — [1]Clausthal University of Technology, Germany — [2]Leibniz-Institut für Kristallzüchtung, Germany — [3]Technische Universität Braunschweig, Germany

Spectroscopic studies of congruent lithium tantalate (cLT) were performed to analyze the optical absorption edge under different thermal treatments in air and to relate its changes to band gap variations with temperature. At room temperature, the material exhibits an absorption edge near 4.45 eV. Thermal measurements, extending up to 900°C, show a systematic shift of about 0.138 eV toward lower photon energies per 100 K with increasing temperature. The treatments at reducing conditions (Ar/5% $H_2$) were found to induce significant changes in the spectra after cooling down to room temperature. These spectra show the formation of extended absorption tails down to photon energies of about 2.5 eV. This may suggest enhanced occupation or reconfiguration of intrinsic defect states, including polaronic states, vacancies, and antisite-related centers. These spectral changes largely evade observation under high-temperature in-situ conditions due to the redshift of the absorption edge. Comparison of spectra recorded after thermal cycling shows partial reversibility of these defect-related features. The present results provide a picture of how temperature and reduction-induced defect chemistry impact the optical response of cLT.

FM 11.31 Tue 18:00 P4

**Analysing the laser-driven tetragonal-to-cubic phase-transition in ferroelectric $BaTiO_3$ using EXAFS spectroscopy as a local probe** — •Janosch Tasto[1], Rajdwip Bhar[1], Simon Rauls[1], Marco Reinhard[2], Dimosthenis Sokaras[2], Uwe Bovensiepen[1], and Heiko Wende[1] — [1]Faculty of Physics and CENIDE, University of Duisburg-Essen — [2]SLAC National Accelerator Laboratory, Stanford University

This work aims to establish time-resolved Extended X-ray Absorption Fine Structure (tr-EXAFS) spectroscopy as a methodology for solids where the structural information of the EXAFS is combined with a pump-probe setup to study local dynamic lattice processes in the time domain.
As a proof of concept, we analyze the structural cubic-to-tetragonal phase-transition in the ferroelectric perovskite $BaTiO_3$. The coexistence of displacive and order-disorder phenomena accompanying this transition is a topic of debate in the literature on this extensively studied material.Difference-EXAFS scans at the Ti K-edge and the Ba $L_3$-edge between the pumped and unpumped state provide a direct way to investigate changes in lattice-structure and thermal-induced disorder in the vicinity of the absorbing atom. We correlate our spectroscopic findings with *ab initio* multiple-scattering calculations using the FEFF10 code to quantify structural dynamics.
We thank the Deutsche Forschungsgemeinschaft (in the framework of the Collaborative Research Center 1242) for financial support.

FM 11.32 Tue 18:00 P4

**Correlation between grain size and dielectric properties in medium entropy titanate-based perovskite oxides** — Amirhosein Paryab, •Doru Lupascu, and Vladimir Shvartsman — Institut für Materialwissenschaft Universität Duisburg-Essen Essen, Germany

High-entropy perovskite oxides have attracted significant attention as promising materials for energy storage applications. The configurational entropy is modulated by substituting different elements at a specific ionic site. If it is in the range of 0.7R-1.6R or above 1.6R, the oxides are called medium-entropy or high-entropy, respectively. We report a study of the influence of the synthesis method on the structure, dielectric, and ferroelectric properties of medium entropy titanate-based perovskite oxides (Ba0.34Sr0.33Ca0.33)TiO3 and (Ba0.25Sr0.25Ca0.25Pb0.25)TiO3. Compared to the solid state method, the sol-gel derived materials have a smaller grain size and higher lattice strain. This results in a more diffuse phase transition and a significant shift in the Curie temperature by 60 and 10 K in (Ba0.34Sr0.33Ca0.33)TiO3 and (Ba0.25Sr0.25Ca0.25Pb0.25)TiO3, respectively. Furthermore, fine grained samples were found to exhibit broader polarization hysteresis loops that could be ascribed to higher barriers to dipole switching and the pinning effect. The interplay of configuration entropy, microstructure, and functional behavior is analyzed.

FM 11.33 Tue 18:00 P4

**Characterization and Fabrication of Silicon Wave Guides for the Study of Quantum Material Properties** — •Sierra Randall Heinrich[1,2], Sebastian Zafra Koch[1,2], Florian Spickmann[1,2], Murat Sivis[1,2], Claus Ropers[1,2], and Hannes Böckmann[1,2] — [1]Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany — [2]University of Göttingen, 4th Physical Institute, Göttingen, Germany

Placing quantum materials into optical cavities promises active control of material properties and functionality. Low-dimensional systems are particularly susceptible and exhibit electronic phases that can be switched by an external stimulus. However, the required extreme light-matter coupling is hampered by intrinsic cavity losses and poor overlap with optical modes. Here, we work towards the integration of a prototypic Peierls insulator at the surface of a silicon waveguide resonator. This project focuses on the creation of the resonator. A resonator couples the light into the sample by always totally internally reflecting it, thus generating the evanescent fields used in light matter coupling. To couple the light into the wafer, the angle of reflection has to be controllable. Here, we used diffraction gratings etched onto the surface with varying periods to achieve this. Next, we used Fabry-Pérot interference to maximize the effect of the evanescent fields. As a result, the resonance conditions of a 25 micrometer thick wafer were observed and accurately predicted for the first four resonance peaks. The two aspects of this project will be combined in future, with etched diffraction gratings on a thin wafer.

FM 11.34 Tue 18:00 P4

**Understanding the formation of metal-semiconductor contacts in ferroelectric p-type oxides** — •Ailu Sackey[1], Ruben Dragland[1], Egil Tokle[1], Zewu Yan[2,3], Edith Bourret[2], Jan Schultheiss[1], Mario Hentschel[4], and Dennis Meier[1,5] — [1]NTNU, Trondheim, Norway — [2]Lawrence Berkeley National Laboratory, Berkeley, CA, USA — [3]ETH Zurich, Zürich, Switzerland — [4]University of Stuttgart, Stuttgart, Germany — [5]University of Duisburg-Essen, Duisburg, Germany

Ferroelectric semiconductors exhibit highly tunable electronic responses, opening new pathways for nanoelectronics beyond Si-based approaches. Of particular interest are functional properties that arise at internal interfaces in ferroelectrics, such as domain walls or phase boundaries, which, when leveraged, can serve as ultra-small active elements or as extended 3D networks, requiring a thorough understanding of the contacts used for current injection and sensing.

Here we investigate metal-semiconductor contacts formed by deposited electrodes on the surface of the model p-type ferroelectric $ErMnO_3$. By cation doping and $O_2$ annealing, we methodically modify the charge carrier distribution and monitor the related changes. We find that donor doping promotes ohmic contact formation, whereas annealing in $O_2$-rich atmospheres leads to Schottky-like barriers. The results align with expected Fermi-level shifts and band-bending phenomena described by traditional semiconductor physics. Our findings offer fundamental guidance for controlling the contact formation in hexagonal manganites and related p-type ferroelectric semiconductors.

FM 11.35 Tue 18:00 P4

**Energy Profile and Hopping Barriers for Small Electron Polarons at Ferroelectric Domain Walls in Bismuth Ferrite from First Principles** — •Sabine Körbel — Friedrich Schiller University Jena, Germany

Evidence from first-principles calculations indicates that excess electrons in $BiFeO_3$ form small polarons with energy levels deep inside the electronic band gap. Hence, n-type electronic transport could occur by polaron hopping rather than by band-like transport. Here, using first-principles calculations, small electron polaron hopping in $BiFeO_3$ is investigated. Both bulk $BiFeO_3$ and a typical ferroelectric domain wall, the neutral 71° domain wall, are considered to account for experimental observations of electrical conductivity at domain walls in otherwise insulating ferroelectrics. The object of this study is to shed light on electron conduction in $BiFeO_3$ and the influence of pristine neutral ferroelectric domain walls. The computed energy barriers for small electron polaron hopping are near 0.2 eV, similar to other perovskite oxides, both in the bulk and within the neutral 71° domain wall. Trapping energies of small electron polarons at the three prevalent domain walls, the 71°, the 109°, and the 180° wall, are determined. The domain walls are two-dimensional traps for small electron polarons, with a trap depth of about twice the thermal energy at room temperature. Based on these findings, the n-type mobility and the diffusion constant in $BiFeO_3$ are estimated, and experimental conductivity data for $BiFeO_3$ are discussed.

FM 11.36 Tue 18:00 P4

**Smart DNA lithography as a tool for nanoelectronics** — •Raufar Shameem[1], Charlotte Kielar[1], Christoph Hadlich[2], Borja Rodriguez-Barea[1], Ralf Seidel[2], and Artur Erbe[1] — [1]Institute of Ion Beam Physics and Materials Research, HZDR, Dresden, Germany — [2]Peter Debye Institute for Soft Matter Physics, University of Leipzig, Leipzig, Germany

Precise nanoscale patterning enables geometry-dependent functions across electrical, optical, and magnetic systems. DNA-templated hybrid lithography employs programmable molecular templates to define complex nanoscale shapes. Here, we use long DNA origami structures in a workflow integrating self-assembly, selective bottom-up oxide growth, and conventional top-down processing. The origami patterns form durable stencil masks on sapphire, guiding etching and metal deposition to create nanowire geometries beyond optical lithography. To generate these masks, DNA origami is assembled on sacrificial silicon, followed by controlled SiOx growth via chemical vapor deposition. Removing the DNA exposes nanowire-like and cavity-like oxide features that accurately reproduce the origami geometry and serve as robust patterning masks. AFM, SEM, and FIB cross sections verify shape transfer, growth behavior, and patterning resolution. This approach extends DNA-assisted lithography toward clean, versatile metal architectures for geometry-sensitive applications. It also improves integration with existing fabrication by providing stable masks, reliable shape transfer, and added flexibility in designing nanoscale features.

FM 11.37 Tue 18:00 P4

**Theory-Guided Discovery of Ion-Exchanged Poly(heptazine Imide) Photocatalysts Using First-Principles Many-Body Perturbation Theory** — •Zahra Hajiahmadi and Thomas D. Kühne — CASUS - Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf e.V. (HZDR), Untermarkt 20, D-02826 Görlitz, Germany

Poly(heptazine imides) (PHI) show strong promise in photocatalysis, but limited control over electronic properties continues to constrain their full potential. We modulated PHI's photocatalytic activity to overcome this limitation by incorporating mono-, di-, and trivalent metal cations into its framework. To elucidate the underlying mechanisms, we employed calculations based on many-body perturbation theory, a highly accurate approach for electronic structure calculations that provides improved accuracy in quasiparticle energy predictions compared to conventional density functional theory, particularly for band gaps and excitonic properties. Our analysis identifies several metal-doped PHI systems with electronic structures well suited for hydrogen and oxygen evolution, $CO_2$ reduction, and $H_2O_2$ production. Guided by these theoretical insights, we synthesized a subset of $M$-PHI materials (where $M$ is either K, Na, Li, Ca, Mg, or Zn) predicted to enhance photocatalytic reactivity.

FM 11.38 Tue 18:00 P4

**Soft X-ray Spectroscopy at the HESEB Beamline, SESAME** — •Ahlam Farhan — SESAME, Allan, Jordan

The ID11-L Helmholtz-SESAME Soft X-ray Beamline (HESEB) represents a significant step forward in soft X-ray research infrastructure in the Middle East. Operating in the 70-2000 eV energy range, HESEB provides photon fluxes between 10-3404 Giga photons/s, with an energy resolution exceeding $E/\Delta E > 8000$. The beamline delivers a focused spot size of $500*250\mu$m and offers tunable circular polarisation, enabling precise investigations of the electronic and magnetic properties of a wide range of materials.

The X-ray absorption spectroscopy (XAS) end station is equipped with a motorised manipulator, magnetic sample holders, and a differential pumping system, allowing measurements under ambient conditions or in a helium atmosphere. This flexibility supports the study of vacuum-sensitive materials, including valuable cultural heritage samples.

Recent XAS and XMCD measurements demonstrate HESEB's excellent stability, high resolution, and precise polarisation control, establishing it as a versatile platform for soft X-ray spectroscopy and magnetic materials research at SESAME.

## FM 12: German-French Focus Session: Materials Research in Polar Oxides – From Domain Engineering to Photonic and Electronic Devices I

chair: Simone Sanna (Justus-Liebig-Universität Gießen, DE)

The focus session is dedicated to bridge the gap between materials research in polar oxides and research fields that apply those materials, such as nonlinear and quantum optics, electronics or sensoring, spanning experimental studies and first-principles simulations.

Time: Wednesday 9:30–13:00 Location: BEY/0138

**Invited Talk** FM 12.1 Wed 9:30 BEY/0138

**Shedding Light on Polar Topological Textures** — •Salia Cherifi-Hertel — CNRS and University of Strasbourg, IPCMS

The study of topological polarization textures in ferroelectric materials represents a rapidly evolving frontier in ferroic research, with implications for solitonic information technologies and emergent phenomena in correlated oxides. Complex configurations, such as non-Ising and chiral domain walls, bubble domains, (anti)vortices, and polar (anti)skyrmions, highlight the diversity of polarization states in low-dimensional systems, where symmetry breaking, strain, and electrostatic boundary conditions produce novel functionalities. While piezoresponse force and transmission electron microscopies remain central to nanoscale characterization, optical methods are emerging as powerful, noninvasive alternatives. Second-harmonic generation (SHG) microscopy, in particular, provides intrinsic sensitivity to symmetry and polarization orientation, enabling three-dimensional mapping of polar architectures. This presentation will outline recent advances in SHG polarimetry combined with machine-learning-assisted analysis, enabling rapid, quantitative reconstruction of 3D polarization textures. This integrated approach offers a robust framework for probing polar topologies and uncovering the intricate coupling between structure, symmetry, and functionality in ferroic materials.

