Crystalline Solids and their Microstructure Division
Fachverband Kristalline Festkörper und deren Mikrostruktur (KFM)

Anna Grünebohm
Experimental Physics 5
Ruhr-Universität Bochum
Universitätsstraße 150
44801 Bochum
anna.gruenebohm@rub.de

Overview of Invited Talks and Sessions

(Lecture halls H9; Poster P1)

Invited Talks

KFM 1.1	Mon	9:30–10:00	H9	**Epitaxial films of layered perovskite-based ferroelectrics: phase stability, polarization enhancement, and pathways to polar metallicity** — •Elzbieta Gradauskaite
KFM 8.1	Tue	9:30–10:00	H9	**Ferrolectric bubble currents** — •Hugo Aramberri
KFM 11.1	Wed	9:30–10:00	H9	**Towards 3D nanoscale chemical mapping with atom probe tomography** — •Kasper Hunnestad, Constantinos Hatzoglou, Antonius van Helvoort, Dennis Meier
KFM 12.1	Wed	11:00–11:30	H9	**Model-assisted Insight into Degradation of Li-Ion Batteries during Thermal Abuse** — •Ulrike Krewer, Leon Schmidt, Jorge Valenzuela
KFM 15.1	Thu	9:30–10:00	H9	**Is CVD diamond now ready to become an electronic material?** — •Philippe Bergonzo
KFM 18.1	Thu	15:30–16:00	H9	**Domain gratings of sub-micrometer period for quantum technologies** — •Carlota Canalias

Invited Talks of the joint SKM Dissertationspreis 2025 (SYSD)

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30–10:00	H2	**Nanoscale Chemical Analysis of Ferroic Materials and Phenomena** — •Kasper Aas Hunnestad
SYSD 1.2	Mon	10:00–10:30	H2	**Advanced Excitation Schemes for Semiconductor Quantum Dots** — •Yusuf Karli
SYSD 1.3	Mon	10:30–11:00	H2	**Aspects and Probes of Strongly Correlated Electrons in Two-Dimensional Semiconductors** — •Clemens Kuhlenkamp
SYSD 1.4	Mon	11:00–11:30	H2	**Mean back relaxation and mechanical fingerprints: simplifying the study of active intracellular mechanics** — •Till Münker
SYSD 1.5	Mon	11:30–12:00	H2	**Coherent Dynamics of Atomic Spins on a Surface** — •Lukas Veldman

Invited Talks of the joint Symposium AI-driven Materials Design: Recent Developments, Challenges and Perspectives (SYMD)

See SYMD for the full program of the symposium.

SYMD 1.1	Mon	15:00–15:30	H1	**Learning physically constrained microscopic interaction models of functional materials** — •Boris Kozinsky
SYMD 1.2	Mon	15:30–16:00	H1	**GRACE universal interatomic potential for materials discovery and design** — •Ralf Drautz
SYMD 1.3	Mon	16:00–16:30	H1	**Multiscale Modelling & Machine Learning Algorithms for Catalyst Materials: Insights from the Oxygen Evolution Reaction** — •Nong Artrith
SYMD 1.4	Mon	16:45–17:15	H1	**Inverse Design of Materials** — •Hongbin Zhang
SYMD 1.5	Mon	17:15–17:45	H1	**Data-Driven Materials Science** — •Miguel Marques

Invited Talks of the joint Symposium Progress and Challenges in Modelling Electron-Phonon Interaction in Solids (SYIS)

See SYIS for the full program of the symposium.

SYIS 1.1	Tue	9:30–10:00	H1	**Electron-phonon and exciton-phonon coupling in advanced materials** — •Claudia Draxl
SYIS 1.2	Tue	10:00–10:30	H1	**Exciton-phonon dynamics from first principles** — •Enrico Perfetto
SYIS 1.3	Tue	10:30–11:00	H1	**Polarons and exciton polarons from first principles** — •Feliciano Giustino
SYIS 1.4	Tue	11:15–11:45	H1	**Wannier-Function-Based First-principle Approach to Coupled Exciton-Phonon-Photon Dynamics in Two-Dimensional Semiconductors** — •Alexander Steinhoff, Matthias Florian, Frank Jahnke
SYIS 1.5	Tue	11:45–12:15	H1	**Phonon influence on (cooperative) photon emission from quantum dots** — •Erik Gauger, Julian Wiercinski, Moritz Cygorek

Invited Talks of the joint Symposium Electronic Structure Theory for Quantum Technology: From Complex Magnetism to Topological Superconductors and Spintronics (SYES)

See SYES for the full program of the symposium.

SYES 1.1	Fri	9:30–10:00	H1	**Ab-initio Design of superconductors** — •Lilia Boeri
SYES 1.2	Fri	10:00–10:30	H1	**Topological superconductivity from first principles** — Bendegúz Nyári, András Lászlóffy, Levente Rózsa, Gábor Csire, Balázs Újfalussy, •László Szunyogh
SYES 1.3	Fri	10:30–11:00	H1	**First-principles study and mesoscopic modeling of two-dimensional spin and orbital fluctuations in FeSe** — •Myrta Grüning, Abyay Ghosh, Piotr Chudzinski
SYES 1.4	Fri	11:15–11:45	H1	**Non-collinear magnetism in 2D materials from first principles: Multiferroic order and magnetoelectric effects.** — •Thomas Olsen
SYES 1.5	Fri	11:45–12:15	H1	**Spin-phonon and magnon-phonon interactions from first principles** — •Marco Bernardi

Sessions

KFM 1.1–1.6	Mon	9:30–11:15	H9	**(Multi)ferroic States: From Fundamentals to Applications (I)**
KFM 2.1–2.13	Mon	9:30–13:00	H13	**Perovskite and Photovoltaics I (joint session HL/KFM)**
KFM 3.1–3.10	Mon	9:30–12:15	H16	**Multiferroics and Magnetoelectric Coupling (joint session MA/KFM)**
KFM 4.1–4.6	Mon	11:30–13:00	H9	**(Multi)ferroic States: From Fundamentals to Applications (II)**
KFM 5.1–5.7	Mon	15:00–17:00	H9	**Instrumentation, Microscopy and Tomography with X-ray Photons, Electrons, Ions and Positrons**
KFM 6.1–6.1	Mon	15:00–15:30	H10	**Invited Talk: X. Fang (joint session MM/KFM)**
KFM 7.1–7.5	Mon	17:15–18:30	H22	**Materials for the Storage and Conversion of Energy (joint session MM/KFM)**
KFM 8.1–8.7	Tue	9:30–11:30	H9	**(Multi)ferroic States: From Fundamentals to Applications (III)**
KFM 9.1–9.5	Tue	11:45–13:00	H9	**(Multi)ferroic States: From Fundamentals to Applications (IV)**
KFM 10.1–10.5	Tue	14:00–15:15	H22	**Materials for the Storage and Conversion of Energy (joint session MM/KFM)**
KFM 11.1–11.4	Wed	9:30–10:45	H9	**(Multi)ferroic States: From Fundamentals to Applications (V)**
KFM 12.1–12.6	Wed	11:00–12:45	H9	**Holistic Structural and Safety Assessment of Lithium-ion and Post-Lithium Cells and their Materials (Modelling of Battery Materials and Degradation)**
KFM 13.1–13.7	Wed	15:00–16:45	H9	**Holistic Structural and Safety Assessment of Lithium-ion and Post-Lithium Cells and their Materials (Experimental Characterisation and Safety Testing)**
KFM 14.1–14.26	Wed	17:00–18:30	P1	**Poster**
KFM 15.1–15.12	Thu	9:30–13:15	H9	**Crystal Structure Defects / Real Structure / Microstructure**
KFM 16.1–16.13	Thu	9:30–13:00	H13	**Perovskite and Photovoltaics II (joint session HL/KFM)**
KFM 17.1–17.5	Thu	11:45–13:00	H23	**Functional Materials: Performance, Reliability and Degradation; and Complex Materials (joint session MM/KFM)**
KFM 18.1–18.7	Thu	15:30–17:45	H9	**Materials Research in Polar Oxides: Perspectives for Optics & Electronics**
KFM 19	Thu	18:00–19:00	H9	**Members' Assembly**

Members' Assembly of the Crystalline Solids and their Microstructure Division

Thursday 18:00–19:00 H9

KFM 1: (Multi)ferroic States: From Fundamentals to Applications (I)

This focus session explores the intricate properties of (multi)ferroic states, spanning from fundamental understanding to cutting-edge applications. Topics include the design and control of (multi)ferroic states and domain structures at interfaces, domain walls, and in heterostructures. Emphasis will be placed on theoretical models, advanced characterization techniques, and the engineering of emergent properties for use in nano-electronic devices.

Chair: Johanna Nordlander (University of Zurich)

Time: Monday 9:30–11:15 Location: H9

Invited Talk KFM 1.1 Mon 9:30 H9

Epitaxial films of layered perovskite-based ferroelectrics: phase stability, polarization enhancement, and pathways to polar metallicity — •Elzbieta Gradauskaite — Laboratoire Albert Fert, CNRS/Thales, Palaiseau, France

Layered perovskite-based compounds offer a range of unconventional properties stemming from their pronounced unit-cell anisotropy. While most renowned for the superconductivity observed in the Ruddlesden-Popper phases, many of these layered compounds are also ferroelectric and exhibit a sizeable in-plane polarization. In this talk, I will review different classes of layered perovskite-based ferroelectrics and the unique functionalities arising from their structural anisotropy.

In particular, the focus will be placed on Carpy-Galy $A_nB_nO_{3n+2}$ phases characterized by 110-oriented perovskite planes interleaved with additional oxygen layers. These compounds have been proposed as platforms for hosting both metallicity and polar displacements. However, their synthesis challenges have hindered integration into devices. Addressing this, our study focuses on $La_2Ti_2O_7$, an n=4 representative of the Carpy-Galy family, exploring its epitaxial growth and concurrent phase stability. Surprisingly, we find that high tensile strain facilitates a controlled layer-by-layer growth mode, yielding films that are ferroelectric from a single unit cell and exhibit polarization enhanced by a factor of four compared to bulk crystals. Most importantly, we show that metallicity in Carpy-Galy films can be induced via interfacial redox processes with a reactive metal, laying the foundation for exploring them as functional polar metals.

KFM 1.2 Mon 10:00 H9

Tailoring ferroelectric to antipolar phase interconversion in multiferroic thin films — •Bixin Yan[1], Marvin Müller[1], Hyeon Ko[1], Yen-Lin Huang[2,3,4], Haidong Lu[5], Alexei Gruverman[5], Ramamoorthy Ramesh[3,4,6], Marta D. Rossell[7], Manfred Fiebig[1], and Morgan Trassin[1] — [1]ETH Zurich, Switzerland — [2]National Yang Ming Chiao Tung University, Taiwan — [3]University of California, Berkeley, USA. — [4]Lawrence Berkeley Laboratory, USA. — [5]University of Nebraska-Lincoln, USA — [6]Rice University, USA. — [7]Empa, Switzerland.