FM 12.2 Wed 10:00 BEY/0138

**Origin and Evolution of Domain-Wall Conductivity in LiNbO3** — •Iuliia Kiseleva[1], Boris Koppitz[1], Matthias Roeper[1], Elke Beyreuther[1], Samuel Seddon[1], and Lukas Eng[1,2] — [1]Institute of Applied Physics, Technische Universität Dresden, Nöthnitzer Straße 61, Dresden, 01187, Germany — [2]ct.qmat: Dresden-Würzburg Cluster of Excellence - EXC 2147, TU Dresden

Ferroelectric domain walls, which effectively serve as two-dimensional interfaces, exhibit functionalities markedly distinct from those of the bulk, such as enhanced conductivity and strong coupling to external fields, making them promising for nanoelectronic applications. Among various systems, lithium niobate (LiNbO3) stands out due to its high Curie temperature, chemical stability, and thoroughly characterized bulk properties. Yet the microscopic origins and dynamic evolution of domain-wall conductivity remain insufficiently understood, largely due to limited in-situ, time-resolved characterization. Here, we combine in-situ second-harmonic-generation (SHG) microscopy with electrical transport measurements and complementary chemical analysis to investigate domain-wall behavior under controlled electric and mechanical loading. This multimodal approach enables real-time visualization of domain restructuring, correlation of conductivity changes with wall inclination, and the dynamics of defects. The results aim to advance the understanding of functional domain-wall states and the mechanism of electrical transport in ferroelectric 2D systems.

FM 12.3 Wed 10:15 BEY/0138

**Persistent photoconductivity in reduced lithium niobate bidomain crystals** — •Philipp Fahler-Muenzer, Marios Hadjimichael, Ana Sanchez-Fuentes, Richard Beanland, Eoin Moynihan, and Marin Alexe — University of Warwick, Coventry, United Kingdom

The uniaxial ferroelectric lithium niobate ($LiNbO_3$) can exhibit significantly enhanced domain wall (DW) conductivity, rendering it an interesting system for DW-based nanoelectronics. Specifically, head-to-head (h2h) DWs exhibit conductivities several orders of magnitude higher than that of the surrounding bulk. We create h2h DWs with a near-90° inclination angle by using the diffusion annealing technique, followed by chemical treatment to change the functional properties. The characterization of the structure and morphology is conducted by piezoresponse force microscopy and transmission electron microscopy.

To characterize electronic transport, we use resistivity measurements under varying temperatures in dark or under UV light illumination, complemented by conductive atomic force microscopy. Our findings indicate only transient conductivity at the DWs, but substantial differences in photoconductivity between monodomain and bidomain crystals, with persistent photoconductivity in crystals with DWs. Furthermore, we report a drastic drop in domain wall photoconductivity upon heating above 80°C, which can be explained by the emptying of charge carrier traps in the DW as the system gains higher thermal energy.

FM 12.4 Wed 10:30 BEY/0138

**Photocurrent-based recognition in time-series tasks using reservoir computing** — •Yan-Meng Chong[1], Atreya Majumdar[2], Ingvild Hansen[1], Karin Everschor-Sitte[2], and Dennis Meier[1,2,3] — [1]Department of Materials Science and Engineering, Norwegian University of Science and Technology (NTNU), Trondheim, Norway — [2]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Duisburg, Germany — [3]Research Center Future Energy Materials and Systems, Research Alliance Ruhr, Bochum, Germany.

In reservoir computing, input data are mapped into higher dimensional space, translating non-linear problems into linearly solvable ones. In general, any physical system that possesses non-linearity, complexity, short-term memory, and reproducibility can serve as reservoir. Here, we investigate the ferroelectric semiconductor ErMnO$_3$ as a potential candidate material for reservoir computing. We show that the system displays pronounced non-linear changes in photocurrent under varying light intensity. The response can be tuned by changing the metal-semiconductor contacts (Schottky- or Ohmic-like behavior) used for readout, determining the timescale on which the photocurrent vanishes after illumination. This relaxation behavior in the OFF state gives fading memory. We perform training on variations in the output (photocurrent), which allows for recognition in time-series tasks. Interestingly, ferroelectric domain walls can also be used as reservoirs with characteristic photocurrent signals, giving new opportunities to down-scale or enhance the complexity of physical reservoirs.

### Coffee break

FM 12.5 Wed 11:00 BEY/0138

**Properties of Charged Interfaces in Uniaxial Ferroelectrics** — •Conor McCluskey, Kristina Holsgrove, Andrew Rogers, James Dalzell, Ronan Lynch, Raymond McQuaid, Tchavdar Todorov, and Marty Gregg — Queen's University Belfast, United Kingdom

When the polarisations of neighbouring ferroelectric domains abut, a bound charge develops at the interface. Often, these charged domain walls show enhanced electrical conductivity, which is typically taken as a sign that the polar divergence is fully screened by the mobile transport carriers. Transport measurements, however, suggest the carrier densities associated with domain wall conductivity lie well below that expected for a fully screened ferroelectric bound charge. In fact, some charged domain walls lack enhanced conductivity entirely. In these cases, polar rotation occurs to fully avoid the development of bound charge, leading to topological patterns in the polarisation field. Here, we discuss the interfaces formed between thermally bonded lithium niobate single crystals generated with intentional head-to-head character. We show that the interfaces formed uniquely host both of these properties: enhanced conductivity, and a striking array of polarisation vortices. Furthermore, since this interface is formed by thermal bonding of two crystalline structures, there is freedom to introduce relative lattice twists between the two parent crystals, which is unavailable at regular domain walls within a single parent crystal. We will discuss the interplay of strain and electrostatics at these unique interfaces in the context of their emergent functionality.

FM 12.6 Wed 11:15 BEY/0138

**Polar Discontinuities, Emergent Conductivity, and Critical Twist-Angle-Dependent Behaviour at Wafer-Bonded Ferroelectric Interfaces** — Andrew Rodgers[1], Kristina Holsgrove[1], Conor McClusky[1], Samuel Seddon[2], Marty Gregg[1], and •Lukas M. Eng[2,3] — [1]Centre for Quantum Materials and Technologies, School of Mathematics and Physics, Queen's University Belfast, UK — [2]Institut für Angewandte Physik (IAP)- Nöthnitzer Str. 61, 01187 Dresden — [3]ct.qmat: Dresden-Würzburg Cluster of Excellence*EXC 2147, TU Dresden, Germany

Probing novel properties, arising from twisted interfaces, has traditionally relied on the stacking of exfoliated 2D materials and the spontaneous formation of van der Waals (vdW) bonds. So far, investigations involving intimate covalent or ionic bonds have not been a focus. Yet, we show here that an established technique, involving thermocompressional wafer bonding, works well for creating twisted non-vdW interfaces. We have successfully bonded z-cut lithium niobate single crystals to create ferroelectric oxide interfaces with strong polar discontinuities and have mapped the associated emergent interfacial conductivity. In some instances, a dramatic change in microstructure occurs, involving local dipolar switching. A twist-induced collapse in the capability of the system to effectively screen interfacial bound charge is implied. Importantly, this only occurs around specific moiré twist angles with sparse coincident lattices and associated short-range aperiodicity. In quasicrystals, aperiodicity is known to induce pseudo-bandgaps and we suspect a similar phenomenon here.

FM 12.7 Wed 11:30 BEY/0138

**Machine learned potential for ferroelectric heterostructure BaTiO3/SrTiO3** — •Lan-Tien Hsu[1], Jonathan Schmidt[2], Aaron Iten[2], Nicola Spaldin[2], and Anna Grünebohm[1] — [1]Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Faculty of Physics and Astronomy, and Center for Interface-Dominated High Performance Materials (ZGH), Ruhr-University Bochum, Germany — [2]Department of Materials, ETH Zürich, Zürich, CH-8093, Switzerland

Ferroelectric heterostructures offer a platform to realize topological patterns with functionalities relevant to future electronic devices.[1] While short-range machine-learned interatomic potentials can capture ferroelectric instabilities in pure materials, long-range dipole interactions remain essential for heterostructures, where depolarizing field plays a role.[2] We address this challenge by combining MACE message-passing networks with a latent Ewald-summation scheme[3] capable of learning long-range interactions and inferring Born effective charges without explicit training on response properties. The model predicts transition temperature and spontaneous polarization of BaTiO$_3$ in close agreement with experiments. It further captures the multidomain formed in heterostructures, consistent with coarse-grained effective-Hamiltonian results, and generalizes well to untrained configurations, including those containing oxygen vacancies.

[1] Das *et al*, Nature **568**, 368-372 (2019)
[2] Yu *et al*, Phys. Rev. B **112**, 104324 (2025)
[3] Zhong *et al*, 10.48550/arXiv.2504.05169

FM 12.8 Wed 11:45 BEY/0138

**From Stacking Faults to Field-Stabilized Polarity: Connecting RP Phases and the MFP Phase in SrTiO$_3$** — •Christian Ludt[1,2], Hartmut Stöcker[1,2], Matthias Zschornak[1,2,3], and Dirk C. Meyer[1,2] — [1]TU Bergakademie Freiberg, 09599 Freiberg, Germany — [2]Zentrum für Effiziente Hochtemperatur-Stoffwandlung, 09599 Freiberg, Germany — [3]Hochschule für Technik und Wirtschaft Dresden, 01069 Dresden, Germany

Polar functionalities in perovskites often arise from a subtle interplay between lattice distortions, defect chemistry, and stacking faults. In this work, particular attention is given to the migration-induced field-stabilized polar (MFP) phase in SrTiO$_3$, a recently identified polar state that arises from field-driven oxygen mobility and picometer-scale cation displacements. To provide a structural framework for understanding and enhancing this phenomenon, the electronic properties of Ruddlesden-Popper-type (RP) stacking faults in SrO(SrTiO$_3$)$_n$ are analyzed using density functional theory. These faults introduce symmetry breaking, modified lattice environments and characteristic changes in the electronic structure that closely resemble the local conditions required to form the MFP phase. By combining insights from RP-layered configurations with the field- and defect-driven mechanisms underlying MFP formation, a unified perspective emerges in which stacking faults act as natural templates that support, amplify, or localize MFP-like polar distortions. This connection highlights new pathways for engineering polar responses and optoelectronic functionalities in complex perovskite oxides.

### Coffee Break

FM 12.9 Wed 12:15 BEY/0138

**Integration of imprint-free and low coercivity ferroelectric BaTiO$_3$ thin films on silicon** — Jingtian Zhao[1,2], Majid Ahmadi[1,2], Beatriz Noheda[1,2], and •Martin F. Sarott[1,2] —

[1]Zernike Institute for Advanced Materials, University of Groningen, The Netherlands — [2]Groningen Cognitive Systems and Materials Center (CogniGron), University of Groningen, The Netherlands

Highly-crystalline ferroelectric oxides integrated on Si hold great promise for energy-efficient memory and logic technologies. Exploiting epitaxial strain engineering in these materials is, however, severely hampered on Si, where the large structural mismatch often results in an inferior interfacial quality and causes a degradation of the ferroelectric switching characteristics. In this work, we present the growth of single-crystalline $BaTiO_3$ thin films on Si, exhibiting imprint-free switching, low coercivity, high remanent polarization, and no fatigue for over $10^{10}$ switching cycles. We accomplish this via the insertion of a $SrSn_{1-x}Ti_xO_3$ layer on $SrTiO_3$-buffered Si. This layer serves as a pseudo substrate that alleviates the *thermal strain* that the Si substrates imposes on the $BaTiO_3$ layer, while simultaneously providing moderate compressive strain that stabilizes a pure out-of-plane polarization. Thus, our work paves the way toward the fabrication of Si-compatible, low-power-consuming ferroelectric devices for non-volatile memory applications.

FM 12.10 Wed 12:30 BEY/0138

**Polarity and polarons in $WO_3$ through epitaxial shear strain** — •Ewout van der Veer[1], Martin Sarott[1,2], Jack Eckstein[3,5], Stijn Feringa[1], Dennis van der Veen[1], Johanna van Gent González[1], Majid Ahmadi[1,2], Horatio Cox[1,2], Ellen Kiens[4], Gertjan Koster[4], Bart Kooi[1,2], Michael Carpenter[3], Ekhard Salje[3], and Beatriz Noheda[1,2] — [1]ZIAM, Uni. of Groningen, Netherlands (E. vd V. now: Fac. of Phys., UDE, Duisburg, Germany and RC FEMS, Bochum, Germany) — [2]CogniGron, Uni. of Groningen, Netherlands — [3]Dept. of Earth Sci., Uni. of Cambridge, UK — [4]MESA+ Inst., Uni. of Twente, Netherlands — [5]Center for Nano. Mater. Sci., ORNL, USA

Tungsten oxides have been investigated for gas sensing, catalytic and electrochromic capabilities. Epitaxial thin films of $WO_3$ on (110)-oriented $YAlO_3$ even exhibit piezoelectricity and conductivity at monoclinic twin walls due to local strain gradients. We grew epitaxial films of $WO_3$ on (001)$YAlO_3$ by pulsed laser deposition and reveal a previously unreported polar phase by imposing epitaxial shear strain, stabilizing a triclinic structure up to large film thicknesses and elevated temperatures. The films have periodic in-plane domains with needle bifurcations and enhanced conductivity at domain walls. STEM shows that these walls exhibit a reduction of a structural distortion, evidence for recently predicted anti-distortive polarons. Our films are structurally and functionally different from known bulk phases and previous epitaxial films due to subtle epitaxial interactions. They are candidates for oxide electronics, neuromorphic computing and catalysis.

FM 12.11 Wed 12:45 BEY/0138

**Inducing Strain Gradients in Transition Metal Oxides using Ferroelastic Domain Patterns** — •Freya Watson[1], Aditya Singh[1], Katarzyna Sopinska[1], Daniel Chaney[2], Marin Alexe[1], and Marios Hadjimichael[1] — [1]University of Warwick, Coventry, United Kingdom — [2]ESRF, avenue des Martyrs, 38043 Grenoble Cedex 9, France

Strain engineering is a powerful tool for accessing new and versatile properties of materials. The use of ferroelectric domain patterns instead of conventional substrates further allows for the modification of the properties of these materials using electric fields. $PbTiO_3$ is a ferroelectric and ferroelastic perovskite which forms a periodic in-plane and out-of-plane domain structure when deposited on (110)-$DyScO_3$ substrates, caused by lattice mismatch. In this work, we explore inducing strain gradients in metallic perovskite thin films grown on this $PbTiO_3$ domain structure. Using this approach we are able to effectively couple strain between heterostructure interfaces and produce large anisotropy in electronic transport and material properties, which are found to be tuneable by altering $PbTiO_3$ layer thickness, and thus domain period. The effects of this strain engineering are demonstrated by scanning probe techniques, microscopy imaging and 4-probe resistivity measurements.

## FM 13: Topical Session: Dislocations in Functional Materials I (joint session MM/FM)

Time: Wednesday 10:15–11:30 Location: SCH/A251

FM 13.1 Wed 10:15 SCH/A251

**Mechanical seeding of dislocations for room-temperature plasticity in ceramics** — •Wenjun Lu[1], Jiawen Zhang[1], and Xufei Fang[2] — [1]Department of Mechanical and Energy Engineering, Southern University of Science and Technology, Shenzhen, 518055, China — [2]Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe,76131, Germany

The pursuit of room-temperature ductile ceramics has long been hindered by their inherent brittleness. Here, we demonstrate a simple strategy to seed mobile dislocations at room temperature with densities up to 1014 m-2, enabling ceramics to sustain plastic compressive strains exceeding 30%. These dislocations multiply through cross-slip and motion, effectively suppressing brittle fracture without high-temperature processing. Using in situ nano-/micromechanical deformation and ex situ bulk tests, we bridge the length scales of plasticity and reveal a strong dependence of yield strength and flow behavior on dislocation density. Specifically, SrTiO3 micropillars transition from brittle fracture (dislocation-free) to plastic yield when mechanically seeded dislocations are present. Yield strength first decreases then rises with increasing dislocation density, reflecting complex structural evolution observed via transmission electron microscopy. These findings highlight dislocation engineering as a viable pathway toward ductile ceramics and open avenues for tuning their mechanical and functional properties through room-temperature dislocation plasticity.

Contribution: Wenjun Lu is the Speaker.

FM 13.2 Wed 10:30 SCH/A251

**Impact of mechanically seeded dislocations on the mechanical properties of perovskite ceramics** — •Jiawen Zhang[1], Xufei Fang[2], and Wenjun Lu[1] — [1]Southern University of Science and Technology, Shenzhen, China — [2]Karlsruhe Institute of Technology, Karlsruhe, Germany

The inherent brittleness of functional ceramics severely hinders their engineering application. The strong ionic and covalent bonds in ceramics make dislocation nucleation, motion, and multiplication difficult at room temperature. Recent research challenges the conventional perception of ceramics as inherently brittle materials, with dislocations emerging as a promising avenue for enhancing their mechanical properties. By using a Brinell ball indenter to perform surface scratching, crack-free plastic deformation zones with tunable dislocation density can be generated on the ceramic surface. The dislocation generation mechanism and dislocation-dominated plastic deformation mechanism were investigated by introducing dislocations into perovskite SrTiO3 and KTaO3. Room temperature micropillar compression tests then revealed that as the mechanical seeded dislocation density increased,SrTiO3 exhibited a *brittle* to *ductile* transition as the dislocation density increased from ~1010 m-2 to ~1014 m-2. However, the (001) KTaO3 single crystal exhibits a *brittle* to *ductile* then to *brittle* transition as the dislocation density increased from ~1010 m-2 to ~1015 m-2. Additionally, the yield strength displayed a complex trend, initially decreasing and then increasing in these two perovskite oxide ceramics.

FM 13.3 Wed 10:45 SCH/A251

**Dislocation interaction with a tilt low angle grain boundary in bi-crystal SrTiO3** — •Kuan Ding[1,2], Atsutomo Nakamura[3], Patrick Cordier[4,5], and Xufei Fang[3,6] — [1]Department of Materials and Earth Sciences, Technical University of Darmstadt, 64287 Darmstadt, Germany — [2]Max Planck Institute for Sustainable Materials, Max-Planck-Straße 1, 40237 Düsseldorf, Germany — [3]Department of Mechanical Science and Bioengineering, Osaka University, 1-3 Machikaneyama-chou, Toyonaka, Osaka, 560-8531, Japan — [4]Unité Matériaux et Transformations, Université de Lille, 59655 Villeneuve d'Ascq Cedex, France — [5]Institut universitaire de France (IUF), 75005 Paris, France — [6]Institute for Applied Materials, Karlsruhe Institute of Technology, Kaiserstr. 12, 76131 Karlsruhe, Germany

For applications of ceramics with dislocation-tuned mechanical and functional properties, it is pertinent to achieve dislocation engineering in polycrystalline ceramics. However, grain boundaries (GBs) are effective barriers for dislocation glide at room temperature. It is critical to understand the fundamental processes for dislocation-GB interaction. We investigated a bi-crystal SrTiO3 with a 4° tilt GB. Brinell indentation was used to generate a plastic zone at the mesoscale without cracking, allowing for direct assessment of GB-dislocation interaction. Together with dislocation etch pits imaging and transmission electron microscopy analysis, we observe dislocation pileup, storage, and transmission across the LAGB. Our observations reveal new insights into dislocation-GB interaction at room temperature at mesoscale.

FM 13.4 Wed 11:00 SCH/A251

**Dislocation-Mediated Extraordinary Room-Temperature Plasticity in Inorganic Semiconductors** — •Xiaocui Li[1] and Yang Lu[2] — [1]Department of Materials Science and Engineering, City University of Hong Kong, Kowloon, Hong Kong SAR, China — [2]Department of Mechanical Engineering, The University of Hong Kong, Pokfulam, Hong Kong SAR, China

Inorganic semiconductors, with their ionic or covalent bonds, are typically brittle at room temperature, restricting their use in flexible electronics. Our recent study reveals that all-inorganic perovskite (CsPbX3, X=Cl, Br, I) single-crystal micropillars can achieve extraordinary room-temperature plasticity with average plastic strain of ~64% (Nat. Mater. 2023, 22, 1175). They can be morphed into distinct geometries without cracks or cleavage. The deformation is mediated by partial dislocations on {011}<0-11> slip system, featuring four equivalent variants that address the lack of deformation pathways in ionic crystals. Sequential activation of variants prevents strain hardening and crack formation caused by dislocation reactions. First-principles calculations attribute this plasticity to low slip barriers enabling sustained deformability and strong Pb-X bonds preserving crystal integrity. Leveraging this deformability, we developed shape-customizable optoelectronic devices that maintain stable functional properties and bandgap energies post-deformation. This discovery overturns the notion of brittleness in inorganic semiconductors, and provides a foundation for advanced applications in flexible electronics and deformable sensors.

FM 13.5 Wed 11:15 SCH/A251

**Dislocations as Key Enablers on the Road to Functional and Resilient Oxide Ceramics** — •Oliver Preuss[1], Enrico Bruder[2], Zhangtao Li[3], Yinan Cui[3], Jinxue Ding[1], Philippe Carrez[4], and Xufei Fang[1] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Division Physical Metallurgy, Department of Materials and Earth Sciences, Technical University of Darmstadt, Darmstadt, Germany — [3]Department of Engineering Mechanics, Tsinghua University, PR China — [4]Materials and Transformations Unit, Université Lille, Lille, France

Designing oxide ceramics that unite high mechanical resilience with strong functional performance is challenging. We show that introducing ultra-high dislocation densities ($\approx 10^{15}$ m$^{-2}$) into materials such as MgO and $SrTiO_3$ provides a direct route to enhance both damage tolerance and functional properties. Cyclic Brinell ball scratching at room temperature generates near-surface, dislocation-rich zones of arbitrary size and shape. These regions markedly alter fracture behaviour, arresting propagating cracks and suppressing crack initiation, as demonstrated by Vickers indentation and quasi-in situ DCDC tests. Crystal-plasticity phase-field simulations reproduce the observed toughening mechanism. The dislocation networks also improve transport properties, increasing electrical conductivity while reducing thermal conductivity by nearly half: an advantageous combination for thermoelectric performance. This work establishes a practical strategy for dislocation engineering to achieve oxide ceramics with combined mechanical robustness and enhanced functionality.

## FM 14: Focus Session: Materials Research in Polar Oxides – From Domain Engineering to Photonic and Electronic Devices II

chair: Conor McCluskey (Queen's University Belfast, UK)

The focus session is dedicated to bridge the gap between materials research in polar oxides and research fields that apply those materials, such as nonlinear and quantum optics, electronics or sensoring, spanning experimental studies and first-principles simulations.

Time: Wednesday 15:00–16:00 Location: BEY/0138

FM 14.1 Wed 15:00 BEY/0138

**Probing ferroelastic domain properties of lanthanum aluminate via spontaneous Raman scattering** — •Robin Buschbeck[1], Susanne C. Kehr[1], Lukas M. Eng[1,2], and Samuel D. Seddon[1] — [1]TU Dresden, Institute of Applied Physics, Nöthnitzer Strasse 61, 01187 Dresden, Germany — [2]ct.qmat: Dresden-Würzburg Cluster of Excellence EXC 2147, TU Dresden, 01062 Dresden, Germany

Lanthanum aluminate ($LaAlO_3$, LAO) is a rhombohedrally distorted oxide perovskite, exhibiting ferroelastic twinning at room temperature. Frequently employed as a thin film substrate [1], it is often overlooked [2] for being optically uniaxial and thus birefringent. The effect of the ferroelastic twins sees an in-plane rotation of this optical axis, with regions of opposing optical axes coexisting (delineated by twin walls).

Here, we present a detailed experimental analysis of LAO(100) using spontaneous Raman scattering (SR). SR is a widely employed technique for obtaining spectral information from a broad range of materials [3]. Using SR, we demonstrate several spatially resolved non-trivial, three-dimensional intrinsic properties of LAO. Special attention is given to the different LAO(100) domains and their behaviour under various SR measurement conditions, including polarization-dependent and spatially resolved in-plane or depth-dependent measurements.

[1] R. W. Simon et al., Springer, Boston, MA (1989)
[2] S. Kustov, et al., Applied Physics Letters 112, 042902 (2018)
[3] A. Orlando et al., Chemosensors 9, 262 (2021)

FM 14.2 Wed 15:15 BEY/0138

**Strain Driven Ferroelastic Switching and Barkhausen Type Behavior in $LaAlO_3$** — •Vladyslav Kovtunovych, Matthias Roeper, Lukas M. Eng, and Samuel D. Seddon — Institut für Angewandte Physik (IAP)- Nöthnitzer Str. 61, 01187 Dresden

Lanthanum aluminate ($LaAlO_3$; LAO) is an oxide perovskite widely used in nano-electronics, and frequently employed as a thin-film substrate therein due to its convienient lattice match to many multiferroic and/or ferroelectric materials. Although oftentimes overlooked, LAO is an improper ferroelastic, posessing crystallographic domains delineated by twin walls, responding to the global application to strain akin to ferromagnetic or ferroelectric materials to magnetic or electric fields respectively. This study focuses on twin wall motion, which was induced and recorded using a commercial Razorbill strain cell with a high-resolution capacitive sensor. Measurements of $LaAlO_3$ under increasing uniaxial compression, revealed the expected jerky domain wall motion indicative of Barkhausen noise, the stochastic stepped reordering of local ordering parameters common among all ferroic materials. This scale invariant physics acts as a power law governing all length scales, from avalanches on mountains down to the nanoscale. Complementary XRD measurements of the expected Bragg peak splitting are correlated with polarised light microscopy imaging all as a function of lattice strain, to observe this effect in a whole new light.