Inversion-symmetry breaking and the emergence of a polar state are essential for technologically relevant effects such as ferroelectricity and nonlinear optical properties. Hence, the ability to reversibly control the onset of such symmetry breaking can be instrumental in establishing emergent computing schemes. In this work, we present a novel approach for reversible control over the ferroelectric-to-antipolar phase transition in epitaxial multiferroic La-substituted $BiFeO_3$ (LBFO) thin films using local pressure and electric field. Utilizing local stress application via a scanning-probe-microscopy tip, we stabilize the antipolar phase. An electric field restores the original ferroelectric phase. Leveraging these insights, we establish the continuous tuning of the ferroelectric/antipolar phase coexistence and can set the net polarization of LBFO to any desired value between its saturation limits. Finally, using optical second harmonic generation as a non-invasive probe, we control the net polarization of our films in device-compliant capacitor heterostructures.

KFM 1.3 Mon 10:15 H9

Unconventional Polarization Response in Titanite-type Oxides due to Hashed Antiferroelectric Domains — •Hiroki Taniguchi[1], Takumi Watanabe[1], Taro Kuwano[2], Akitoshi Nakano[1], Yukio Sato[3], Manabu Hagiwara[4], Hiroko Yokota[2], and Kazuhiko Deguchi[1] — [1]Department of Physics, Nagoya University, Nagoya, Japan — [2]School of Materials and Chemical Technology, Institute of Science Tokyo, Yokohama, Japan — [3]Research and Education Institute for Semiconductors and Informatics, Kumamoto University, Kumamoto, Japan — [4]Department of Applied Chemistry, Keio University, Yokohama, Japan

$CaTiSiO_5$, a titanite-type oxide, consists of one-dimensional chains of TiO_6 octahedra bridged by SiO_4 tetrahedra and CaO_7 polyhedra. While $CaTiSiO_5$ has potential antiferroelectric properties, these have not been directly verified until now. In this study, we demonstrate the antiferroelectricity of $CaTiSiO_5$ by observing a double $P-E$ hysteresis loop. Moreover, we show an unconventional enhancement of permittivity through partial substitution of Si with Ge, resulting in a doubling of permittivity over a wide temperature range in the antiferroelectric phase. Transmission electron microscopy and second harmonic generation measurements have revealed the formation of microscopic polar regions in the antiferroelectric phase of $CaTi(Si_0.5Ge_0.5)O_5$. Antiphase boundaries are suggested to play a role in the generation of these microscopic polar regions. This study provides new insights into boosting the permittivity of antiferroelectric materials from the perspective of domain engineering.

KFM 1.4 Mon 10:30 H9

Dielectric crossover and its structure-function relationship in pseudo Ruddlesden-Popper-type oxides — •Akitoshi Nakano and Hiroki Taniguchi — Nagoya University, Nagoya, Japan

A phase variation of a pseudo-Roddlesden-Popper-type ferroelectric oxide Li2Sr1-xCax(Nb1-xTax)2O7 is systematically investigated using dielectric measurements, and x-ray diffraction experiments. We find an exotic x-T phase diagram, including paraelectric Cmcm, antiferroelectric Pmcn, and in-plane antiferroelectric and out-of-plane ferroelectric P21cn phases. At low x, we observe large and divergent dielectric anomalies associated with phase transitions from Cmcm to P21cn, whereas it crosses over into a small kink as x increases. Structural analyses reveal an internal distortion, and the rotation of octahedra also strongly depends on x. These results demonstrate the great tunability of dielectric properties in layered perovskite-type oxides by tuning the chemical bonding state in the octahedron.

KFM 1.5 Mon 10:45 H9

Stoichiometry of CoFe2O4 as a key to phase control and improved functional properties of multiferroic BaTiO3-CoFe2O4 bulk composites — •Daniil Lewin, Sofia Shamsulbahrin, Vladimir V. Shvartsman, and Doru C. Lupascu — Institute for Materials Science and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, Universitätsstrasse 15, 45141, Essen, Deutschland

Composite multiferroics have been widely studied as materials with a large magnetoelectric effect at room temperature. Barium titanate – cobalt ferrite composites are among the first and most reliable composite systems of such kind. Unfortunately, high-temperature sintering can result in the formation of secondary phases and undesirable chemical modifications, particularly that of barium hexaferrite (BaFe12O19). We present a method to suppress the formation of this phase both by sintering in nitrogen and by changing the stoichiometry of cobalt ferrite to incorporate more cobalt. The latter restricts the diffusion of the iron cations into the barium titanate during sintering. Moreover, composite samples with non-stoichiometric cobalt ferrite show up to a threefold improvement in magnetoelectric coefficient when compared to samples made with stoichiometric cobalt ferrite.

KFM 1.6 Mon 11:00 H9

Stabilization and Characterization of the LiNbO3-type Phase in NiTiO3 Thin Films: Towards Ferroelectricity — •Meriem Chettab[1], Quentin Simon[1], Mustapha Zaghrioui[1], Oleg I. Lebedev[2], Xavier Rocquefelte[3], Gwenhael Duplaix-Rata[3], Richard Retoux[2], and Patrick Laffez[1] — [1]University of Tours, GREMAN, UMR 7347-CNRS, IUT de Blois 15 Rue de la Chocolaterie, 41029 Blois Cedex, France — [2]University of Caen, CRISMAT, UMR

6508 - CNRS, ENSICAEN 6 Bd Maréchal Juin, 14000 Caen, France — [3]Univ Rennes, CNRS, ISCR (Institut des Sciences Chimiques de Rennes) UMR 6226 - F-35000 Rennes, France

Nickel titanate (NiTiO3) exhibits polymorphic structures, including ilmenite (IL), LiNbO3-type (LN), and corundum (CR), with the LN phase being potentially ferroelectric. NiTiO3 thin films were deposited by RF sputtering in an Ar/O2 plasma on Si(100) substrates at temperatures between 400 °C and 650 °C. XRD, Raman spectroscopy, and HRTEM revealed a mixture of IL, LN, and CR phases at lower temperatures, with pure IL films obtained at 650 °C. All films showed a [00W] fiber texture. Post-annealing at 800 °C transformed the films into pure IL while preserving the texture. DFT simulations predicted Raman spectra for LN and CR phases, offering insight into phase behavior. This study highlights the potential of the LN phase for ferroelectric applications.

KFM 2: Perovskite and Photovoltaics I (joint session HL/KFM)

Time: Monday 9:30–13:00 Location: H13

KFM 2.1 Mon 9:30 H13

Oxygen-Mediated (0D) Cs4PbX6 Formation during Open-Air Thermal Processing Improves Inorganic Perovskite Solar Cell Performance — Rafikul Ali Saha[1], •Wei-Hsun Chiu[2], Giedrius Degutis[1], Peng Chen[3], Matthias Filez[4], Eduardo Solano[5], Nikolai Orlov[6], Francesco De Angelis[7], Carlo Meneghini[7], Christophe Detavernier[4], Sawanta S. Mali[8], Minh Tam Hoang[2], Yang Yang[2], Erik C. Garnett[9], Lianzhou Wang[3], Hongxia Wang[2], Maarten B. J. Roeffaers[1], and Julian A. Steele[3] — [1]KU Leuven, Belgium — [2]Queensland University of Technology, Brisbane, Australia — [3]The University of Queensland, Brisbane, Australia — [4]Ghent University, Belgium — [5]ALBA synchrotron, Barcelona, Spain — [6]AMOLF, Amsterdam, The Netherlands — [7]Roma Tre University, Rome, Italy — [8]Chonnam National University, Gwangju, South Korea — [9]University of Amsterdam, The Netherlands

We highlight the beneficial role of ambient oxygen during the open-air thermal processing of metastable γ-CsPbI3-based perovskite thin films and devices. Physiochemical-sensitive probes elucidate oxygen intercalation and the formation of Pb-O bonds in the perovskite, entering via iodine vacancies at the surface, creating superoxide (O2-) through electron transfer reactions, which drives the formation of a zero-dimensional (0D) Cs4PbI6 protective capping layer during annealing (>330°C). Applied to γ-CsPbI2Br perovskite solar cells, it boosts the operational stability and photo-conversion efficiency of champion devices from 12.7% to 15.4% when annealed in dry air.

KFM 2.2 Mon 9:45 H13

Compositional Engineering of Mixed-Metal Chalcohalides for Photovoltaic Applications — •Pascal Henkel[1], Jingrui Li[2], and Patrick Rinke[1,3] — [1]Department of Applied Physics, Aalto University, P.O.Box 11100, 00076 AALTO, Finland — [2]School of Electronic Science and Engineering, Xi'an Jiaotong University, Xi'an 710049, China — [3]Technical University of Munich, 85748 Garching, Germany

Perovskite-inspired quaternary mixed-metal chalcohalides (MMCHs, M(II)$_2$M(III)Ch$_2$X$_3$) are an emerging materials class for photovoltaic's [1], that could overcome the stability and toxicity problems of halid perovskites [2], and still deliver high conversion efficiencies [3]. Compositional engineering enables the optimization of MMCH materials properties en route to commercialization.

We study the stability of MMCH alloys for three different compositional positions: the M(III), the Ch and the X site. We use a combination of density functional theory and machine learning to explore the compositional space of the alloys [4] and to compute their convex hulls. For x site alloying, for example [Sn$_2$InS$_2$(Br$_{1-c}$I$_c$)$_3$], we obtained stable structures for $c = \frac{1}{3}$ and $c = \frac{2}{3}$ for the $Cmcm$ phase and for $c = \frac{1}{6}$ and $c = \frac{1}{3}$ for the $Cmc2_1$ phase, but not for $P2_1/c$. The energetically favored structures (at $c = \frac{1}{3}$) are highly symmetrical and exhibit a layered pattern. Every third halogen layer is fully occupied by iodine whereas the other two layers are filled with bromine.

[1] *Chem. Mater.* **35**, 7761-7769 (2023), [2] *Z. Anorg. Allg. Chem.* **468**, 91-98 (1980), [3] *Mater. Horiz.* **8**, 2709 (2021). [4] *Phys. Rev. Materials* **6**, 113801 (2024).

KFM 2.3 Mon 10:00 H13

Versatile Two-Step Process for Enhanced Stability and Efficiency in Perovskite Top Cells for Tandem Photovoltaics — •Ronja Pappenberger[1,2], Roja Singh[1,2], Alexander Diercks[2], and Ulrich W. Paetzold[1,2] — [1]Institute of Microstructure Technology, KIT, Germany — [2]Light Technology Institute, KIT, Germany

To achieve highly efficient 2T perovskite/silicon (Si) tandem solar cells (TSCs), textured-front Si bottom cells provide superior light-harvesting capabilities, making higher short-circuit current densities of TSC possible. A promising approach to fabricating uniform, high-quality perovskite films on these textured Si cells is the solution-based two-step method. One of the main challenges for perovskite solar cells (PSCs) remains their long-term stability. While methylammonium (MA)-based PSCs have demonstrated some of the highest efficiencies, their instability continues to pose a major obstacle. In this work, a versatile two-step process is employed – replacing MA with formamidinium – which maintains high efficiency, improves open-circuit voltage and enhances stability. A further performance boost is achieved by implementing a dual passivation strategy using PDAI$_2$ and BAI for bulk and surface passivation. This leads to a stable power output exceeding 20.8% for E_g = 1.67 eV due to reduced non-radiative recombination at the perovskite/ETL interface and improved film crystallization, enhancing charge carrier extraction. The long-term stability is also distinctly improved. When implemented on textured Si bottom cells, this process delivers efficiencies exceeding 24% for lab-scale monolithic perovskite/Si TSCs with a 1 cm^2 active area.