FM 14.3 Wed 15:30 BEY/0138

**Single crystal growth of stoichiometric lithium tantalate** — •Sebastian Inckemann, Roberts Blukis, Angélique Hoffmann, Matthias Bickermann, and Steffen Ganschow — Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, 12489 Berlin, Germany

A material isomorphous to the intensively investigated lithium niobate (LiNbO3, LN) that has the same inherent non-stoichiometry is lithium tantalate (LiTaO3, LT). Despite similar characteristics to LN, the properties of LT are significantly less studied, even though there are notable differences that favor the use of LT in certain applications. Of special interest is the investigation of stoichiometric LT (sLT) compared to congruent LT (cLT), as the lithium deficiency in cLT causes a high concentration of defects (Kim et al., 2001). Literature describes multiple methods to achieve stoichiometric LN single crystals, exemplary via the double crucible method. However, the growth method reporting a crystal composition closest to the stoichiometric ratio is the growth via the flux method (Polgár et al., 2002). Due to the similarities between LN and LT an analogous approach is the most promising, with the use of $K_2O$ as a solvent showing the best results in the case of LN (Polgár et al., 1997). To ensure an efficient single crystal growth in this system, knowledge about the $Li_2O$-$K_2O$-$Ta_2O_5$ phase diagram is vital (Mühlberg et al., 2008). As there is no literature regarding this phase diagram, this presentation will present our current progress by combining DTA, PXRD and SEM measurements. Furthermore, results regarding the single crystal sLT growth attempts will be presented.

FM 14.4 Wed 15:45 BEY/0138

**Poling and acoustic characterization of near-stoichiometric Li(Nb,Ta)O$_3$ crystals** — •Éva Tichy-Rács[1], Stepan Hurskyy[1], Steffen Ganschow[2], Fatima El Azzouzi[1], Holger Fritze[1], and Yuri Suhak[1] — [1]Clausthal University of Technology, Goslar, Germany — [2]Leibniz Institut für Kristallzüchtung, Berlin, Germany

Li(Nb,Ta)O$_3$ solid solutions bridge the high Curie temperature of $LiNbO_3$ and the thermal stability of $LiTaO_3$, while maintaining a strong piezoelectric performance, making them attractive for high-temperature sensing and actuation. The intrinsic properties of $LiNbO_3$, $LiTaO_3$ and, consequently, their Li(Nb,Ta)O$_3$ solid solutions are well known to be highly sensitive to lithium stoichiometry. In the present work the acoustic properties of near-stoichiometric $LiNb_{1-x}Ta_xO_3$ (x=0; 0.45; 1) single crystals are investigated as a function of temperature and time by resonant piezoelectric spectroscopy. The near-stoichiometric compositions were obtained by the vapor transport equilibration (VTE). Subsequently, the samples were electrically poled to ensure a single-domain state. The study shows that acoustic losses in nsLT remain in the range of $10^{-4}$–$10^{-3}$ up to 620 °C, i.e., within the ferroelectric phase, and increase monotonically with temperature, though only weakly, with an activation energy of about 0.05 eV. In contrast, nsLN and nsLNT45 exhibit a pronounced loss increase above 600 °C, attributed to the conductivity-related relaxation mechanism. Under constant operation at 600 °C for 350 h, all samples demonstrate excellent long-term stability, with resonance frequency deviations not exceeding ± 100 ppm of the initial value.

## FM 15: Nanoscale Probing of Functional Properties

chair: Jiali He (Norwegian University of Science and Technology, Norway)

Time: Wednesday 15:00–15:45 Location: BEY/0E40

FM 15.1 Wed 15:00 BEY/0E40

**Nanoscale Phonon Dynamics Studied In-Situ by Laser Stimulated Vibrational Electron Energy-Gain Spectroscopy** — •Mairi McCauley[1,2], Joel Martis[3], Ondrej Krivanek[3], Ben Plotkin-Swing[3], Tolga Wagner[1,2], Hüseyin Çelik[1,4], Grigory Kornilov[1], Katrina Coogan[1,2], Meng Zhao[1,2], Andreas Mittelberger[3], Matthias Meffert[5], Luca Piazza[5], Tracy Lovejoy[3], Guillaume Radtke[6], Christoph Koch[1,2], and Benedikt Haas[1,2] — [1]Department of Physics, Humboldt-Universität zu Berlin, Berlin, Germany — [2]Center for the Science of Materials Berlin, Humboldt-Universität zu Berlin, Berlin, Germany — [3]Bruker AXS LLC, Kirkland, WA, USA — [4]Institute for Physics and Astronomy, Technische Universität Berlin, Berlin, Germany — [5]DECTRIS AG, Baden-Daettwil, Switzerland — [6]Sorbonne Université, CNRS UMR 7590, MNHN, IMPMC, Paris, France

Advances in instrumentation allow to directly probe phonon dispersions at the nanoscale using electron energy gain and loss spectroscopy (EEGS/EELS) within a scanning transmission electron microscope (STEM). By integrating a laser injection system, we enable the investigation of stimulated phonons at the spatial resolution determined by the electron beam. A synchronised laser-detector configuration enables nanosecond-scale time-resolved measurements. The thermal conductivity of amorphous carbon and silicon nitride was investigated by local time-resolved temperature measurements and is compared to numerical simulations. Ongoing work applies the system to study phonon transport through defects and interfaces at atomic resolution.

FM 15.2 Wed 15:15 BEY/0E40

**Photoluminescence Spectroscopy of Platinum (II) and Palladium (II) Dimers in Organic Molecular Single Crystals Under Pressure** — Paul Steeger[1], Tobias Theiss[2], Dominik Schwab[3], Ivan Maisuls[2], •Vedhanth Senthiappan Vellaiappan Uthayasurian[1], Robert Schmidt[1], Ilya Kupenko[4], Carmen Sanchez Valle[4], Steffen Michaelis de Vasconcellos[1], Nikos L. Doltsinis[3], Cristian A. Strassert[2], and Rudolf Bratschitsch[1] — [1]Institute of Physics, University of Münster — [2]Institut für Anorganische und Analytische Chemie, University of Münster — [3]Institute of Solid State Theory, University of Münster — [4]Institute of Mineralogy, University of Münster

Cyclometalated transition-metal complexes are promising for applications ranging from bioimaging to light-emitting diodes. We investigate two tailored biscyclometalated Pd(II) and Pt(II) complexes, which feature ligands that promote head-to-tail dimer formation to enable interactions between their metal centers [1]. We prepare molecular single crystals and apply hydrostatic pressure with a diamond anvil cell in the GPa range [2]. The photoluminescence shows a prominent redshift under pressure. Density functional theory calculations link this effect to a reduced metal-metal distance. Importantly, the observed mechanochromism is reversible, which holds the promise for pressure sensing and optical storage applications. References: [1] T. Theiss et al., J. Am. Chem. Soc. 145, 3937 (2023), [2] P. Steeger et al., Nano Lett. 25, 2628 (2025)

FM 15.3 Wed 15:30 BEY/0E40

**A novel Approach to parametrize a ferroelectric Phase-Field Model from atomistic Simulation Data** — •Frank Wendler[1], Dilshod Durdiev[2], Xuejian Wang[1], Hikaru Azuma[3], Takahiro Tsuzuki[3], Tomohiro Ogawa[3], Ryo Kobayashi[3], Masayuki Uraganase[4], Shuji Ogata[3], and Michael Zaiser[1] — [1]Institute of Materials Simulation, FAU Erlangen-Nürnberg, Dr.-Mack-Str. 77, 90762 Fürth, Germany — [2]Division Mechanics of Functional Materials, TU Darmstadt, Germany — [3]Physical Science and Engineering Department, Nagoya Institute of Technology, Japan — [4]RIKEN Center for Biosystems Dynamics Research, Japan

Based on molecular dynamics simulations using a core-shell potential for polarization switching in ferroelectric BaTiO3 (BTO) with and without vacancy defects, a parametrization framework for phase-field simulations is established. Crucial material properties such as elastic and piezoelectric tensor components, kinetic coefficients, as well as domain wall characteristics are extracted from the MD results to adjust the anisotropic gradient energy. The 6th order Landau polynomial coefficients are derived from statistical analysis of polarization switching data, including the activation parameters for BTO that govern domain nucleation. The proposed energy landscape favours polarization switching in two subsequent 90° steps over 180° switching, which was observed experimentally and in recent MD simulations. The method is important for phase-field simulations of domain nucleation and domain wall motion in presence of point defects carrying mono- or dipolar electric fields as well as elastic strain fields.

# FM 16: Topical Session: Dislocations in Functional Materials II (joint session MM/FM)

Time: Wednesday 15:45–17:15 Location: SCH/A251

**Topical Talk** FM 16.1 Wed 15:45 SCH/A251

### Dislocations in perovskite oxides: similarities and differences

— •Pierre Hirel — Univ. Lille, CNRS, INRAE, Centrale Lille, UMR 8207 - UMET - Unité Matériaux et Transformations, F-59000 Lille, France

The experimental discovery of room-temperature ductility in strontium titanate $SrTiO_3$ in 2001, has revealed the surprising mobility of dislocations in $\langle 110\rangle\{110\}$ slip systems. Atomic-scale simulations have contributed to resolving the core structure of these dislocations, and their role in the ductile-brittle transition. Since then, similar ductile behaviour was found in related perovskite oxides $KNbO_3$ and $KTaO_3$. However, other perovskites like $BaTiO_3$ or $CaSiO_3$ remain essentially brittle at room temperature, despite having the same crystal lattice and similar chemical compositions as ductile perovskites.

FM 16.2 Wed 16:15 SCH/A251

### Probing the Known Unknown of the Dislocation Dynamics in Oxides and Semiconductors

— •Liming Xiong — NC State University, Raleigh, NC, USA

Dislocation dynamics in oxides and semiconductors are widely aware, but its exact nature and impact on the properties and functionality of these materials are not fully understood yet. One reason is that the well-established knowledge for dislocation dynamics in metals often can't fully explain or even fail when used for oxides and semiconductors. To fill this knowledge gap, here we will present a concurrent atomistic-continuum computational tool for probing the dislocation dynamics in oxides and semiconductors. This tool has a unique feature to accommodate the motion/multiplication of $\mu$m-long dislocations together with the atomic-scale core structure evolution along the dislocation within all within one single model. Taking dislocation-seeded SrTiO3 and ZnS as sample materials, we will: (i) map the core structure/stress along a dislocation line to its local charge states and motion mechanism; (ii) measure the dislocation mobility and its dependence on stress, temperature, dopant concentration, charge states, electrical field, light illumination, and dislocation line lengths ranging from nanometers to micrometers; (iii) predict how local internal stress builds up when a mesoscale dislocation slip interacts with an atomically structured grain boundaries, and how such a high local stress may initiate a crack in turn. A consolidation of such simulation data into constitutive rules needed by higher-scale models for interpreting experimental observations will be also discussed.

FM 16.3 Wed 16:30 SCH/A251

### Electric Field Effects on Dislocation Motion in SrTiO3 via Mesoscale Indentation

— •Alexander Frisch[1], Daniel Isaia[2], Oliver Preuss[2], and Xufei Fang[1] — [1]Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany — [2]Department of Materials and Earth Sciences, Technical University of Darmstadt, Darmstadt, Germany

Dislocations in perovskite oxides have the potential of tuning functional properties of electroceramics, however their behavior and stability under externally applied electric fields remain elusive. Therefore, we investigated the effect of high densities of dislocations onto the dielectric breakdown behavior of SrTiO3, a model perovskite material. Lower dielectric breakdown strengths were found in the high-dislocation-density samples, engineered through the Brinell scratching method. Further, the effect of a 2 kV/mm electric field on the introduction and mobility of dislocations in SrTiO3 was investigated. While no changes to the dislocation plastic zone size, depth, or dislocation distribution were observed, the results suggest the stability of pre-engineered dislocation structures in perovskite oxides under applied electric fields. These results will be interpreted in the context of the dislocation charge state, associated electric field forces, and defect-modified electrical/thermal conductivity.

FM 16.4 Wed 16:45 SCH/A251

### Generating a “ferroelectric metal” by preferential reduction of dislocations in $BaTiO_3$

— •Christian Rodenbücher[1], Gustav Bihlmayer[2], Carsten Korte[1], and Kristof Szot[3] — [1]Forschungszentrum Jülich GmbH, Institute of Energy Technologies (IET-4), 52425 Jülich, Germany — [2]Forschungszentrum Jülich GmbH, Peter Grünberg Institut (PGI-1), 52425 Jülich, Germany — [3]University of Silesia, Institute of Physics, 41-500 Chorzów, Poland

Redox processes in transition metal oxides are of high relevance for sensors, information technology, superconductivity, and energy conversion. Perovskites with mixed ionic-electronic conductivity, such as $BaTiO_3$, are of particular interest because oxygen nonstoichiometry controls electronic charge carriers and thus conductivity. Surprisingly, thermal reduction in vacuum can induce metallic behaviour with conductivities far exceeding predictions from point-defect chemistry. To clarify the origin of this metallic state, we investigate the electronic transport, electronic structure, and chemical composition of $BaTiO_3$ single crystals during annealing and cooling under ultrahigh vacuum. Surface-sensitive techniques such as XPS and LC-AFM allow us to correlate electronic structure changes with the insulator-to-metal transition. We find that surface-layer dislocations act as preferential reduction sites, forming conducting filaments that yield macroscopic metallic behaviour despite minimal overall oxygen loss. Metallic behaviour persists into the ferroelectric phase. Nanoscale mapping shows that metallic filaments and piezoelectrically active regions coexist thus explaining how a “ferroelectric metal” can exist.

FM 16.5 Wed 17:00 SCH/A251

### Dislocation dynamics in Ni-based superalloys: atomistic simulations and uncertainty quantification

— •Geraldine Anis, Thomas Hudson, and Peter Brommer — University of Warwick, Coventry CV4 7AL, UK

Ni-based superalloys exhibit extraordinary strength at high temperatures. This strengthening effect is largely attributed to precipitation strengthening, where dislocations are hindered by precipitates present in their microstructure. In our work, we model dislocation trajectories obtained from Molecular Dynamics (MD) simulations of $Ni$-$Ni_3Al$. A reduced model was developed to describe dislocation-interface interactions within this system, which captures important features of the MD dislocation trajectories. The developed model was tested on a representative system and was shown to capture a range of qualitatively different dislocation behaviour. The model parameter distributions were then determined using Differential Evolution Monte Carlo (DE-MC) sampling and a Gaussian process surrogate model. The present approach offers a means of identifying atomistic-scale parameters, which can be used to inform larger length scale simulations of dislocations. Determining parameter distributions using DE-MC means that parameter uncertainties can be propagated through a hierarchy of multiscale models. We illustrate how such uncertainty propagation can be achieved by considering a dislocation mobility law with quantified uncertainties in pure Ni. This work is part of a wider study aiming to model the deformation behaviour of Ni-based superalloys with a focus on quantifying and propagating uncertainties.

# FM 17: Highlighted Talk: Piled higher, probed deeper: X-ray insights into ferroelectric devices (Martina Müller)

Chair: Anna Grühnebohm (Ruhr-Universität Bochum), Jan Schultheiß (NTNU Trondheim)

Time: Thursday 9:30–10:00 Location: BEY/0138

**Invited Talk** FM 17.1 Thu 9:30 BEY/0138

**Piled higher, probed deeper: X-ray insights into ferroelectric devices** — •Martina Müller — Fachbereich Physik, Universität Konstanz

In ferroelectrics, the nothing is mighty: The key to shaping the ferroelectric functionalities of oxide/nitride materials and devices lies in the tunability of their oxygen/nitrogen sublattice, particularly their defect structure. While dopants and vacancies are a key aspect of emerging ferroelectricity in $HfO_2$ and AlScN, their detection is much more subtle than that of atomic properties. This is because the experimental observation of e.g. oxygen vacancies means the detection of something absent. This requires access to indirect signatures, which often are of very low intensity and located within a device structure - a combination of experimental conditions that are challenging to meet in practice.

This talk presents recent advances in the expertise required to detect defects and dopants related ferroelectric functionality in $HfO_2$ and AlScN using synchrotron radiation. Bulk-sensitive hard X-ray photoelectron spectroscopy (HAXPES) enables the non-destructive depth profiling of heterostructures, revealing spectroscopic fingerprints also in subtle core-level signatures. Performing HAXPES 'in operando' is a powerful tool for determining the band alignment and chemical state of interfaces under operating conditions of real-world ferroelectric devices.

# FM 18: German-French Focus Session: (Anti)ferroic states – ferroelectrics, ferroelastics and antiferroelectrics II

chair: Elzbieta Gradauskaite (CNRS/Thales, FR)

This focus session explores recent advances in understanding and control of (anti)ferroic states. Emphasis will be placed on theoretical modelling, advanced characterization techniques, and the engineering of emergent properties for use in nano-electronic devices. The session aims to bridge fundamental research with emerging device-relevant functionalities, bringing together experimental, and theoretical perspectives on ferroic materials.

Time: Thursday 10:15–12:45 Location: BEY/0138

**Invited Talk** FM 18.1 Thu 10:15 BEY/0138

**Stabilizing antiferroelectricity in PbZrO3 thin films using epitaxial tensile strain** — •Vincent Garcia — Laboratoire Albert Fert, CNRS, Thales, Univ. Paris-Saclay, France

The antiferroelectric nature of lead zirconate, the historical and most studied antiferroelectric material, has recently been challenged. Progress in atomic-level characterization using aberration-corrected scanning transmission electron microscopy (STEM) has revealed the complex nature of polar textures in PbZrO3. In single crystals, ferrielectric phases have been detected, while in PbZrO3 epitaxial films, thickness reduction engenders competition among antiferroelectric, ferrielectric and ferroelectric phases. All studies so far on PbZrO3 films have utilized commercially-available oxide single crystals with large compressive lattice mismatch, causing the films to undergo strain relaxation within a few nanometres. Interestingly, first principles calculations have predicted that tensile strain can stabilize antiferroelectricity down to the nanometre scale. Here we use tensile strain imposed by artificial substrates of LaLuO3 to stabilize a pure antiferroelectric phase in epitaxial ultrathin films of PbZrO3. Sharp double hysteresis loops of polarization vs electric field in these PbZrO3-based capacitors show zero remanent polarization, and atomic scale mapping of polar displacements using STEM reveals the characteristic antipolar pattern of the Pbam phase in film thicknesses down to 9 nanometres. These results highlight the critical role of coherent epitaxial strain in the phase stability of PbZrO3.

**Invited Talk** FM 18.2 Thu 10:45 BEY/0138

**Strain effects in free-standing membranes of antiferroelectric Lead Zirconate** — •Umair Saeed[1,2], Huazhang Zhang[3,4], David Pesquera[1], Philippe Ghosez[3], Nini Pryds[5], Jose Santiso[1], Felip Sandiumenge[6], and Gustau Catalan[1,7] — [1]ICN2, Catalonia — [2]UAB, Spain — [3]ULiège, Belgium — [4]WUT, China — [5]DTU, Denmark — [6]ICMAB, Catalonia — [7]ICREA, Catalonia

Antiferroelectrics like PbZrO3 (PZO) exhibit reversible switching between antiferroelectric and ferroelectric phases. However, complex energy landscape of PZO and few lattice matching substrates render strain engineering challenging. In this context, free-standing membranes provide a unique opportunity for strain tuning due to their flexibility.

We studied PZO membrane capacitors under homogeneous in-plane strain applied via bending, observing that the hysteresis decreases under in-plane compression and increases under tension. The results suggest that the changes in the switching behavior originate from the modification of energy barriers between the phases under the influence of strain rather than the energies of the phases. Molecular dynamic simulations show that this response depends on crystallographic directions of strain and electric field.

In wrinkled stand-alone PZO membranes, on the other hand, high strain gradients induce flexoelectric effects, leading to non-canonical antiferroelectric-like ordering under tensile and ferroelectric phases under compressive strain, highlighting strain as a tool to control PZO functionalities.

FM 18.3 Thu 11:15 BEY/0138

**Strain induced ferroelastic twin-domain dynamics in lanthanum aluminate** — •Matthias Roeper[1], Robin Buschbeck[1], Jakob Wetzel[1], Lukas M. Eng[1,2], and Samuel D. Seddon[1] — [1]Institute of Applied Physics, TU Dresden, Nöthnitzer Strasse 61, 01187 Dresden, Germany — [2]ct.qmat: Dresden-Würzburg Cluster of Excellence - EXC 2147, TU Dresden, 01062 Dresden, Germany

Over the last decades scientific attention of the oxide perovskite lanthanum aluminate ($LaAlO_3$) has turned (due to the absence of ferroelectric contributions) from originally only an active interfacial substrate material into a model system of ferroelastic twin domain walls. Our new results explore ferroelastic twin-domain dynamics induced by the controlled application of uniaxial strain in single crystalline samples. The domains are spacially resolved by Atomic Force Microscopy and $\mu$-Raman Spectroscopy as a function of applied strain, as well as structural analysis by X-ray diffraction. All experimental investigations are complemented by density functional perturbation theory calculations.

FM 18.4 Thu 11:30 BEY/0138

**MD data-driven physics-informed neural network for multiscale modelling of ferroelectric: parameter identification and field reconstruction** — •Xuejian Wang[1], Frank Wendler[1], Hikaru Auzuma[2], and Shuji Ogata[2] — [1]Institute of Materials Simulation, Department of Materials Science and Engineering, Friedrich-Alexander-Universität Erlangen-Nürnberg, Fürth, Germany — [2]Graduate School of Engineering, Nagoya Institute of Technology, Nagoya, Japan

A persistent challenge in multiscale ferroelectric modeling is connecting atomistic information with continuum phase-field descriptions. Here, we develop a PINN framework driven by MD polarization data. The loss function combines supervised fitting of MD-derived polarization fields with physics-based residuals of the steady-state phase-field PDEs. Minimizing the total loss enables the network to reconstruct polarization, strain, stress, and electric field distributions, while simultaneously identifying key phase-field parameters, including characteristic energy and length scales, gradient anisotropy, and Landau coefficients. Using these PINN-identified parameters in COMSOL reproduces ferroelectric domain structures and their electromechanical responses with high fidelity. This approach provides an efficient route to establishing atomistic-to-continuum links and inferring physical properties directly from polarization configurations.

FM 18.5 Thu 11:45 BEY/0138

**Evidence of ferroelectricity in epitaxially strained tungsten trioxide thin films** — •Nives Strkalj[1,2], Zhuotong Sun[1], Ming Xiao[1], Ziyi Yuan[1], Xuan T. Nguyen[1], Simon M. Fairclough[1], Caterina Ducati[1], Giuliana Di Martino[1], and Judith L. MacManus-Driscoll[1] — [1]University of Cambridge, UK — [2]Institute of Physics, Zagreb, Croatia

Ferroelectric films offer a promising path to faster, more energy-efficient CMOS technologies. Here, we report the deposition of epitaxial tungsten trioxide films at temperatures below 400°C using atmospheric pressure spatial chemical vapour deposition. In these films, epitaxial strain imposed by the substrate promotes the formation of the low-temperature polar phase at room temperatures, evidenced by x-ray diffraction, scanning transmission electron microscopy, piezoresponse force measurements, and Raman spectroscopy. Exploring ferroelectricity in ultrathin tungsten trioxide films could provide a new platform for polarization-controlled electronic and optical applications.

FM 18.6 Thu 12:00 BEY/0138

**Investigating metallicity in layered Carpy-Galy ferroelectrics through topotactic transformation.** — •Lilia Huynh[1], Marko Kuvezdic[1], Dongxin Zhang[1], Annouk Goossens[1], Luis Moreno[1], Alexandre Gloter[2], Lucia Iglesias[1], Manuel Bibes[1], and Elzbieta Gradauskaite[1] — [1]Laboratoire Albert Fert, Palaiseau, France — [2]Laboratoire de Physique du Solide, Orsay, France

Combining seemingly incompatible properties within a single material can yield unconventional functionalities. For instance, polar metals host inversion-symmetry breaking displacements despite finite metallicity. However, they remain scarce, as conventional ferroelectricity usually relies on orbital rehybridization and gets suppressed by free charge carriers. Here, we report the epitaxial stabilization of the layered Carpy-Galy ferroelectric $Sr_2Nb_2O_7$ ($A_nB_nO_{3n+2}$, $n = 4$), which exhibits a geometric in-plane polarization driven by collective octahedral rotations. These films can be successfully transformed into the metallic perovskite $SrNbO_3$ through a topotactic interfacial reduction mediated by an Al overlayer, which drives oxygen-vacancy migration and electron doping. This redox-engineering route enables fine, continuous and even reversible tuning of oxygen stoichiometry, allowing us to stabilize intermediate $Sr_2Nb_2O_{7-x}$ phases, as confirmed by XRD, XPS, STEM, and transport measurements. In contrast to bottom-up synthesis of polar metals, this top-down strategy provides fine control of metallicity in a geometric ferroelectric host and opens avenues for exploring charge- and spin-transport phenomena in polar metals.

FM 18.7 Thu 12:15 BEY/0138

**Dynamical tuning of the depletion region at a single ferroelectric domain wall** — •Jiali He[1], Ruben Dragland[1], Jan Schultheiss[1], Zewu Yan[2,3], Edith Bourret[3], and Dennis Meier[4] — [1]NTNU, Norway — [2]ETH Zurich, Switzerland — [3]LBNL, USA — [4]University of Duisburg-Essen, Germany

Ferroelectric domain walls (DWs) are promising building blocks for future nanoelectronics, combining ultra-small feature size with emergent device-relevant behaviors. Most studies so far focused on bulk crystals and thin films, where the measured response reflects convoluted contributions from, e.g., the hidden sub-surface wall structures and the networks they form. The intrinsic behavior of individual DWs thus often remains unclear. In my talk, I will present the extraction of a single insulating ferroelectric DW, situated in a 1-$\mu$m-thick $ErMnO_3$ lamella, mounted on a conductive back electrode. This configuration enables a well-defined top-bottom current path using an AFM tip as movable top electrode. Consistent with previous measurements on single crystals, we observe that the initially thin insulating wall (∼200 nm electronic width) transforms under applied bias into a narrow conductive core surrounded by a broad asymmetric depletion region, leading to a fivefold increase in apparent wall width. Systematic bias variation demonstrates a highly tunable electronic wall width, manifesting as voltage-controlled expansion and contraction of the depletion region. The results corroborate that functional DW properties known from crystals are transferable to nano-structured device-relevant systems, revealing new possibilities for electronic signal control.