KFM 2.4 Mon 10:15 H13

Recombination at grain boundaries in Cd(Te,Se) thin films in comparison with other photovoltaic absorber layers — •Luka Blazevic[1], Sebastian Weitz[1], Elisa Artegiani[2], Alessandro Romeo[2], and Daniel Abou-Ras[1] — [1]Helmholtz-Zentrum Berlin, Germany — [2]Universita di Verona, Italy

The role of grain boundaries on the device performance is of concern for all polycrystalline absorbers in photovoltaic solar cells. In the present work, recombination velocities s_{GB} at grain boundaries in Cd(Te,Se) thin-film absorbers were determined from cathodoluminescence (CL) intensity distributions, which were acquired together with electron backscatter diffraction (EBSD) and energy-dispersive X-ray spectroscopy (EDXS) maps. The resulting s_{GB} values exhibited ranges over several orders of magnitude ($10^1 - 10^3$ cm/s). These wide value ranges are in good agreement with those obtained on other photovoltaic absorber materials (multicrystalline Si, Cu(In,Ga)Se$_2$, Cu$_2$ZnSn(S,Se)$_4$). The present work suggests a model comprising the enhanced, nonradiative Shockley-Read-Hall recombination at grain boundaries as well as the upward/downward band bending (± several 10 meV) at these planar defects. This model can reproduce successfully the experimental s_{GB} values from various photovoltaic absorber materials and provides also ranges for the effective defect densities as well as their capture cross-sections at the grain boundaries. It will be shown that typical losses in the open-circuit voltage of the corresponding solar cells due to grain-boundary recombination in the absorbers are few 10 mV.

KFM 2.5 Mon 10:30 H13

Microscopic origins of band-gap broadening and its relationship with Urbach tails in photovoltaic absorbers — •Daniel Abou-Ras — Helmholtz-Zentrum Berlin, Germany

The broadening of absorption edges is a general feature found in numerous semiconductors used as absorber layers for thin-film solar cells. Since this broadening gives rise to radiative losses of the open-circuit voltage, it is of importance to control the broadening by corresponding material design of the photovoltaic absorber materials. The present work provides an overview of the microscopic origins of band-gap broadening, addressing not only compositional aspects and microstrain, but also electrical and optoelectronic properties on the sub-μm scale. In addition, the Urbach energy extracted from absorptance or quantum efficiency spectra has been used broadly to quantify disorder in a material. However, up to date, it has not only not been clarified what the microscopic origins of Urbach tails are; the present contribution also shows that there is no direct correlation between the broadening of the absorption edge and the Urbach energy of a semiconductor, as verified for about 30 different photovoltaic absorbers.

KFM 2.6 Mon 10:45 H13

Minimizing V_{OC} losses in high bandgap perovskite solar cells for the application in perovskite/perovskite/silicon triple-junction solar cells — •Athira Shaji[1,2], Minasadat Heydarian[1,3], Oliver Fischer[1,3], Michael Günthel[1], Orestis Karalis[4], Maryamsadat Heydarian[1], Alexander J. Bett[1], Hannes Hempel[4], Martin Bivour[1], Florian Schindler[1], Martin C. Schubert[1], Stefan W. Glunz[1,3], Andreas W. Bett[1,2], Juliane Borchert[1,3], and Patricia S. C. Schulze[1] — [1]Fraunhofer Institute for Solar Energy Systems ISE, Germany — [2]University Freiburg, Institute of Physics, Germany — [3]University of Freiburg, Department of Sustainable Systems Engineering, Germany — [4]Helmholtz-Zentrum Berlin, Solar Energy Division, Germany

The high bandgap (HBG) top cell is the main source of V_{OC} loss in perovskite/perovskite/silicon triple junction solar cells due to photoinduced phase segregation, non-radiative recombination at the perovskite bulk and interface with the charge transport layers (CTLs), as well as energetic misalignment between the perovskite layer and the CTLs. The starting point of this work was a triple-cation double-halide perovskite composition with a bandgap of 1.83 eV. By implementing a multi-faceted optimization approach, an average improvement in V_{OC} of 250 mV was achieved for HBG perovskite solar cells. Replacing the reference HBG perovskite with the optimised top cell in perovskite/perovskite/silicon triple-junction solar cells results in the improvement of V_{OC} by 124 mV, and the champion device achieves a voltage above 3 V.

15 min. break

KFM 2.7 Mon 11:15 H13

The Effect of Overdamped Phonons on the Fundamental Band Gap of Perovskites — •Xiangzhou Zhu and David A. Egger — Physics Department, TUM School of Natural Sciences, Technical University of Munich, 85748 Garching, Germany

Different from conventional semiconductors, halide perovskites (HaPs) exhibit unique anharmonic fluctuations that strongly influence optoelectronic properties. Recent studies have shown that in specific temperature regimes, the strong phonon-phonon interactions in HaPs lead to overdamped phonons, where vibrational lifetimes drop below one oscillation period. However, the relationship between these overdamped phonons and atomic fluctuations, as well as their impact on optoelectronic properties, are not fully understood. Here, using molecular dynamics (MD) simulations and augmented stochastic Monte Carlo methods that account for phonon renormalization and imaginary modes, we contrast the band gap behavior of two anharmonic perovskite materials, $SrTiO_3$ and $CsPbBr_3$, of which only the latter exhibits overdamped phonons.[1] Our results show that the overdamped phonon dynamics in $CsPbBr_3$ drive slow atomic fluctuations that are not adequately captured by conventional phonon quasiparticle descriptions. Importantly, we show that these overdamped phonon lead to significant renormalization of the band gap. Our work disentangles the consequences of anharmonic effects on the optoelectronic properties and electron-phonon interactions in perovskites.

[1] Zhu, X. & Egger, D. A. arXiv:2406.05201 (2024).

KFM 2.8 Mon 11:30 H13

Polymorphism at surface in $CsPbI_3$ from first principles — •Jasurbek Gulomov[1], Guido Roma[1], Jacky Even[2], and Marios Zacharias[2] — [1]Université Paris-Saclay, CEA, Service de recherche en Corrosion et Comportement des Matériaux, SRMP, Gif sur Yvette, 91191, France — [2]Université Rennes, INSA Rennes, CNRS, Institut FOTON - UMR 6082, F-35000 Rennes, France

Halide perovskites show great potential for optoelectronics and photovoltaics, but challenges with ion migration and phase stability remain.Atomic-scale phenomena at surfaces and interfaces must be understood to block ion migration and enhance passivation. A peculiar property of these materials is the tendency to gain energy by disordered structural distortions, dubbed polymorphism, in contrast to the view of a perfectly symmetric monomorphous structure. Using first-principles calculations, we investigate the electronic and structural properties of polymorphous bulk $CsPbI_3$ and its 100 surface with two terminations. For the bulk, we generate a dynamically stable polymorphous structure for the cubic high-temperature phase using the method recently proposed by M. Zacharias et al. [1]. The energy gain and band gap opening are essentially linked to the increased average length of Pb-I bonds. Then we extend the concept of polymorphism to the surface, analyzing surface dipoles and work functions by comparing monomorphous and polymorphous slabs with experimental data. Our results tend to confirm the occurrence of polymorphism at surfaces in $CsPbI_3$.

[1] Zacharias, M., et al., npj Comput. Mater. 9, 153 (2023).

KFM 2.9 Mon 11:45 H13

Benchmarking approximations for the theoretical prediction of positron lifetimes in halide perovskites — Kajal Madaan[1], •Guido Roma[1], Jasurbek Gulomov[1], Pascal Pochet[2], Catherine Corbel[3], and Ilja Makkonen[4] — [1]Université Paris-Saclay, CEA, Service de recherches en Corrosion et Comportement des Matériaux, SRMP, 91191 Gif sur Yvette, France — [2]Department of Physics, IriG, Univ. Grenoble-Alpes and CEA, Grenoble, France — [3]LSI, CEA/DRF/IRAMIS, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, Palaiseau, 91120, France — [4]Department of Physics, University of Helsinki, P.O. Box 43, FI-00014 Helsinki, Finland

Positron annihilation spectroscopy is a well recognized tool for probing vacancies in materials. Recent applications of this technique to $APbX_3$ halide perovskites are sparse, and the rare theoretical predictions of positron lifetimes in these materials, published in association with experiments, do not fully agree with each other. These works suggest that vacancies on the A site are not detected. In our theoretical study we thoroughly revisit and compare several approximations for the electron-positron correlation functional, applied to methylammonium lead iodide ($MAPbI_3$) and $CsPbI_3$ and their vacancies. The discrepancies between the approaches make it difficult to unequivocally exclude the presence of methylammonium vacancies in $MAPbI_3$. Moreover, when using a truly nonlocal electron-positron correlation functional, the predicted positron density in a vacancy presents peculiar features and a much lower binding energy to the vacancy with respect to semilocal approximations.

KFM 2.10 Mon 12:00 H13

Dynamics of electronic surface states in halide perovskites using machine-learning force fields — •Frederico Delgado[1], Frederico Simões[1], Waldemar Kaiser[1], Leeor Kronik[2], and David A. Egger[1] — [1]Physics Department, TUM School of Natural Sciences, Technical University of Munich, Germany — [2]Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Israel

The photovoltaic performance exhibited by bulk halide perovskites (HaPs) hinges on their excellent optoelectronic properties, which have been extensively investigated. Nonetheless, extended defects like surfaces are ubiquitous, and as such, their impact on such properties requires further, careful investigation. Rigorous examination of dynamics in this context through ab-initio molecular dynamics implies large computational costs, which are here circumvented by the use of machine learning (ML) force fields. In this study, we demonstrate the transient and shallow nature of surface states in $CsPbBr_3$. We shed light on the mechanisms which underpin the behaviour of such states through the framework of local, internal dipoles. Our results aid in rationalizing the benign nature of surfaces in $CsPbBr_3$, and further the understanding of the correlation between structural dynamics and optoelectronic properties of HaP surfaces.

KFM 2.11 Mon 12:15 H13

Comprehensive High-Throughput DFT Study of Intrinsic Defects and Dopability in p-type Zn3P2 for Photovoltaic Applications — •Nico Kawashima[1,2,3] and Silvana Botti[1,3] — [1]Ruhr-Universität, Bochum, Germany — [2]Friedrich-Schiller-Universität, Jena, Germany — [3]RC FEMS, Bochum, Germany

Zn_3P_2 has attracted significant interest as a thin-film absorber material for photovoltaic applications due to its intrinsic p-type conductivity and earth-abundant constituents. However, the nature of the dominant native defects – whether phosphorus interstitials (P_i) or zinc vacancies (V_Zn) – remains a subject of debate, with implications for the material's electronic structure and dopability through mechanisms such as Fermi-level pinning and defect compensation.