FM 18.8 Thu 12:30 BEY/0138

**Hybrid antiferroelectric-ferroelectric-ferroelastic domain walls in noncollinear antipolar oxides** — •Ivan N. Ushakov[1], Mats Topstad[1], Muhammad Z. Khalid[1], Niyorjyoti Sharma[2], Christoph Grams[3], Ursula Ludacka[1], Jiali He[1], Kasper Hunnestad[1], Mohsen Sadeqi-Moqadam[1], Julia Glaum[1], Sverre M. Selbach[1], Joachim Hemberger[3], Petra Becker[3], Ladislav Bohatý[3], Amit Kumar[2], Jorge Íñiguez-González[4,5], Antonius T.J. van Helvoort[1], and Dennis Meier[1,6] — [1]NTNU, Trondheim — [2]QUB, Belfast — [3]University of Cologne — [4]LIST, Luxembourg — [5]University of Luxembourg — [6]University of Duisburg-Essen

Antiferroelectrics are emerging as advanced functional materials and are fertile ground for unusual electric effects. Here, we demonstrate how antiferroelectricity induces noncollinearity in dipolar order and establish it as an additional degree of freedom, unlocking physical nanoscale properties that are symmetry-forbidden in classical antiferroelectrics. We show that antiferroelectrically driven noncollinear order of electric dipole moments in $K_3[Nb_3O_6|(BO_3)_2]$ leads to a coexistence of antiferroelectric and ferroelectric behaviors. Besides the double-hysteresis loop observed in antiferroelectrics, a pronounced piezoresponse and electrically switchable hybrid domains are observed, forming atomically sharp and micrometer long charged domain walls with inseparably entangled antiferroelectric and ferroelectric properties. Hybrid antiferroelectric-ferroelectric responses are expected in a wide range of noncollinear systems, giving a new dimension to the research on antiferroelectrics and multifunctional oxides in general.

# FM 19: Advanced Microscopy and Tomography for Functional Materials

chair: Manuel Zahn (University of Augsburg)

Time: Thursday 10:15–12:45 Location: BEY/0E40

FM 19.1 Thu 10:15 BEY/0E40

**Electron Beam-Induced Currents as a Quantitative Probe for Nanoscale Semiconductor Devices** — •Sebastian Schneider[1], Sebastian Beckert[1], René Hammer[2], Markus König[3], Grigore Moldovan[2], Darius Pohl[1], and Bernd Rellinghaus[1] — [1]Dresden Center for Nanoanalysis (DCN), TU Dresden, Dresden, Germany — [2]Point Electronic GmbH, Halle (Saale), Germany — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Electron beam-induced current (EBIC) mapping in the scanning transmission electron microscope (STEM) enables the direct visualization of charge carrier transport with nanometer resolution. We present a comparative STEM-EBIC study on silicon photodiode lamellae prepared by gallium and xenon focused ion beam milling. The EBIC mapping reveals the p-n junction and allows for the extraction of the effective electron and hole diffusion lengths as a function of local thickness. These values are up to three orders of magnitude smaller than bulk EBIC results, highlighting strong surface recombination and preparation-induced artifacts. Complementary I-V measurements show significant deviations from the expected diode-like behavior, which we attribute to high resistive contacts at the metal-semiconductor interfaces. Our findings emphasize the critical role of sample preparation for quantitative EBIC analysis.

Financial support by the DFG through TRR 404, project no. 528378584, is gratefully acknowledged.

FM 19.2 Thu 10:30 BEY/0E40

**X-ray Stress Tensor Tomography** — •Peter Modregger[1,2], Ahmar Khaliq[1,2], and Felix Wittwer[1,2] — [1]Physics Department, University of Siegen — [2]Center for X-ray and Nano science, CXNS, DESY, Hamburg

The possibility for tomographic reconstrution of strain and stress tensor present in poly-crystalline samples has been discussed for nearly two decades. We will demonstrate the successful retrieval of all 6 strain/stress tensor components in martensitic steel samples from experimental data acquired at the ID11 beamline of the ESRF. Compared to established techniques this novel approach for the depth-resolved determination of stress states offers the tantalizing advantages of a simple experimental setup, isotropic gauge volumes and faster scans. In our presentation, we will discuss the possible adverse effects of detector parallax and crystallographic texture. Further, we will provide specific experimental requirements such as the required photon flux or the available scattering angles. With these in mind, we have achieved a strain sensitivity of $10^{-4}$ and a stress sensitivity of 20 MPa.

FM 19.3 Thu 10:45 BEY/0E40

**Developing a resuable optical fiber-based sensing system for in-situ X-ray radiaiton monitoring** — Ali Karatutlu[1,2], Esra Kendir Tekgül[2], Zehra Gizem Mutlay[1], Andriy Budnyk[1], Gianluca Iori[3,4], Philipp Hans[5], Fareeha Hameed[5], and •Bülend Ortaç[1] — [1]Bilkent University, Institute of Materials Science Nanotechnology and National Nanotechnology Research Center (UNAM), Ankara, 06800 Turkey — [2]Sivas University of Science and Technology, Department of Engineering Basic Sciences, Sivas, 58100 Turkey — [3]Swiss Light Source, Paul Scherrer Institute, Villigen, Switzerland — [4]GratXray, Villigen, Switzerland — [5]Synchrotron-light for Experimental Science and Applications in the Middle East (SESAME), Allan, 19252, Jordan

Specialty optical fibers doped with rare-earths such as Yb, and Tm are utilized for various applications from medical to high-power beam delivery for materials processing. Nevertheless, radiation-induced defects can occur due to irradiation, causing a degradation of beam quality. In this study, we utilize this type of degradation, referred to as radiation-induced attenuation, as an X-ray sensing and the conditions in the in-situ recovery of color centers. The experiments were conducted at hard X-ray beamline at BEATS, SESAME, using different monochromatic beams such as 10 keV and 20 keV, suggesting the origin of color centers playing role in the RIA and the sensing and recovery behavior that are related to the optical and morphological effects of the X-ray irradiation.

FM 19.4 Thu 11:00 BEY/0E40

**Multiscale characterization of porous carbon fibers** — •Markus Löffler[1], Mohsen Sadeghi Bogar[2,3], Paul Bertram[3,4], Jan Wolf[2,3], Darius Pohl[1], Thomas Behnisch[2,3], Iris Kruppke[3,4], Chokri Cherif[3,4], Maik Gude[2,3], and Bernd Rellinghaus[1] — [1]Dresden Center for Nanoanalysis (DCN), cfaed, TUD Dresden University of Technology (TUD), Dresden, Germany — [2]Institute of Lightweight Engineering and Polymer Technology (ILK), TUD, Dresden, Germany — [3]Research Center Carbon Fibers Saxony, TUD, Dresden, Germany — [4]Institute of Textile Machinery and High Performance Material Technology (ITM), TUD, Dresden, Germany

Porous carbon fibers (PCF) are valued for structural energy storage because they combine low density, high thermal and electrical conductivity, low thermal expansion, strong mechanical properties, and a large specific surface area. Key pore features - volume, shape, and connectivity - determine their suitability for use as electrodes in batteries, supercapacitors, and as structural materials. A hierarchical pore structure with sizes from 2 nm to over 50 nm is desirable. These PCFs are made by wet-spinning polyacrylonitrile (PAN) with nanocellulose as a pore-forming additive, followed by electron beam irradiation, stabilization, and carbonization. To understand how processing affects pore development, fibers are analyzed at various stages and scales using submicro-XCT, FIB, SEM, and TEM. All fibers show a low density of large pores, while precursor and irradiated fibers also have a high density of nanoscale pores.

FM 19.5 Thu 11:15 BEY/0E40

**Tomographic Electron Holography reveals 3D-Potential Variations from Surface Segregation in p-n doped InGaAs Nanowires** — •Kai-Luis Jakob[1], Laura Niermann[1], Tore Niermann[1], Frederik Otto[1], Rahel Specht[1], Daniel Wolf[2], Esmaielpour Hamidreza[3], Gregor Koblmüller[1], and Michael Lehmann[1] — [1]TU Berlin — [2]IFW Dresden — [3]TU München

Mapping the three-dimensional electrostatic potential distribution at the nanoscale is crucial for tuning the electrical properties of semiconductor nanostructures, such as InGaAs nanowires utilized in optoelectronics. Off-axis electron holography enables measurement of the projected electrostatic potential with nanoscale spatial resolution; however, the 3D information typically remains inaccessible. In this work, we combine electron holography with tomography to reconstruct 3D potentials, thereby investigating subtle effects such as surface segregation, Fermi-level pinning, and damages induced by Focused Ion Beam preparation. Here, we focus on MBE-grown InGaAs nanowires featuring an axial p-n junction. A tilt series of holograms is acquired over a wide tilt range in a FEI Titan 80-300 TEM. Projected electrostatic potentials are reconstructed individually and aligned for tomographic reconstruction. This approach allows us to access the electrostatic potential and resolve both axial and radial changes from the wire core to its surface. We observed a largely constant potential step across the axial p-n junction of 0.5 V, however, near-surface regions exhibited deviations from it. At the surface of the n-doped segment, we found a thin p-type layer, likely attributable to known surface segregation.

### Coffee break

FM 19.6 Thu 11:45 BEY/0E40

**Advanced Polymer-Tungsten Nanocomposites for Radiation Shielding and X-ray Computed Tomography Applications** — Taylan BAŞKAN[1], Saliha MUTLU[2,3], Bülend ORTAÇ[3], Ali KARATUTLU[3,4], Sevil SAVAŞKAN YILMAZ[2,3], and •Ahmet Hakan YILMAZ[1] — [1]Karadeniz Technical University Physics Department, Trabzon, 61080, Türkiye — [2]Karadeniz Technical University Chemistry Department, Trabzon, 61080, Türkiye — [3]National Nanotechnology Research Center (UNAM) and Institute of Materials Science Nanotechnology, Bilkent University, Ankara, 06800, Türkiye — [4]Sivas University of Science and Technology, Department of Engineering Basic Sciences, Sivas, 58100 Turkey

The growing trend of ionizing radiation in biomedicine and industry has intensified the need for efficient and reliable radiation shielding materials. In our current work, we incorporated W nanoparticles and WO3 nanoparticles with varying proportions in the PMSQ polymer to synthesize dual-functional nanocomposites with simultaneous gamma ray shielding and contrast enhancement in computed tomography imaging. This study will present the three-dimensional micro-evolutions of biodegraded polymer-metal/polymer-metal oxide composite materials using synchrotron-based X-ray computed tomography methods upon post $\gamma$-radiolysis exposure from 0.5 kGy to 5 kGy. The synchrotron-based XCT available at BEATs in SESAME demonstrates the internal structural defects and morphology non-destructively in the vicinity of resolved micro-scales with 650 nm resolution.

FM 19.7 Thu 12:00 BEY/0E40

**Defects in Materials: Limitations of the Trapping Model - the Influence of Corrupt Components in Positron Lifetime Spectra - cured by a New Spectrometer?** — Torsten Staab, •Dominik Boras, and Danny Petschke — LCTM / IFB, Department of Chemistry, University of Wuerzburg, Roentgenring 11, D-97070 Wuerzburg, Germany

Positron lifetime spectroscopy is able to extract densities for defects (e.g. vacancies or dislocations) from the measured spectroscopic data by applying the so-called trapping model, which describes the decomposition of lifetime spectra into two or more components (lifetimes and intensities). Since the procedure of fitting several exponential decays folded by a mimicked instrumental resolution function (IRF) is a so-called ill-posed problem, the goodness of the fit relies heavily on the quality of the recorded data. By our digital twin of a positron lifetime spectrometer we could clearly see the strong influence of back scattered and corrupted coincidences on recorded spectra. Unfortunately, even by physically filtering digitised pulses, those events cannot be removed. One way to reduce their effect are changes in the geometry (90° instead of 180°) of the detector set-up leading to heavy losses in efficiency (about 90%). However, this leads to much more realistic bulk positron lifetimes of light materials (Mg, Al, Si) in accordance with calculations, and enables correct decompositions by the trapping model. We present here a new fully digitised spectrometer with an IRF described by one singe Gaussian and a FWHM of 128ps together with 22-Na sources without positronium having a single lifetime component.

FM 19.8 Thu 12:15 BEY/0E40

**Characterising electron vortex beams inside crystalline materials via vorticity** — •Christian Bick, Dorothee Hüser, and Tobias Klein — Physikalisch-Technische Bundesanstalt, Braunschweig, Germany

Convergent electron beams with an orbital angular momentum (OAM), also known as electron vortex beams or twisted electrons, have been investigated for multiple applications in material science. Recently, first measurements of vortex electron magnetic circular dichroism (EMCD) in the electron microscope have been reported.

We present a simulation-based study on vortex beam behaviour inside crystalline material utilising vorticity as a local property to characterise the beam. This quantity, which is widely used in fluid mechanics, can be understood as a local measure of OAM . We relate it to commonly used integrated quantities like the total OAM and channelling strength in order to further the understanding of the beams behaviour inside of model crystals and discuss possible measurements.

FM 19.9 Thu 12:30 BEY/0E40

**Toward Atomic-scale Imaging of Resistive Switching Mechanisms in Prussian Blue Memristors** — •Mohammed Fayis Kalady[1], Johannes Schultz[1], Michael Pohlitz[2], Falk Röder[1], Darius Pohl[3], Daniel Wolf[1], and Axel Lubk[1,4] — [1]Leibniz Institute for Solid State and Materials Research, Dresden, Germany — [2]Faculty of Physical Engineering/Computer Sciences, University of Applied Sciences, Zwickau, Germany — [3]DCN, TU Dresden, Germany — [4]IFMP, TU Dresden, Germany

Prussian blue and its analogues are promising materials for memristive devices based on resistive switching. To obtain a microscopic understanding of the structural and chemical processes responsible for switching, we employed a detailed high-resolution transmission electron microscopy (HRTEM), scanning transmission electron microscopy combined with electron energy loss and energy dispersive x-ray spectrum imaging (STEM-EELS and STEM-EDX) studies on pristine films and on films previously subjected to electrical biasing. The pristine film exhibits a homogeneous distribution of K, Fe, C, N, and O, whereas the electrically biased regions display clear nanoscale modifications, including local changes in elemental distribution and a phase transition from Prussian blue to Prussian white. The electrical measurements on the bulk reveal transitions between low-resistance and high-resistance states, demonstrating bipolar switching behavior across multiple cycles. These results provide the first steps toward in-situ TEM biasing experiments aimed at directly resolving elemental migration pathways and phase evolution under applied voltages.

## FM 20: Excursion and Network-Event at Infineon Dresden AG (joint session FM/HL)

We are organizing an Excursion and Network-Event to Infineon Dresden AG.
Only for registered and selected participants.
Please register until latest February 12th here: https://www.icams.de/news-events/events/registration-infineon/?api=561b8d7cfcb678e9f0938830d78cf979

Time: Thursday 13:30–17:00 Location: Infineon

**Only for registered and selected participants.**

## FM 21: Members Assembly

We will elect our spokespersons, plan the programme for the coming years, and award the poster prize. This is also your opportunity to suggest topics for focus sessions, symposia, and plenary speakers for the next DPG conference!

chairs: Jan Schultheiß (NTNU, NO), Anna Grünebohm (Ruhr University Bochum, DE), FM spokespersons

Time: Thursday 18:00–18:45 Location: BEY/0138

**All members of the Functional Materials Division are invited to participate.**

# FM 22: Focus Session: Materials Discovery III – New materials and functionalities by general principles

chairs: Hiroki Taniguchi (Nagoya University, JP), Akitoshi Nakano (Nagoya University, JP)

Discovering new functional materials is crucial to advance today's technologies, ranging from caloric cooling via catalysis to next-generation energy conversion and storage, such as thermoelectric, ferroelectric, and ionic conductor materials. New materials also form the basis for potential applications in quantum information technologies. This session provides a platform to highlight functional materials discoveries and how they come about. Notably, systematic searches with high-throughput synthesis approaches, as well as predictions from materials informatics, have helped to go beyond serendipitous discoveries in recent years. However, intuition guided by general principles remains an important factor. In this session, we particularly welcome contributions that showcase the discovery of new functional materials with original approaches. Diverse material systems - from well-established to emerging and niche classes across condensed-matter and materials physics - will be featured. Bringing together diverse discoveries in a single session will help delineate general principles and inspire future work.

Time: Friday 9:30–12:45 Location: BEY/0138

**Invited Talk** FM 22.1 Fri 9:30 BEY/0138

**Topological thermoelectrics for solid state cooling** — •Yu Pan[1] and Claudia Felser[2] — [1]Chongqing University, Chongqing, China — [2]Max Planck Institute for Chemical Physics of Solids

Thermoelectric effects enable the direct conversion between thermal energy and electrical energy, and has broad application potential in areas such as thermoelectric power generation, solid-state cooling, and precise temperature control. Classic thermoelectric materials mainly focus on heavily doped narrow bandgap semiconductor materials, whose thermoelectric performance is limited above room temperature (> 300 K). So far, further enhancement of thermoelectric performance at low temperatures (<300 K) faces significant challenges, severely restricting the application of thermoelectric materials in low-temperature solid-state cooling. In recent years, the surge of topological quantum materials has triggered many novel thermoelectric transport behaviors, especially the significantly enhanced low-temperature thermoelectric performance under magnetic fields, providing new opportunities to greatly improve low-temperature thermoelectric performance. For example, their linear-dispersion energy band structures and ultrahigh mobility significantly enhance the magneto-Seebeck effect and Nernst effect. On the other hand, topological quantum materials with broken symmetry can exhibit an anomalous Nernst thermoelectric potential far higher than that of conventional ferromagnets due to the presence of nonzero Berry curvature, laying a scientific foundation for thermoelectric applications of the anomalous Nernst effect under low or even zero magnetic fields.

FM 22.2 Fri 10:00 BEY/0138

**Topological quantum materials for high performance heterogenous catalysis** — •Xia Wang and Claudia Felser — Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany

The electronic structure of a catalyst plays a pivotal role in governing its performance1. Topological quantum materials, known for their symmetry-protected electronic states, offer a unique platform to bridge solid-state topology and heterogeneous catalysis. When combined with chirality, topological quantum materials give rise to novel material systems exhibiting distinct chiral phenomena, opening new avenues for the development of next-generation chiral catalysts. Situated at the interface of condensed matter physics and chemistry, the emerging field of topological catalysis exploits the exotic quantum properties of topological quantum materials to not only enhance catalytic activity and selectivity but also to enable fundamental studies of reaction mechanisms. Our recent experimental and theoretical work demonstrates a direct link between spin-orbit coupling and the kinetics of oxygen electrocatalysis, including both the oxygen reduction and evolution reactions. Furthermore, we show that external stimuli such as magnetic fields can effectively tune catalytic performance by modifying the topological features of the electronic structure. Together, these insights establish topological quantum materials as a compelling framework for designing high-performance, field-tunable catalysts, with far-reaching implications for asymmetric synthesis to probing the origins of life.

FM 22.3 Fri 10:15 BEY/0138

**Ta2PdSe6: A guide towards high performance thermoelectric semimetals** — •Akitoshi Nakano — Nagoya University, Nagoya, Japan

We have recently discovered that a transition-metal chalcogenide Ta2PdSe6 exhibits an extraordinary thermoelectric property despite its semimetal character. Ta2PdSe6 crystallizes in a layered structure, each layer of which consists of quasi-one-dimensional chains formed by prismatic TaSe6 and square-planner PdSe4. The thermoelectric property measured along this direction is highly exotic; an ultra-high conductivity ($\sigma$) above 10^6 Ω^-1cm^-1 is compatible with a substantial thermopower (S) of 40 μVK^-1 at 20K. As a result, the power factor (= S^2$\sigma$) reaches above 2000 μWcmK^-2, which is top level among bulk thermoelectric materials thus far.

Furthermore, we have found that the thermal conductivity of Ta2PdSe6 is relatively small (˜ 100 Wm^-1K^-1) for such a good electrical conductor associated with a serious violation of the Wiedemann-Franz law. As a result, the thermoelectric figure of merit Z (= S^2$\sigma\kappa$^-1) of Ta2PdSe6 at 14 K reaches as high as 3*10^-3 (K^-1), which is comparable to Bi2Te3 at 300 K.

In the presentation, we will discuss the origin of the anomalous transport properties of Ta2PdSe6 from the viewpoint of the carrier dynamics.

FM 22.4 Fri 10:30 BEY/0138

**Symmetry-Driven Transitions Between Flat Bands and Dirac Cones in Bilayer Kagome Lattices** — •Taylan Gorkan — Bilkent University-UNAM

Flat bands (FBs) and Dirac cones represent two distinctive features of topological electronic systems, yet a unified mechanism enabling transitions between them has remained elusive to date. Here, we demonstrate a symmetry-governed and tunable transition from flat bands to Dirac cones in AB-stacked bilayer kagome lattices. This transition is mediated by the interplay between destructive quantum interference (DQI), C3 rotational symmetry, and spatial inversion symmetry. Strong interlayer coupling enhances DQI and stabilizes compact localized states that produce FBs, while weaker coupling allows C3 and inversion symmetries to dominate, giving rise to robust Dirac nodal points. Using a minimal tight-binding model, we map the continuous evolution of topological states-including type-II and type-III Dirac cones, spin-1 Dirac nodes, and partial flat bands-as a function of interlayer coupling. We further demonstrate this transition mechanism by examining an AB-stacked bilayer derived from the experimentally synthesized Nb3TeCl7 structure. In particular, first-principles calculations on bilayer Nb3TeCl7 reveal that vertical strain/pressure modulates interlayer interactions, enabling the entire FB-Dirac cones transition sequence. These findings establish a realistic novel pathway for gaining further insights into flat-band physics and engineering tunable topological phases in two-dimensional materials.

FM 22.5 Fri 10:45 BEY/0138

**Emergent High Conductivity Transport Channel in $Bi_{12}Rh_3Ag_6I_9$ Single-Crystalline Multilayer Heterostructure** — •Nicolas Perez[1], Eduardo Carrillo-Aravena[2], Christian Niclaas Saggau[1], Kornelius Nielsch[1], and Michael Ruck[2] — [1]Leibniz Institute for Solid State and Materials Research Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany — [2]Faculty of Chemistry and Food Chemistry, Technische Universität Dresden, 01062

Dresden, Germany

$Bi_{14}Rh_3I_9$-type weak 3D topological insulators (TIs) can be seen as nano-periodic multilayer heterostructures of 2D TIs spaced by topologically trivial insulators. The newest member $Bi_{12}Rh_3Ag_6I_9$ exhibits 2D cationic conductivity in the silver iodide spacer, which allows to electrochemically adjust the Fermi level, and has the widest band gap so far in this family of compounds, 286 meV. It shows strongly increasing diamagnetism at low temperatures in a field perpendicular to the layers. Magnetoresistance measurements in macroscopic crystals reveal confinement and oscillatory behaviour, which coincides with a drastic drop in resistivity both parallel and across the layers. The observation of such an effect in a crystalline multilayer structure is compatible with the theoretically predicted formation of a collective [1+1]-dimensional sheath state involving all lateral crystal faces and probably arising from tunneling between the protected edge states of the numerous closely spaced 2D TI layers. A macroscopic system of some $10^5$ coupled spin channels appears promising for applications in spintronics and quantum computation.

FM 22.6 Fri 11:00 BEY/0138

**Simulating the Schrödinger equation in anti-Hermitian electrical circuits** — •Ivan Scolan[1], Ronny Thomale[2], Jasper Van Wezel[3], Viktor Könye[3], Ali Moghaddam[4], Jeroen Van Den Brink[1], and Joseph Dufouleur[1] — [1]Leibniz Institute for Solid State and Materials Research Dresden — [2]Institute for Theoretical Physics and Astrophysics, University of Würzburg — [3]Institute for Theoretical Physics Amsterdam — [4]Faculty of Engineering and Natural Sciences, Tampere Finland

In recent years, a number of condensed matter lattice models have been realized using classical electric circuits, exploring topological phases hitherto inaccessible experimentally. In these previous works, the Hamiltonian of a system was implemented in a topo-electronic circuit, thus possessing the same spectrum as any equivalent condensed matter system, but the dynamics of the electronic circuit remained distinct from the quantum dynamics given by the Schrödinger equation. Here we propose a new way to realize electronic circuits that are equivalent to solid-state lattices based on anti-hermitian circuits the dynamic of which perfectly follows the Schrödinger dynamics.

Intrinsic symmetries of these circuits allow the experimental measurement of all eigenstates. Using this framework, we apply it to a 1D atomic chain with position-dependent hopping terms and experimentally retrieve the theoretical results presented in Mertens et al. (2022), Morice et al. (2021). Finally, we show how our method can be used to develop novel electronics which can be used for concrete applications and also for solving fundamental physics problems.

## Coffee Break

FM 22.7 Fri 11:30 BEY/0138

**Photo-dielectric synaptic plasticity in Zn-substituted $BaAl_2O_4$** — •Hiroki Taniguchi — Department of Physics, Nagoya University, Nagoya 464-8602, Japan

Optical control of material properties is pivotal for advancing the evolution from conventional electronics to next-generation photoelectronics. Although a variety of photo-induced phenomena, including the photovoltaic effect and photoconduction, have been well established as key mechanisms for photoelectronic devices, the optical manipulation of dielectric responses has remained comparatively unexplored.

Here, I demonstrate a photo-dielectric effect in partially Zn-substituted $BaAl_2O_4$, in which the dielectric permittivity increases under below-bandgap photo-irradiation without inducing photoconduction. First-principles calculations indicate that Zn substitution creates a unique defect complex. Upon photo-irradiation, photo-generated electron*hole pairs form a local dipole around this defect complex, producing an additional polarization contribution and consequently enhancing the dielectric permittivity. Furthermore, transient permittivity measurements under sequential pulsed optical excitation reveal synaptic-plasticity-like responses in Zn:$BaAl_2O_4$, highlighting its potential for neuromorphic device applications.

FM 22.8 Fri 11:45 BEY/0138

**Triclinic distortion in titanite-type oxides CaSnGeO5 and SrSnGeO5** — •Taro Kuwano[1], Hiroko Yokota[1], Manabu Hagiwara[2], Toshiya Uohashi[3], Akitoshi Nakano[3], and Hiroki Taniguchi[3] — [1]4259 Nagatsuta-cho, Midori-ku, Yokohama, Kanagawa, 226-8501 Japan — [2]3-14-1 Hiyoshi, Kohoku-ku, Yokohama, Kanagawa, 223-8522 Japan — [3]Furo-cho, Chikusa-ku, Nagoya, Aichi, 464-8602 Japan

Titanite-family oxides have been emerging as a novel vein of antiferroelectric materials owing to their unique pseudo-one-dimensional structure hosting "antipolar arrangement of polar chains." In this study, we focus on another characteristic feature of the titanite-type structure: ferroelastic phase transition associated with triclinic distortion. We will propose one couple of representatives, SrSnGeO5 and CaSnGeO5, which exhibit the phase transition at about 150 and 600 K, repectively. In comparison with the cases of SrZrGeO5 and CaZrGeO5, the origin of the triclinc distortion will be discussed.