We perform a high-throughput density functional theory (DFT) analysis to systematically investigate both intrinsic point defects and potential extrinsic dopants. By resolving the ground-state configurations and formation energies of key native defects, we provide a clearer understanding of their impact on the electronic landscape. This insight is then applied to evaluate a range of extrinsic dopants, predicting their incorporation and activation potentials in the presence of native defects.

Our study offers a comprehensive framework that links intrinsic defect behavior with extrinsic doping strategies, providing critical guidance for tuning the electrical properties of Zn_3P_2. The findings present experimentally actionable insights that can drive the optimization of Zn_3P_2 for next-generation photovoltaic devices.

KFM 2.12 Mon 12:30 H13

Density functional theory study of hydrogen passivation mechanisms in defective silicon — •Hania Azzam[1], Tobias Binninger[1], and Michael Eikerling[1,2] — [1]Theory and Computation of Energy Materials (IET-3), Institute of Energy Technologies, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Chair of Theory and Computation of Energy Materials, Faculty of Georesources and Materials Engineering, RWTH Aachen University, 52062 Aachen, Germany

Silicon heterojunction (SHJ) solar cells offer high-effeciency energy conversion, with reported efficiencies up to 27%. Their performance and durability depend on effective passivation of dangling bonds at the amorphous/crystalline silicon interface, where electron-hole recombination reduces efficiency. Hydrogen atoms play a crucial role in passivating those dangling bonds, minimizing recombination loses. Recent experimental studies by IMD-3 at Forschugnszentrum Jülich showed performance improvements after light soaking, a process where solar cells are exposed to intensive light at elevated temperatures. It is hypothesized that light soaking activates hydrogen migration toward defect sites. This theoretical study explores hydrogen passivation mechanisms in defective silicon for SHJ solar cells. Using Density Functional Theory (DFT), we analyze how silicon vacancies alter the electronic structure of Si-H systems, introducing localized defect states within the band gap and shifts in Fermi level, and subsequently investigate the changes induced by hydrogen passivation. These insights contribute to understanding the beneficial effects of light soaking on SHJ solar cells.

KFM 2.13 Mon 12:45 H13

First principles theory of nonlinear long-range electron-phonon interaction — •Matthew Houtput[1,2], Luigi Ranalli[2], Jacques Tempere[1], and Cesare Franchini[2] — [1]University of Antwerp, Belgium — [2]University of Vienna, Austria

Electron-phonon interactions in a solid are crucial for understanding many interesting material properties, such as transport properties and the temperature dependence of the electronic band gap. For harmonic materials, the linear interaction process where one electron interacts with one phonon is sufficient to quantitatively describe these properties. However, this is no longer true in anharmonic materials with significant electron-phonon interaction, such as quantum paraelectrics and halide perovskites. Currently, the only available models for nonlinear electron-phonon interaction are model Hamiltonians, written in terms of phenomenological parameters. Here, we provide a microscopic semi-analytical expression for the long-range part of the 1-electron-2-phonon matrix element, which can be interfaced with first principles techniques. We show that unlike for the long-range 1-electron-1-phonon interaction, the continuum approximation is not sufficient and that the entire phonon dispersion must be taken into account. We calculate an expression for the quasiparticle energies and show that they can be written in terms of a 1-electron-2-phonon spectral function. To demonstrate the method in practice, we calculate the 1-electron-2-phonon spectral function for $KTaO_3$ from first principles. The framework in this article bridges the gap between model Hamiltonians and first-principles calculations for the 1-electron-2-phonon interaction.

KFM 3: Multiferroics and Magnetoelectric Coupling (joint session MA/KFM)

Time: Monday 9:30–12:15 Location: H16

KFM 3.1 Mon 9:30 H16

Trilinear coupling and toroidicity in multiferroics — Andrea Urru[1] and •Vincenzo Fiorentini[2,3] — [1]Dept. of Physics, Rutgers University, USA — [2]Chair of Materials Science and Nanotech, TU Dresden — [3]Dept. Physics, University of Cagliary, Italy

We discuss the properties of the triple-order-parameter (ferromagnet, ferroelectric, ferrotoroid) layered-perovskite metal Bi5Mn5O17, as predicted from first-principles calculations, in the light of a Landau expansion with trilinear coupling, with particular reference to its multiple degenerate ground states with mutually orthogonal vector order parameters, giant cross-coupling magnetoelectricity, and magnetotoroidic effects.

KFM 3.2 Mon 9:45 H16

Engineering magnetic domain wall energies in $BiFeO_3$ via epitaxial strain: A route to assess skyrmionic stabilities in multiferroics from first principles — •Sebastian Meyer[1,2], Bin Xu[3,4], Laurent Bellaiche[4], and Bertrand Dupé[1,2] — [1]Université de Liège, Belgium — [2]Fonds de la Recherche Scientifique, Belgium — [3]Soochow University, China — [4]University of Arkansas, USA

Epitaxial strain has emerged as a powerful tool to tune magnetic and ferroelectric properties in functional materials such as in multiferroic perovskite oxides. Here, we use first-principles calculations to explore the evolution of magnetic interactions in the antiferromagnetic multiferroic $BiFeO_3$ (BFO), one of the most promising multiferroics for future technology [1]. The epitaxial strain in BFO is varied between $\varepsilon \in [-2\%, +2\%]$. We find that both strengths of the exchange interaction and Dzyaloshinskii-Moriya interaction decrease linearly from compressive to tensile strain whereas the uniaxial magnetocrystalline anisotropy lifts the energy degeneracy of the (111) easy plane of bulk BFO. From the trends of magnetic interactions we can explain the destruction of cycloidal order in compressive strain as observed in experiments due to the increasing anisotropy energy. For tensile strain, we predict that the ground state remains unchanged as a function of strain. By using the domain wall energy, we envision a region where isolated chiral magnetic textures might occur as a function of strain [2].

[1] R. Ramesh, N. Spaldin, *Nature Mater* **6**, 21-29 (2007)
[2] S. Meyer *et al.*, *Phys. Rev. B* **109**, 184431 (2024)

KFM 3.3 Mon 10:00 H16

Hidden order in Cr_2O_3 and α-Fe_2O_3 as a predictor for (anti-)magnetoelectricity — •Xanthe Verbeek[1,2], Andrea Urru[2,3], and Nicola Spaldin[2] — [1]Insitut für Physik, Johannes Gutenberg-Universität Mainz, D-55099 Mainz, Germany — [2]Materials Department, ETH Zurich, 8093 Zürich, Switzerland — [3]Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA

With first-principles calculations of Cr_2O_3 and α-Fe_2O_3, we show that the different magnetoelectric effects in these materials result from the ordering of hidden magnetic multipoles. We reveal for the first time anti-ferroically ordered magnetic multipoles in both Cr_2O_3, and isostructural α-Fe_2O_3, in which the global inversion symmetry is preserved by the different magnetic dipolar ordering. We can relate each of these multipoles and their ordering to linear, quadratic, and cubic (anti-) magnetoelectric effects, where in an anti-magnetoelectric effect the induced moments are ordered antiferromagnetically in the unit cell. We confirm the predicted induced moments using first-principles calculations, showing the lowest response in α-Fe_2O_3 a centrosymmetric magnetic material, to be a linear anti-magnetoelectric effect, revealing the presence of the magnetoelectric coupling despite the preserved global inversion symmetry. Our results demonstrate the existence of hidden magnetic multipoles leading to local linear magnetoelectric responses, even in centrosymmetric magnetic materials, and broaden the definition of magnetoelectric materials by including those showing such local magnetoelectric responses.

KFM 3.4 Mon 10:15 H16

Non-trivial Spin Structures and Multiferroic Properties of the DMI-Compound $Ba_2CuGe_2O_7$ — •Peter Wild[1], Korbinian Fellner[1], Michał Dembski-Villalta[1], Markus Garst[2], Eric Ressouche[5], Tommy Kotte[3], Bertrand Roessli[4], Alexandra Turrini[4], and Sebastian Mühlbauer[1] — [1]Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Garching, Germany — [2]Karlsruhe Institute of Technology, (KIT), Karlsruhe, Deutschland — [3]Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Dresden, Germany — [4]Paul Scherrer Institut (PSI), Villigen, Switzerland — [5]Institut Laue-Langevin (ILL), Grenoble, France

Antiferromagnetic $Ba_2CuGe_2O_7$, characterized by a quasi-2D structure with Dzyaloshinskii-Moriya interactions (DMI), is a non-centrosymmetric insulator that exhibits spiral spin structures with potential non-trivial topology and a variety of unconventional magnetic phase transitions. Below the Néel temperature $T_N = 3.05$K, the DMI term leads to a long-range incommensurate, almost AF cycloidal spin spiral in the ground state. Recently, a new phase with a vortex-antivortex magnetic structure has been theoretically described and experimentally confirmed in a pocket in the phase diagram at around 2.4K and an external field along the crystalline c-axis of around 2.2T. A lack of evidence for a thermodynamic phase transition towards the paramagnet in specific heat measurements and a finite linewidth in E and Q of the incommensurate peaks in neutron scattering, as opposed to the cycloidal ground state, seem to mark the vortex phase as a slowly fluctuating structure at the verge of ordering.

KFM 3.5 Mon 10:30 H16

A comparison of Γ-point symmetries and phonon selection rules of spin-space and magnetic point group in $Co_2Mo_3O_8$ — •Onur Ercem[1], Felix Schilberth[1,2], Lilian Prodan[1], Vladimir Tsurkan[1], Alexander Tsirlin[3], István Kézsmárki[1], and Joachim Deisenhofer[1] — [1]Experimental Physics V, Center for Electronic Correlations and Magnetism, Institute for Physics, University of Augsburg, D-86135 Augsburg, Germany — [2]Department of Physics, Budapest University of Technology and Economics, 1111 Budapest, Hungary — [3]Felix Bloch Institute for Solid-State Physics, Leipzig University, 04103 Leipzig, Germany

$Co_2Mo_3O_8$, which has recently come into the focus of research, as different magnetically ordered ground states can be formed and tuned by external magnetic fields or doping. $Co_2Mo_3O_8$ has a hexagonal structure, the polarization along the c-axis, and a collinear antiferromagnetic order below $T_N = 40$ K. Reflectivity measurements were performed using the FTIR spectrometer, in the frequency range from 100 to 8000 cm^{-1}, and the temperature range from 10 to 300 K could be covered. A preliminary analysis of the infrared-active modes for $E \parallel c$ reveals that 8 out of the 9 predicted A_1 modes are observed at the expected eigenfrequencies and the emergence of the mode at around 300 cm^{-1} below T_N. In $E \perp c$ at room temperature 10 modes were observed. Below T_N two new modes at 301 cm^{-1} and at 362 cm^{-1} observed. Comparison was made with lattice dynamical calculations.

KFM 3.6 Mon 10:45 H16

Ferroelectric hafnium oxide-based multiferroic bilayers for magnetoelectric spin-orbit devices — •Maximilian Lederer, Johannes Hertel, Christoph Durner, Tatiana Gurieva, and Benjamin Lilienthal-Uhlig — Fraunhofer IPMS, Center Nanoelectronic Technologies, Dresden, Germany

This study investigates multiferroic heterostructures comprising $Hf_{0.5}Zr_{0.5}O_2$ (HZO) with Co/Pt top and TiN bottom electrodes on Si substrates. Using advanced deposition techniques, sub-nanometric thin films were fabricated. The research highlights achieving both ferroelectricity and perpendicular magnetic anisotropy simultaneously through a two-step annealing process. These properties are crucial for magnetoelectric spin-orbit (MESO) devices, which offer significant advantages such as lower power consumption and enhanced data storage capabilities. Insights into crystallization and diffusion processes were gained through various structural investigation methods. Additionally, the study demonstrates the manipulation of magnetic and ferroelectric domains using different microscopy techniques, underscoring the potential of MESO devices in next-generation electronic applications.

15 min. break

KFM 3.7 Mon 11:15 H16

Internal fields at the V-sites and magnetic structure of the lacunar spinel GeV_4S_8 — •Thomas Gimpel[1], Norbert Büttgen[1], Hiroyuki Nakamura[2], Vladimir Tsurkan[1], and István Kézsmárki[1] — [1]University of Augsburg — [2]Graduate School of Engineering, Kyoto

GeV_4S_8 is a multiferroic lacunar spinel that undergoes both structural (T_{JT}=30 K) and magnetic (T_N=13 K) transitions upon which the four V-sites of the V_4 tetrahedra that are equivalent in the cubic phase transform into three distinct sets of V-sites with zero-field ^{51}V NMR frequencies of 21.7, 53.6 and 65.6 MHz. This indicates that only two V-sites have the same internal magnetic field, while the other two have different ones. Based on the angular dependence of the resonance field upon the rotation of the field, we conclude that the direction of the internal field is common for the four V-sites and is parallel to one of the cubic [110]-type axes, which indicates that the magnetic space group is $Pmn2_1$.

KFM 3.8 Mon 11:30 H16

Fast control of antiferromagnetic domains via pulsed electric fields in Co_3O_4 — •Isabel Täuber, Maximilian Winkler, Somnath Ghara, Lilian Prodan, and Istvan Kezsmarki — Universität Augsburg, Deutschland

Co_3O_4 shows the linear magnetoelectric effect below the Neel-temperature of 30K, with a large magnetoelectric coefficient of 14 ps/m. Besides the typical control of the AFM state by colling with electric and magnetic fields across TN, the domains can be switched by voltage pulses as short as a few ns far below the transition temperature. To improve the application ability, we focus on switching of thin films of Co_3O_4 single crystals, paving the way for the next generation of spintronics.

KFM 3.9 Mon 11:45 H16

Anomalously strong magnetoelectric coupling in hexaferrite films — •Jakub Vít[1], Kwang-Tak Kim[2], Hyunju Hwang[2], Radomír Kužel[3], Milan Dopita[3], Darina Smržová[4], Kee Hoon Kim[2], and Josef Buršík[4] — [1]Institute of Physics, Czech Academy of Sciences, Czechia — [2]Center for Novel States of Complex Materials Research, Seoul National University, Korea — [3]Faculty of Mathematics and Physics, Charles University, Czechia — [4]Institute of Inorganic Chemistry, Czech Academy of Sciences, Czechia

Bulk hexaferrites are well known to exhibit strong magnetoelectric (ME) effects, often extending up to room temperature. In contrast, ME properties of hexaferrite films have been investigated only in a single recent study: In Z-hexaferrite films, the ME effect was found significantly stronger than in a crystal. [1] We continued this research by studying Y-hexaferrite films $Ba_{2-x}Sr_xCo_2Fe_{11.1}Al_{0.9}O_{22}$ on $SrTiO_3$ (111), grown by chemical solution deposition. For x=1, the magnetic-field-induced polarization reached 6.5 mC/m^2 at 10 K , i.e. 10x more than in the Z-hexaferrite films [1] and 50x more than in Y-hexaferrite crystals. [2] To elucidate these intriguing observations, microstructure of the films was studied in detail by real (SEM, TEM) and reciprocal (XRD) space techniques. Possible influence of the substrate on ME measurements was also taken into account.

[1] K. Shin et al., *Adv. Electron. Mater.* 2101294, (2022) [2] C. B. Park, et al., *Phys. Rev. Mater.* **5**, 034412 (2021)

KFM 3.10 Mon 12:00 H16

Higher-order Magnetizations of Non-centrosymmetric Antiferromagnets — •Michael Paulsen[1], Silvia Knappe-Grüneberg[1], Jens Voigt[1], Allard Schnabel[1], Rainer Körber[1], Michael Fechner[2], Ivan Ushakov[3], and Dennis Meier[3] — [1]Physikalisch-Technische Bundesanstalt, Berlin, Germany — [2]Max Planck Institute for the Structure and Dynamics of Matter, CFEL, Hamburg, Germany — [3]NTNU Norwegian University of Science and Technology, Trondheim, Norway

Antiferromagnetic materials lack macroscopic magnetic dipole fields, due to their compensated magnetic spin texture. In his seminal work, Dzyaloshinskii predicted that higher-order magnetization contributions arise in non-centrosymmetric antiferromagnets, in particular quadrupolar magnetic field contributions, and first experimental data suggested the presence of such fields in the antiferromagnetic model system Cr_2O_3. Here, we present calculations and measurements gained at cryogenic and room temperature using Superconducting Quantum Interference Devices (SQUIDs) and Optically Pumped Magnetometers (OPMs) setups, respectively, in ultra-low magnetic field environments. The results demonstrate the existence of quadrupolar far-fields and characteristic signatures in different classes of antiferromagnets. Importantly, our SQUID-based approaches are universal and can be applied to a wide range of systems, establishing new methods for characterizing materials with ultra-small magnetic remanence in general.

KFM 4: (Multi)ferroic States: From Fundamentals to Applications (II)

This focus session explores the intricate properties of (multi)ferroic states, spanning from fundamental understanding to cutting-edge applications. Topics include the design and control of (multi)ferroic states and domain structures at interfaces, domain walls, and in heterostructures. Emphasis will be placed on theoretical models, advanced characterization techniques, and the engineering of emergent properties for use in nano-electronic devices.

Chair: Nives Strkalj (Institute of Physics, Zagreb)

Time: Monday 11:30–13:00 Location: H9

KFM 4.1 Mon 11:30 H9

Oersted Mapping of Current Flow in Ferrorelectric Domain Walls with a Single-spin Magnetometer — •James Dalzell, Conor McCluskey, Marty Gregg, and Amit Kumar — Queen's University Belfast

Nitrogen vacancy (NV) [1] based magnetometers offer outstanding sensitivity for detecting static or dynamic magnetic fields at the nanoscale. As a result, this technique can be employed to evaluate current flow in materials with complex topologies and microstructures through direct measurement of the Oersted fields generated along any current pathways [2]. This creates an opportunity to evaluate fundamental aspects of electron transport in conducting ferroelectric domain walls, employed recently in lab-level ephemeral transistors and neuromorphic domain-wall based computing. We exploit the capability of the NV-AFM system to measure the current density along conducting domain walls in erbium manganite. By integrating high field sensitivity with exceptional spatial resolution, NV-based Oersted mapping has been shown to potentially offer a non-invasive approach to characterizing current flow in ferroelectrics. This advancement paves the way for a deeper understanding of electron transport phenomena in ferroelectric systems with current densities >1x104A/cm2, with improvements capable of being achieved by following pulse probe methods.

[1] Rondin, L. et al, Rep.Prog.Phys. 77 056503,(2014) [2] Tetienne, Jean-Philippe. et al, Sci. Adv. 3, e1602429 (2017). [3] Broadway,D.A, et al, Physics Review Applied 14(2) (2020).

KFM 4.2 Mon 11:45 H9

Transport behavior at domain walls in a depleted ferroelectric semiconductor — •Jiali He[1], Ruben Dragland[1], Leonie Richarz[1], Zewu Yan[2,3], Edith Bourret[3], Gustau Catalan[4,5], and Dennis Meier[1] — [1]NTNU Norwegian University of Science and Technology — [2]ETH Zurich, Switzerland — [3]Lawrence Berkeley National Laboratory, USA — [4]Institut Català de Nanociencia i Nanotecnologia (ICN2), Spain — [5]Institucio Catalana de Recerca i Estudis Avançats (ICREA), Spain

Electronic depletion regions naturally form at metal-semiconductor interface, which enables control of electrical currents in pn-junctions and is widely used in CMOS technology. Here, we expand the research towards ferroelectric domain walls, studying their functional properties under electronic depletion. Using ferroelectric p-type semiconductor $ErMnO_3$ as the model system, we deposit W electrodes and systematically investigate changes in the local transport behavior as the material is thinned down to the sub-10 nm range. Combined imaging experiments in terms of scanning electron microscopy (SEM) and scanning probe microscopy (SPM) reveal that for a critical thickness, t_c, a step-like drop occurs in the electronic conduction, which we associate with the width of the depletion region at the $W/ErMnO_3$ interface. Interestingly, ferroelectric domain walls within the depletion region exhibit qualitatively different transport behavior than in the p-type regions. Our results give new insight into the physics of domain walls and demonstrate additional opportunities for controlling their electronic responses, which is of interest for domain-wall-based electronics.

KFM 4.3 Mon 12:00 H9

Domain and domain wall conductance in the vicinity of metal-semiconductor contacts — •Ruben Dragland[1], Leonie Richarz[1], Ingvild Hansen[1], Manuel Zahn[1], Jiali He[1], Zewu Yan[2], Edith Bourret[2], Mario Hentschel[3], and Dennis Meier[1] — [1]NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]Lawrence Berkeley National Laboratory, Berkeley, CA,USA — [3]University of Stuttgart, Stuttgart, Germany

Ferroelectric domain walls hold promise as functional quasi-2D systems and are intensively studied as key electronic elements for next-generation nanotechnology. Despite their outstanding application potential, however, little is known about the performance in actual device geometries and the contact phenomena that co-determine the current injection. In this study, we perform a systematic analysis of the local transport behavior of the ferroelectric semiconductor $ErMnO_3$ in the vicinity of different electrode materials. By applying electron beam lithography and evaporation, we design metal-semiconductor contacts with varying work functions and investigate the impact on the electronic conductance and respective barrier formation. Combining conductive atomic force microscopy (cAFM), Kelvin probe force microscopy (KPFM), as well as mesoscopic probe techniques, we correlate the band bending at the interface to the measured conductance of domains and domain walls. Our results are relevant for the integration of ferroelectric domain walls and the understanding of the nanoscale physics at metal-semiconductor junctions in ferroelectrics in general.