FM 22.9 Fri 12:00 BEY/0138

**Interplay between Lattice Dynamics and Free Electrons in Polar Metals: A Chemical-Bonding Perspective** — •Hiroto Kikuchi[1], Suguru Yoshida[1], Hiroshi Takatsu[1], Kantaro Murayama[1], Peter Lemmens[2], and Hiroshi Kageyama[1] — [1]Department of Energy and Hydrocarbon Chemistry, Graduate School of Engineering, Kyoto University, Nishikyo-ku, Kyoto 615-8510, Japan — [2]Institute for Condensed Matter Physics, Technische Universitat Braunschweig; Braunschweig 38106, Germany

Polar-nonpolar (P-NP) transitions in metals such as $LiOsO_3$ show that polar order can coexist with metallicity, defining "polar metals" as a new class of quantum materials. However, the microscopic mechanism remains under debate, with competing scenarios invoking electron-phonon coupling and coordination bonding.

We recently found that metallic $LiReO_3$, isostructural with $LiOsO_3$ and adopting the $LiNbO_3$-type structure, undergoes a P-NP structural transition at $T_s = 170$ K. Unlike the second-order transition in $LiOsO_3$, $LiReO_3$ shows thermal hysteresis and strong lattice softening, indicating enhanced fluctuations between polar and nonpolar phases.

We investigated Raman scattering across $T_s$, combined with phonon calculations and crystal orbital Hamilton population (COHP) analysis, and reveals strongly redshifted $LiO_6$-related optical phonons in $LiReO_3$ compared with $LiOsO_3$. These results, supported by computed force constants and bond strengths, provide a unified picture of phonon softening and polar stability in metallic $LiReO_3$.

FM 22.10 Fri 12:15 BEY/0138

**NaSICON with Mg and Ca as charge carriers** — •Katharina Helmbrecht and Axel Gross — Institute of Theoretical Chemistry, Ulm University, 89069 Ulm, Germany

While the $Mo_6S_8$ chevrel phase is frequently used as cathode material in Mg–ion batteries, theoretical studies on this material are comparatively scarce. $Mo_6S_8$ as a cathode material for mono– and multivalent–ion batteries is an interesting candidate. Furthermore, magnesium and calcium both show much promise a charge carriers for a suitable battery system of the future.

In this work we study the behavior of mono– and multi–valent charge carriers (Li, Na, K, Mg, Ca, Zn, Al) at the low vacancy limit of intercalation and its influence on stability and kinetics of $Mo_6S_8$ intercalation compounds to reach fundamental understanding of the material and its properties.

Upon varying the charge carriers in the Chevrel phase at the upper vacancy limit in a previous study [1], their diffusion barriers were observed to scale linearly with the ion size, almost independent of the charge of the considered ions. This indicates a rather unique and geometry dominated diffusion mechanism in the chevrel phase and raises the question whether this trend persists at the lower vacancy limit.

[1] K. Helmbrecht, H. Euchner, A. Groß, Batteries Supercaps **5**, e202200002 (2022).

FM 22.11 Fri 12:30 BEY/0138

**High pressure crystallography: from mineral physics to material sciences** — •Leonid Dubrovinsky — BGI, Bayreuth University, Bayreuth, Germany

Modern science and technology rely on the fundamental knowledge of matter that is provided by crystallographic studies. About a decade ago, our group pioneered an approach to the SCXRD data collection and analysis for the products of chemical reactions in laser heated DACs. Since then we have designed and built new instrumentation to enable sophisticated in situ experiments in house and on synchrotron radiation facilities. Our efforts have pushed the range of static pressures achievable in a DAC up to 1 TPa and enabled single-crystal X-ray diffraction experiments at such extreme conditions. Structural studies at simultaneous high pressures of over ~200 GPa and temperatures of several thousand degrees have also become possible. This has led to remarkable findings in solid state physics, mineral physics, and chemistry at extreme conditions.We illustrate application of new methodology for simultaneous high-pressure and high-temperature single crystal diffraction studies using examples of investigations of chemical and phase relations in the halides, nitrides, and carbonates.

## FM 23: Focus Session: (Anti)ferroic states – Magnetic and magnetoelectric III (joint session FM/MA)

chair: Morgan Trassin (ETH Zurich, CH)

This focus session explores recent advances in understanding and control of (anti)ferroic states. Emphasis will be placed on theoretical modelling, advanced characterization techniques, and the engineering of emergent properties for use in nano-electronic devices. The session aims to bridge fundamental research with emerging device-relevant functionalities, bringing together experimental, and theoretical perspectives on ferroic materials.

Time: Friday 9:30–11:30 Location: BEY/0E40

**Invited Talk** FM 23.1 Fri 9:30 BEY/0E40

**Mapping topological textures in compensated magnets with X-rays** — •Claire Donnelly — Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Extending spin systems to three dimensions promise significant opportunities for applications, for example providing higher density devices and new functionalities associated with complex topology and greater degrees of freedom. Until now, however, insight into three dimensional spin systems has mainly been limited to ferromagnetic and ferrimagnetic systems through X-ray magnetic tomography [1], where a variety of topological textures [1,2], as well as 3D dynamics [3,4], have been observed. In this talk I will describe our recent work mapping topological textures in compensated systems. I will first describe the development of X-ray linear orientation tomography [5], which we have harnessed to map three-dimensional orientation fields - both crystallographic [5], and antiferromagnetic - at the nanoscale. Second, I will present our recent mapping of topological textures in altermagnets [6], harnessing both X-ray circular and linear magnetic dichroism. These insights into the formation of topological textures in compensated magnets not only paves the way for enhanced understanding of these systems, but also towards the next generation of technological devices.

[1] C. Donnelly et al., Nature 547, 328 (2017). [2] C. Donnelly et al., Nat. Phys. 17, 316 (2021) [3] C. Donnelly et al., Nature Nanotechnology 15, 356 (2020). [4] S. Finizio et al., Nano Letters (2022) [5] A. Apseros et al., Nature 636, 354 (2024) [6] R. Yamamoto et al., Phys. Rev. Appl. 24, 034037 (2025)

FM 23.2 Fri 10:00 BEY/0E40

**Exploring Magnetoelectric Effects in 1T-$FeCl_2$/bilayer-GaSe Multiferroic Heterostructures** — •Fahmida Fakhera[1], Oliver J. Conquest[1], Carla Verdi[1,2], and Catherine Stampfl[1] — [1]School of Physics, The University of Sydney, NSW 2006, Australia — [2]School of Mathematics and Physics, The University of Queensland, QLD 4072, Australia.

Multiferroic materials exhibit multiple ferroic orders simultaneously, including ferromagnetism and ferroelectricity [1]. A recent study [2] on sliding ferroelectricity in bilayer GaSe adds a novel dimension, making it useful as a ferroelectric (FE) sublayer in multiferroic heterostructures. We employ first-principles density functional theory (DFT) to investigate the interlayer and intralayer sliding mechanisms of FE GaSe. Moreover, this study investigates the structural and electronic properties, energy band alignments, magnetic anisotropy, binding energies, electric dipole moments, and interfacial charge transfer of different stackings of 1T-$FeCl_2$/bilayer GaSe. For all stackings, the magnetic anisotropy energies indicate an in-plane easy axis of magnetization in both upward and downward polarization directions. The contact interfaces form Ohmic contacts, enabling sufficient charge transfer between the layers. As the first study on sliding-induced FE and ferromagnetic interfaces, this work offers new insights into the design and understanding of multiferroic materials for the future.

[1] X. Feng, J. Liu, X. Ma, and M. Zhao, Physical Chemistry Chemical Physics 22, 7489 (2020). [2] F. Fakhera, O.J. Conquest, C. Verdi, and C. Stampfl, Physical Review Materials 9, 054402 (2025).

FM 23.3 Fri 10:15 BEY/0E40

**Nonlinear phononic slidetronics** — •Pooja Rani and Dominik Juraschek — Eindhoven University of Technology, Eindhoven, Netherlands

We investigate ultrafast switching of ferroelectricity in bilayer hexagonal boron nitride using nonlinearly driven phonons. Conventional coherent phonon excitation mechanisms such as infrared absorption, Raman-based techniques, and terahertz sum-frequency excitation produce too small a shear-mode amplitude to overcome the barrier between stacking orders. Using first-principles calculations and phenomenological modeling, we demonstrate instead that strong excitation of high-frequency intralayer phonons dynamically tilts the interlayer potential, enabling efficient and deterministic switching at experimentally accessible pulse strengths. Our results establish nonlinear phononic slidetronics as a powerful method for ultrafast, energy-efficient control of stacking order and related electronic phases in van der Waals materials, with potential for future all-optical ferroelectric memory devices.

**Coffee break**

FM 23.4 Fri 10:45 BEY/0E40

**Resolving the chemical depth profile of ultrathin EuO films by grazing incidence HAXPES measurements** — •Katharina Wehrstein[1], Umut Parlak[1], Pia Düring[1], Oliver Rehm[1], Andrei Gloskovskii[2], Christoph Schlueter[2], and Martina Müller[1] — [1]FB Physik, Uni Konstanz — [2]DESY, Hamburg

Magnetic proximity effects enable control of magnetic order in ferromagnetic insulators without altering their intrinsic properties. Europium oxide (EuO) thin films coupled with heavy metals (HM) are promising systems for spintronic applications, in which spin-polarized states are induced, altered or converted via interface coupling. These systems require a sharp interface between the metal and the EuO layer, as well as stoichiometric EuO. As ferromagnetic Eu(II)O is metastable and tends to oxidize to paramagnetic $Eu(III)_2O_3$, investigating the depth-resolved chemical and thus magnetic nature of an EuO layer is mandatory to observe and eventually tune magnetic proximity effects.

Ultrathin EuO films (2-15 nm) were prepared by molecular beam epitaxy on Pt/$SrTiO_3$ and W/$SrTiO_3$ substrates. Grazing incidence hard X-ray photoelectron spectroscopy (GIXPES) enables high X-ray intensity at the sample surface due to reflection of the X-ray beam on the heavy metal layer, leading to the formation of X-ray standing waves. By changing the incidence angle of the X-ray beam, spectra with modulated depth-sensitivity were recorded, revealing variations in the $Eu^{3+}$ content at different depths of the ultrathin EuO layer. This yields a chemical depth profile and thus a magnetic profile that provides insight into the magnetic behavior of the EuO/HM system.

FM 23.5 Fri 11:00 BEY/0E40

**Optical manipulation of multiferroic phases in $BiFeO_3$ thin films** — •Bixin Yan[1], Lauren J. Riddiford[1,2], Ales Hrabec[1,2], Annika Mechnich[3], Christian L. Degen[3], Manfred Fiebig[1], and Morgan Trassin[1] — [1]Department of Materials, ETH Zurich, Switzerland — [2]PSI Center for Neutron and Muon Sciences, Paul Scherrer Institute PSI, Switzerland — [3]Department of Physics, ETH Zurich, Switzerland

Employing light as a means of actively tuning material properties unlocks the potential for non-invasive, remote, and macroscopic control over technology-relevant functionalities. In our work, we demonstrate optical control over multiferroic phases in prototypical magnetoelectric $BiFeO_3$ (BFO) thin films, utilizing above-bandgap UV light illumination. Taking advantage of the enhanced response at the strain-driven morphotropic phase boundary, we show that by modifying the electrostatic boundary conditions with photoinduced charge carriers, the rhombohedral-like (R-like) phase of BFO can be selectively suppressed within the tetragonal-like (T-like) phase BFO matrix. Furthermore, the electronic origin of such an optical response permits a pronounced polarization-dependent R-to-T-phase conversion. Finally, using scanning nitrogen-vacancy magnetometry, we correlate optically induced ferroelectric phase conversion with a change from uncompensated magnetic ordering to G-type antiferromagnetic ordering. Our work thus presents a novel approach to writing multiferroic states, which is key to magnetoelectric oxide electronics.

FM 23.6 Fri 11:15 BEY/0E40

**Time resolved X-ray diffraction study of polarization reversal in uniaxial ferroelectric $BaMgF_4$ single crystals** — •Nathan Leubner[1,4], Sara Polo-Filisan[2], Gaetano Bonetti[2], Hiroki Tanaka[2], Matthias Zschornak[3], Dirk C. Meyer[1], Carsten Richter[2], and Semën Gorfman[4] — [1]Institut für Experimentelle Physik, TU Bergakademie Freiberg — [2]Leibniz-Institut für Kristallzüchtung, Berlin — [3]Fakultät Maschinenbau, HTW Dresden — [4]Department of Materials Science and Engineering, Tel Aviv University, Israel

$BaMgF_4$ (BMF) is a uniaxial ferroelectric material crystallizing in the orthorhombic space group $Cmc2_1$ and being a compelling candidate for frequency conversion in far ultraviolet regime. In this work, we present time-resolved X-ray diffraction (XRD) studies of single-crystalline BMF under applied electric fields, enabling direct observation of atomic-scale structural changes during domain switching. Complementary dielectric measurements provide insights into the kinetics of domain wall motion. The XRD data reveal the electric-field dependence of strain, allowing for the determination of the components of the piezoelectric tensor of BMF. Furthermore, by exploiting the resonant Friedel pair contrast between oppositely polarized domains, we achieve a direct determination of the crystal structure of each domain. This approach eliminates the need for conventional correction factors (e.g., absorption, extinction), offering a robust and accurate alternative to traditional structure refinement methods. Our findings advance the fundamental understanding of ferroelectric switching in BMF.