KFM 4.4 Mon 12:15 H9

Exploring ferroelectric oxides for reservoir computing — •Yan Meng Chong[1], Atreya Majumdar[2], Ingvild Hansen[1], Karin Everschor-Sitte[2], and Dennis Meier[1] — [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

In reservoir computing, input data is 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 or fading memory, and reproducibility can serve as reservoir. Here, we investigate ferroelectric semiconductor $ErMnO_3$ as 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) used for readout, determining the timescale on which photocurrents vanish after illumination. This relaxation behavior in the OFF state gives the fading memory. We perform training for recognition on variations in the output (photocurrent), which allows for reconstructing the sequential input (light pulses). Interestingly, both ferroelectric domains and domain walls can be used as reservoirs with characteristic photocurrent signals, giving new opportunities for downscaling or enhancing the complexity of physical reservoirs.

KFM 4.5 Mon 12:30 H9

Coupling between small polarons and ferroelectricity in $BaTiO_3$ — •Darin Joseph[1] and Cesare Franchini[1,2] — [1]Dipartimento di Fisica e Astronomia, Università di Bologna, 40127 Bologna, Italy — [2]University of Vienna, Faculty of Physics, Center for Computational Materials Science, Vienna, Austria

Ferroelectric properties of materials are found to be modified upon polaron formation. In this study, we investigate the formation of electron and hole small polarons in the prototypical ferroelectric material barium titanate ($BaTiO_3$), with a focus on their interaction with ferroelectric distortive fields. To accurately describe the ferroelectric phase in $BaTiO_3$, we employ the HSE06 hybrid functional, which addresses the limitations of conventional DFT and DFT+U models, providing a more precise depiction of both ferroelectric and polaronic behaviours. Our analysis spans three structural phases of $BaTiO_3$: cubic, tetragonal, and rhombohedral. We uncover a phase-dependent trend in electron polaron stability, which progressively increases across the structural phases, peaking in the rhombohedral phase due to the constructive coupling between the polaron and ferroelectric phonon fields. In contrast, hole polarons exhibit a stability pattern largely unaffected by the phase transitions. Furthermore, we observe that polaron self-trapping significantly alters the local ferroelectric distortive pattern, which propagates to neighbouring sites but has a minimal effect on the long-range macroscopic spontaneous polarization. Charge trapping is also associated with localized spin formation, opening new possibilities for enhanced functionalities in multiferroic materials.

KFM 4.6 Mon 12:45 H9

Energy barriers for small electron polaron hopping in bismuth ferrite from first principles — •Sabine Körbel[1,2] and Harini Priyanka Shanmugasundharam Swaminathan[2,3] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena — [2]Institute of Condensed Matter Theory and Optics, Friedrich Schiller University, Fürstengraben 1, 07743 Jena, Germany — [3]University of Applied Sciences Jena, Carl-Zeiss-Promenade 2, 07745 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 transport could occur by hopping of small electron polarons rather than by band-like transport. Here, by means of first-principles calculations, small electron polaron hopping in $BiFeO_3$ was investigated. Both bulk $BiFeO_3$ and a typical ferroelectric domain wall, the neutral 71° domain wall, were considered. The latter was included to account for experimental observations of currents that appear to be localized within domain-wall planes. The object of this study is to shed light on the intrinsic n-type conduction mechanism in rhombohedral $BiFeO_3$ and the role of the ferroelectric domain walls in electrical conductivity. Based on the computed energy barriers for small electron polaron hopping, the intrinsic n-type mobility in bulk $BiFeO_3$ and at 71° domain walls is estimated.

KFM 5: Instrumentation, Microscopy and Tomography with X-ray Photons, Electrons, Ions and Positrons

Chair: Theo Scherer (Karlsruhe Institute of Technology)

Time: Monday 15:00–17:00 Location: H9

KFM 5.1 Mon 15:00 H9

Simulation study of beam splitting of vortex electron beams inside crystals — •Christian Bick and Dorothee Hüser — Physikalisch-Technische Bundesanstalt, Braunschweig, Germany

Electron vortex beams have long been of interest for applications such as electron magnetic circular dichroism (EMCD), beam shaping and nanoparticle manipulation. They have attracted new attention with the recent development of an orbital angular momentum (OAM) sorter, theoretical developments in analysis of momentum transfer and as a quantum logic gate.

When propagating through a crystal, the vortex electron wave interacts with the asymmetric crystal potential, causing the wave to split into intensity centres around atomic columns, called channelling. This behaviour gives rise to a total OAM that can no longer be described by an integer vortex quantum number. In this simulation-based study we track the behaviour of electron beams inside different crystals. We show an in-depth analysis of the wave phase propagating through the crystal for different materials, focussing our research on beam splitting into intensity centres with their own OAM. This study was carried out using multislice simulations of the electron beam propagation through the crystal potential together with vector analysis to identify the local vortex centres.

KFM 5.2 Mon 15:15 H9

Single-phase valence band structure of a $Ge_{0.85}Si_{0.15}$ Crystal - Insights by momentum microscopy — •Andreas Fuhrberg[1], Pia M. Düring[1], Kevin Gradwohl[2], Olena Fedchenko[3], Yaryna Lytvynenko[3], Olena Tkach[3], Sergii Chernov[4], Christoph Schlueter[4], Gerd Schönhense[3], Hans-Joachim Elmers[3], and Martina Müller[1] — [1]Universität Konstanz — [2]IKZ, Berlin — [3]Universität Mainz — [4]DESY, Hamburg

Spin qubits are the fundamental components of quantum computing devices. Planar $Ge/Ge_{1-x}Si_x$ heterostructure qubits have proven to be advantageous for upscaling and fabrication. The Si concentration of the $Ge_{1-x}Si_x$ buffer has been shown to be an important parameter for tuning the valence band (VB) electronic structure of $Ge/Ge_{1-x}Si_x$ qubits by homoepitaxial strain, which is difficult to realize experimentally without phase separation.

Synchrotron-based hard X-ray momentum microscopy (MM) is used to study the VB electronic structure of a $Ge_{0.85}Si_{0.15}$ single crystal grown to provide well-defined small strain. Our MM experiments reveal an individual VB structure of $Ge_{0.85}Si_{0.15}$, that is clearly distinct from Si and Ge references. The shape of the heavy/light hole band and split-off band follows that of Ge, but with lower binding energies at Γ, X and L points and a reduced split-off band gap, hence no evidence for phase separation. Additional diffraction experiments, supported by Bloch wave calculations, show that the Si atoms occupy Ge lattice positions within the crystal. This result is very promising for the future experimental realization of single-phase GeSi-based spin qubits.

KFM 5.3 Mon 15:30 H9

Miniature device for in situ application of strain inside Scanning Tunnelling Microscope — •Uladzislau Mikhailau, Rashed Alhamli, and Peter Wahl — University of St Andrews, St Andrews, United Kingdom

Recent studies [1] have demonstrated that uniaxial strain significantly affects the macroscopic properties of strongly correlated electron systems. Scanning Tunneling Microscopy (STM) is a powerful technique for investigating changes in the electronic structure induced by such lattice deformation. Controlled application of strain adds an additional degree of freedom to tune, e.g., Van Hove singularities in quantum materials [2] and thereby control their ground state. To perform such studies, we have developed a specialized STM sample holder capable of applying strain at cryogenic temperatures and in high magnetic fields. Strain is applied by bending a plate beneath the sample, with stress adjustable up to the crystal's buckling limit. The device allows for the application of uniaxial or biaxial strain, depending on the configuration of the bending plate. With these capabilities, the system provides a versatile platform for exploring strain-induced phenomena through a powerful combination of atomic scale imaging in strain tuning.

[1] Clifford W. Hicks et al., Strong Increase of T_c of Sr_2RuO_4, Under Both Tensile and Compressive Strain. Science 344, 283 (2014).

[2] Chandrasekaran, A., Rhodes, L.C., Morales, E.A. et al. On the engineering of higher-order Van Hove singularities in two dimensions. Nat Commun 15, 9521 (2024).

KFM 5.4 Mon 15:45 H9

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

Since the early days of positron lifetime spectroscopy, the meaningful decomposition of lifetime spectra into two or more components has been highly disputed. This procedure is extremely important to extract correct defect densities. Since the procedure of fitting several exponential decays folded by a mimicked instrumental resolution function to extract positron lifetimes and intensities is an "ill-posed problem", the goodness of the fit relies heavily on the quality of the recorded data. In the past there have been several simulation attempts to create and decompose spectra into two or three components (lifetimes and intensities). However, those attempts always assumed "ideal", random number Monte Carlo simulated data. Hence, the following data analysis has been fairly straight forward. By our recently developed digital twin of a positron lifetime spectrometer we could clearly see the strong influence of back scattered and corrupted coincidences on the lifetime spectrum. Unfortunately, those events cannot be removed by physically filtering digitised pulses. Changes in the geometry of the set-up lead to much more realistic bulk positron lifetimes of light materials (Mg, Al, Si) in accordance with calculations and correct decompositions in accordance with the trapping model, while the efficiency is reduced by 95%.

15 min. break

KFM 5.5 Mon 16:15 H9

Investigating Mechanical Properties of Porous Materials with Brillouin Light Scattering and Machine-Learned Force Fields — •Florian Lindner[1], Nina Strasser[1], Sandro Wieser[2], Egbert Zojer[1], and Caterina Czibula[3] — [1]Institute of Solid State Physics, Graz University of Technology, Austria — [2]Institute of Materials Chemistry, TU Wien, Austria — [3]Institute of Bioproducts and Paper Technology, Graz University of Technology, Austria

Brillouin light scattering (BLS) is based on the inelastic scattering of light from thermally activated gigahertz acoustic phonons. As the later are correlated with a material's elastic tensor via the Christoffel dispersion the elastic constants can be determined in a non-destructive and contactless manner. From these, practically relevant mechanical properties like the Young's modulus can be derived. In this contribution we show, how BLS can be used to study the mechanical properties of metal organic frameworks (MOFs), a class of porous crystalline materials with a plethora of possible applications. The measured mechanical properties are then compared to state-of-the-art dispersion corrected DFT calculations and simulations based on machine learned interatomic potentials [1], which speed up simulations by many orders of magnitude [2]. This allows to additionally determine thermoelastic properties of MOFs at elevated temperatures, which in combination with suitable experiments will portray the full potential of the used methodology.

[1] arXiv:2409.07039 (submitted to JPCL, currently under review); [2] npj Comput Mater 10, 18 (2024);

KFM 5.6 Mon 16:30 H9

TwinPALS: A Digital Twin for Laboratory-Based Positron Annihilation Lifetime Spectroscopy — •Dominik Boras — Julius-Maximilians University, Würzburg, Germany

In this work, we present a comprehensive digital twin of a laboratory-based Positron Annihilation Lifetime Spectroscopy (PALS) system. This digital twin is capable of simulating entire spectra while incorporating all effects of the hardware used in the PALS system, as well as varying source strengths. For the first time, it is possible to visualize unwanted components within the lifetime spectrum and assess their impact on the interpretability of these spectra. The digital twin enables the identification of issues within one's own setup and allows for digital testing of potential optimizations before physical implementation. The TwinPALS system is designed in a modular structure. The first module is responsible for constructing the digital world, taking into account the influences of position, dimension, and the materials used. The second module combines a customized version of the DLTPulsgenerator with software to process the information from the first module, incorporating considerations of radioactivity, positron lifetime, and PMT blurring. The third and final module serves to visualize the output stream from the second module, utilizing the DDRS4PALS software. In summary, this system is a modular digital twin that can be adapted to the requirements of the system being simulated.

KFM 5.7 Mon 16:45 H9

TwinPALS: A digital Twin for laboratory-based Positron Annihilation Lifetime Spectroscopy — •Dominik Boras, Danny Petschke, and Torsten Staab — LCTM / IFB, Department of Chemistry, University of Wuerzburg, Roentgenring 11, D-97070 Wuerzburg, Germany

In this work, we present a comprehensive digital twin of a laboratory-based Positron Annihilation Lifetime Spectroscopy (PALS) system. This digital twin is capable of simulating entire spectra while incorporating all effects of the hardware used in the PALS system, as well as varying source strengths. For the first time, it is possible to visualize unwanted components within the lifetime spectrum and assess their impact on the interpretability of these spectra. The digital twin enables the identification of issues within one's own setup and allows for digital testing of potential optimizations before physical implementation. Additionally, this approach facilitates the validation of software-based physical filters and provides a unique opportunity to visualize their effects on unwanted components in the spectra. The digital twin represents a comprehensive simulation framework that allows for a multitude of hardware investigations in the digital realm, effectively functioning as a digital mirror of the complete hardware setup. This enables researchers to conduct extensive, risk free experiments and optimize system configurations, ultimately improving the quality and reliability of PALS data.

KFM 6: Invited Talk: X. Fang (joint session MM/KFM)

Time: Monday 15:00–15:30 Location: H10

Invited Talk KFM 6.1 Mon 15:00 H10

Room-temperature dislocations in oxide ceramics: from understanding to active engineering — •Xufei Fang — Institute for Applied Materials, Karlsruhe Institute of Technology, Karlsruhe, Germany

In the conventional picture, dislocations are most relevant for metals while ceramics are considered brittle and exhibit little or no plasticity at room temperature. However, recent years' research on dislocations in ceramics suggests that dislocations may have been much under-appreciated in ceramics. Proofs-of-concept for dislocation-tuned functional properties suggest that dislocations may hold great technological potential in advanced ceramics. As the prerequisite to harvest dislocation-tuned properties, engineering dislocations into ceramics without brittle fracture has thus become a pressing bottleneck. To tackle this challenge, we have separately examined the dislocation behavior including dislocation nucleation, multiplication and motion, enabling us to tune dislocations into ceramic oxides at room temperature. We can now achieve a dislocation density up to ~10^15/m^2 with a plastic zone size of up to milli-/centimetres using a mechanical deformation toolbox. We further extend the material toolbox by discovering and reporting more oxide perovskites that can be plastically deformed at room temperature across the length scale. The combined deformation and material toolboxes offer a new platform for studying the dislocation-tuned functional properties (e.g., electrical and thermal conductivity) and the mechanical properties (such as plasticity, toughness, and damage tolerance) over a wide range of length scales.

KFM 7: Materials for the Storage and Conversion of Energy (joint session MM/KFM)

Lithium-based Materials

Time: Monday 17:15–18:30 Location: H22

KFM 7.1 Mon 17:15 H22

Lithium diffusion pathways in modern solid state Li conductors — •Mykhaylo Monchak[1], Volodymyr Baran[2], Stefan Strangmüller[3], and Anatoliy Senyshyn[3] — [1]Institut für Angewandte Materialien, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [2]Deutsches Elektronen Synchrotron, 22607 Hamburg, Germany — [3]Heinz Maier-Leibnitz Zentrum, Technical University of Munich, 85748 Garching, Germany

The rapid development of energy storage demands cheaper, more robust electrode and electrolyte materials with improved electrochemical performance. Energy storage and conversion primarily rely on diffusion-based processes, making understanding diffusion pathways crucial. However, determining diffusion pathways in polycrystalline (non-cubic) materials is challenging using bulk or local measurements. Theoretical approaches like molecular dynamics simulations face numerous computational limitations. Alternatively, diffusion processes can be predicted from crystal structures using scattering density maps (electron for X-ray or nuclear for neutrons). These maps analyzed via probability density functions or reconstructed through the maximum entropy method (MEM) are highly reliable. MEM is particularly effective for powder-averaged diffraction data, detecting weak structural disorders. This study applies high-resolution neutron powder diffraction and MEM analysis to explore state-of-the-art lithium conductors considered for application in all-solid-state Li-ion batteries, providing insights into their diffusion pathways and systematics.

KFM 7.2 Mon 17:30 H22

"Effortless Embedding": Non-Parametric Solid-State Embedding for NMR Computations using All-Electron DFT — •Federico Civaia[1], Simone S. Köcher[2,1], Karsten Reuter[1], and Christoph Scheurer[1,2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Institute of Energy Technologies (IET-1), Forschungszentrum Jülich GmbH, Jülich

Solid-state electrolytes are crucial in lithium-ion battery research, because of the pressing need for safe and durable high-energy storage solutions. Understanding Li-ion dynamics in these materials is essential for developing improved battery technologies. Owing to its non-destructive nature and sensitivity to atomic environments, solid-state nuclear magnetic resonance (SS-NMR) spectroscopy has become an invaluable tool for probing diverse Li-ion environments and investigating Li-ion mobility.

To facilitate the interpretation of experimental Li SS-NMR spectra, we are developing a method for computing NMR parameters of diamagnetic Li compounds using the linear-scaling, all-electron, density functional theory code FermiONs++ [1]. To allow the description of both crystalline and disordered materials, we employ a SS embedding method. In this regard, we present a consistent, non-parametric hybrid Quantum Mechanics/Molecular Mechanics (QM/MM) methodology for systematic and reproducible structure generation and SS embedding calculations.

[1] J. Kussman *et al.*, J. Chem. Phys. **138**, 134114 (2013); J. Chem. Theory Comput. **11**, 918 (2015).

KFM 7.3 Mon 17:45 H22

Insights into Li-ion battery cathode redox chemistry via charge transfer multiplet simulations of $\mathbf{LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2}$ — •Ruiwen Xie[1], Maximilian Mellin[2], Wolfram Jaegermann[2], Jan. P Hofmann[2], and Hongbin Zhang[1] — [1]Theory of Magnetic Materials Group, Department of Materials and Geosciences, Technical University of Darmstadt — [2]Surface Science Laboratory, Department of Materials and Geosciences, Technical University of Darmstadt

The evolution of electronic structure during discharging and charging processes with Li intercalation and deintercalation in transition metal oxide cathode materials involves changes in oxidation states, non-rigid band behavior, and oxygen's role in charge compensation, which significantly impact cathode performance. To gain deeper insights, we combine experimental x-ray photoelectron spectroscopy (XPS) at various voltages with many-body electronic structure simulations. The electronic structures of $\mathrm{Li}_x\mathrm{CoO}_2$ and $\mathrm{Li}_x\mathrm{NiO}_2$ were calculated using Density Functional Theory and Dynamical Mean-Field Theory (DFT+DMFT). We found that Li intercalation and deintercalation shift the hybridization between Co/Ni d and O p orbitals relative to the Fermi energy, altering Co/Ni d occupancy. Based on this, we performed XPS calculations using the multiplet ligand-field model in Quanty to revisit the transition metal 2p satellite structure evolution. This study provides crucial insights into the interplay between electronic structure and Li intercalation dynamics for enhancing cathode performance.

KFM 7.4 Mon 18:00 H22

Modelling LLZO Grain Boundaries with Amorphous Domains by Adaptively Trained Machine-Learning Interatomic Potentials — •Yuandong Wang, Yute Chan, Hao Wan, Kyeonghyeon Nam, Karsten Reuter, and Christoph Scheurer — Fritz-Haber-Institut der MPG, Berlin

Garnet $\mathrm{Li_7La_3Zr_2O_{12}}$ (LLZO) is a highly promising solid state electrolyte (SSE) for lithium batteries. However, its practical application faces challenges, primarily arising from Li dendrite formation and the impact of grain boundaries (GBs) on Li transport and stability. Amorphous LLZO combines several desirable properties like blocking Li dendrite growth, high Li mobility and high electronic impedance. Controlling amorphous domains between crystalline grains could therefore offer an intriguing approach to tune electrolyte performance. For this, an atomistic understanding of the interplay between composition, structure and the properties of LLZO glass-ceramics is crucial.

This study introduces a Machine Learning Interatomic Potential (MLIP) tailored to accurately represent amorphous and GB structures in LLZO. Developed through an iterative training protocol using simulated annealing, this MLIP includes diverse structures in its training set, ensuring comprehensive modeling of complex LLZO phases. The MLIP enables large-scale molecular dynamics simulations, allowing the construction of realistic amorphous and GB models, and providing a foundation for in-depth analysis of LLZO structural and electrochemical behavior.

KFM 7.5 Mon 18:15 H22

Early Stage of Li Cluster Nucleation at the Li Anode-Solid Electrolyte Interface in Solid-State Batteries — •Yun An[1,2], Taiping Hu[2], Quanquan Pang[2], and Shenzhen Xu[2] — [1]Fritz-Haber- Institut der MPG, Berlin, Germany — [2]School of Materials Science and Engineering, Peking University, Beijing, China

Li dendrite formation inside all-solid-state lithium batteries (ASSBs) strongly impedes their practical applications. Despite this recognized challenge, a comprehensive understanding of the Li dendrite nucleation mechanism remains elusive. In particular, the initial sites of Li dendrite formation are still ambiguous: do Li clusters form directly at the Li anode surface, or do they nucleate at a distance from the Li metal surface?

Here, based on deep-potential molecular dynamics simulations combined with enhanced sampling techniques, we investigate the atomic-level mechanism of Li cluster nucleation sites in ASSBs. We observe isolated Li clusters initially forming inside the solid electrolyte interphase (SEI), located approximately 1 nm away from the Li anode/SEI boundary, rather than directly connected to the Li anode. The local electronic structure of the spontaneously formed SEI is a key factor enabling the Li cluster formation within SEI. Our work provides atomic-level insights into initial Li-dendrite nucleation sites in ASSBs and could guide future design for developing Li-dendrite-inhibiting strategies.

KFM 8: (Multi)ferroic States: From Fundamentals to Applications (III)

This focus session explores the intricate properties of (multi)ferroic states, spanning from fundamental understanding to cutting-edge applications. Topics include the design and control of (multi)ferroic states and domain structures at interfaces, domain walls, and in heterostructures. Emphasis will be placed on theoretical models, advanced characterization techniques, and the engineering of emergent properties for use in nano-electronic devices.

Chair: Morgan Trassin (ETH Zurich)

Time: Tuesday 9:30–11:30 Location: H9

Invited Talk KFM 8.1 Tue 9:30 H9

Ferrolectric bubble currents — •Hugo Aramberri — Luxembourg Institute of Science and Technology

Frustrated ferroelectrics can display complex dipole textures displaying rich physical phenomena. In ferroelectric/paraelectric superlattices, built-in or applied electric fields can result in bubble domains of nanometric size akin to magnetic skyrmions.

Our atomistic calculations predict these bubbles to be quasiparticles that display thermally activated Brownian motion, enabling the conceptualization of some of the all-electric unconventional computing schemes that have already been developed for their magnetic counterparts.

However, control over the bubble motion, which is key for many potential technological applications, is still essentially lacking. In this talk I will present our latest ideas to induce bubble currents. Our simulations indicate that bubbles can be accelerated up to at least 50 m/s in the absence of electric currents, which holds the promise of a competitive alternative to magnetic skyrmion-based technologies.

KFM 8.2 Tue 10:00 H9

Exploring (110) epitaxial strain in ferroelectric films and superlattices — •Lan-Tien Hsu, Chien-Wen Hao, and Anna Grünebohm — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS) and Center for Interface-Dominated High Performance Materials (ZGH), Ruhr-University Bochum, Universitätsstr. 150, 44801 Bochum, Germany

Epitaxial strain in low-symmetry orientations significantly influences the phase stability and polarization orientation of ferroelectric thin films and superlattices,[1] offering the potential for advanced nanoelectronic applications.[2] We explore the phase diagrams of (110)-oriented $BaTiO_3$, $KNbO_3$, and superlattice $BaTiO_3/SrTiO_3$ under strain and electric field using ab initio based coarse-grained molecular dynamics.[3] We reveal how the epitaxial (110) strain affects polarization, transition temperatures, and the emergence of topological features. Complex multidomain structures appear, particularly in superlattices due to depolarization fields.

[1] Das *et al*, Nature **568**, 368-372 (2019)

[2] Grünebohm *et al*, J.Phys.:Condens.Matter **34**, 073002 (2021)

[3] Nishimatsu *et al*, Phys. Rev. B **78**, 104104 (2008)

KFM 8.3 Tue 10:15 H9

Vortex dynamics in incommensurate 2D and 3D bulk ferroics — •Aaron Merlin Müller[1], Quintin Meier[2], Andrés Cano[2], Manfred Fiebig[1], and Thomas Lottermoser[1] — [1]Department of Materials, ETH Zurich, 8093 Zurich, Switzerland — [2]Univ. Grenoble Alpes, CNRS, Grenoble INP, Institut Néel, 25 Rue des Martyrs, 38042, Grenoble, France

We reveal that in 3D ferroic systems with competing incommensurate stripe phases of ferroic order and topological defects in the form of vortex lines, these vortex lines exhibit fundamentally different dynamics compared to their 2D counterparts. We show that loops of vortex lines can exhibit long relaxation times resulting from their positioning at saddle points in the energy landscape. Using phase-field simulations and analytical approaches, we demonstrate that the distinctive relaxation behavior in 3D systems arises from the interplay between dimensionality and the energy landscape of incommensurate stripe phases. Many ferroically ordered materials, such as hexagonal manganites and planar spin systems, feature periodic order parameters that support such competing orders. Hence, we employ a general model of two-component ferroic order whose findings generalize to all ferroic systems that exhibit vortices and incommensurate stripe phases. We analyze the dynamics of topological defects during the transition from inhomogeneous order without stripes to an incommensurate stripe phase in both 2D and 3D systems. We conclude by discussing the critical role of dimensionality in shaping the system's energy landscape and broader implications for ferroic systems.

KFM 8.4 Tue 10:30 H9

Valence bond solid states in IrTe2 — •Sergey Artyukhin[1], Francesco Foggetti[2], and Daniel Khomskii[3] — [1]Italian Institute of Technology — [2]Uppsala University — [3]University of Cologne

We study the phase diagram of IrTe2. This material manifests, below 280 K, a sequence of states where some Ir-Ir bonds shorten forming dimers, which results in a striped order. Ab-initio calculations suggest that the total energy is decreasing approximately linearly with the dimer fraction for the previously observed phases. The phonon density of states is shifted to higher frequencies, into the dimer-localized phonon bands. We describe the interactions between dimers using the force constant matrix from ab-initio calculations, and find features, similar to those driving striped orders in orthorhombic manganites. The strain texture is consistent with the observed striped orders. A simplified model, based on dimer energetics and phonon entropy, is formulated and the phase diagram of IrTe2 is obtained.

KFM 8.5 Tue 10:45 H9

Ultrafast control of interlayer ferroelectricity in h-BN — •Pooja Rani and Dominik M. Juraschek — Eindhoven University of Technology, Eindhoven, Netherlands

Two-dimensional ferroelectrics in nanoscale systems have received increasing interest due to their potential applications in the areas of memory storage and sensing. Among these materials, bilayer hexagonal boron nitride (h-BN) is a promising material for studying interlayer ferroelectricity because of its out-of-plane polarization that can be reversed by changing the stacking order. Using the first-principles simulation, we investigate the theoretical aspects of ultrafast control of interlayer ferroelectricity in h-BN to determine how the polarization can switch by light-induced shear motion. This phononic sliding mechanism would be particularly favourable since it provides a potential way of modulating ferroelectric behaviour at the nanoscale, creating an entirely novel path for the development of tuneable ferroelectric materials. Specifically, we focus on the excitation of the high-energy degenerate modes by an ultrashort mid-infrared pulse coupled to the low-energy shear and out-of-plane modes. Our findings suggest that the shear modes can significantly enhance the ferroelectric polarisation in h-BN, and we explore whether the ferroelectricity can be switched through this mechanism. With this, observing how out-of-plane modes affect ferroelectric polarization or interlayer ferroelectricity in h-BN will be interesting.

KFM 8.6 Tue 11:00 H9

Phonon-induced multiferroicity — Carolina Paiva[1], Michael Fechner[2], and •Dominik Juraschek[3] — [1]Tel Aviv University, Tel Aviv, Israel — [2]Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany — [3]Eindhoven University of Technology, Eindhoven, Netherlands

A well-known mechanism for multiferroicity involves an electric polarization arising from a spatially varying magnetization, such as a spin spiral or cycloid. Reciprocally, optical phonons can produce a magnetization through a temporally varying electric polarization, an effect also known as dynamical multiferroicity. Here, we go a step beyond this phenomenon and describe a mechanism by which both a ferroelectric polarization and a magnetization can be created in nonpolar, nonmagnetic materials. Using a combination of phenomenological modeling and first-principles calculations, we demonstrate that a ferroelectric polarization, a magnetization, or both simultaneously can be transiently induced by an ultrashort laser pulse upon linearly, circularly, or elliptically polarized excitation of phonon modes in γ-$LiBO_2$. The direction and magnitude of the multiferroic polarization can be controlled by the chirality of the laser pulse and the phonon modes, offering a pathway for controlling multiferroicity and magnetoelectricity on ultrafast timescales.

KFM 8.7 Tue 11:15 H9

Ferroelectric and piezoelectric molecular crystals: From database mining to computational design — •Kristian Berland[1], Elin D. Sødahl[1], Seyedmojtaba Seyedraofi[1], Carl H Gørbitz[2], Ola Nilsen[2], Manjunath Balagopalan[2], Maxi Litterst[3], Martijn Kemerink[3], Jesus Carrete[4], Georg K. H. Madsen[4], Graeme Day[5], and Julian Walker[6] — [1]NMBU, Ås, Norway — [2]U. Oslo, Norway — [3]Heidelberg University, Heidelberg, Germany — [4]TU Wien, Vienna, Austria — [5]U. Southampton, UK — [6]NTNU, Trondheim, Norway

Molecular crystals offer great potential for piezoelectric and ferroelectric devices due to their vast chemical tuneability. Plastic (ionic) crystals hosts malleable orientationally disordered mesophases and their rotational freedom can yield high shear piezoelectric response[CrystGrowthDes. 2023, 23, 729]. Proton-transfer Making new crystals with desired properties, however, is not straightforward. We devised new tools to screen the Cambridge Structural Database (CSD), identifying 60 new potential ferroelectrics[PhysRevMaterials 8, 054413, 2024; CrystGrowthDes 2023, 23, 8607], 5 of which we have experimentally confirmed. Crystal structure prediction (CSP) was used to design additional ones [arXiv:2410.20481]. Finally, machine-learning force fields (MLFFs) can provide insight into dynamical properties of mesopphases [arXiv:2410.15746]. With these examples, I will argue how computational methods can be pivotal in advancing the field of small-molecule ferroic crystals.

KFM 9: (Multi)ferroic States: From Fundamentals to Applications (IV)

This focus session explores the intricate properties of (multi)ferroic states, spanning from fundamental understanding to cutting-edge applications. Topics include the design and control of (multi)ferroic states and domain structures at interfaces, domain walls, and in heterostructures. Emphasis will be placed on theoretical models, advanced characterization techniques, and the engineering of emergent properties for use in nano-electronic devices.

Chair: Morgan Trassin (ETH Zurich)

Time: Tuesday 11:45–13:00 Location: H9

KFM 9.1 Tue 11:45 H9

Investigating Self-Heating of Conducting Domain Walls Using Scanning Thermal Microscopy — •Lindsey Lynch, Kristina Holsgrove, Marty Gregg, and Raymond McQuaid — Queen's University Belfast

Domain walls (DWs) in ferroelectrics are an exciting category of reconfigurable functional interface, with properties that can differ from bulk. Lab-level transistor [1] and memristor devices [2] have been demonstrated, where functionality is derived entirely from electrically conducting DWs. Here, the DWs perform the equivalent role of conductive nanofilaments in metal-oxide resistive switching memories. While self-heating and local temperature are important factors in oxygen-vacancy based resistive switching [2,3], much less is known about the intrinsic self-heating of domain walls and its influence on device operation. We have been investigating the electrothermal properties of LiNbO3 domain wall devices using Scanning Thermal Microscopy (SThM). This involves using the scanning probe as a mobile nanoscale temperature sensor to map self-heating in domain wall devices. Temperature hot spots on the order of 10K are detected and PFM corroborates that their origin is due to sub-surface domain wall heating. Since heat spreading occurs within the surrounding ferroelectric film and top electrode, the measured surface temperatures likely represent a lower bound for the intrinsic rise in domain wall temperature.

[1] Nat. Commun. 11, 2811 (2020). [2] Adv. Funct. Mater. 30, 2000109 (2020). [3] Sci. Adv. 8, eabk1514 (2022). [4] ACS Appl. Mater. Interfaces 14, 29025 (2022).

KFM 9.2 Tue 12:00 H9

Thermoelectricity from domain wall formation in a polar metal — •Feifan Wang[1,2], Carl Romao[1], and Manfred Fiebig[1] — [1]Dept. of Materials, ETH Zurich, Switzerland — [2]Institute of Physics, Beijing 100190, China

Simultaneous optimization of the electronic and phononic properties of a thermoelectric material is essential to achieve a high thermoelectric performance. This has been realized in the polar metal compounds by making use of the high configurational entropy, Rashba effect and ferroelectric anharmonicity, tuned at the atomic level. What has been overlooked in this process is the role of macroscopic effect such as the role of domain and domain wall formation in further enhancing the thermoelectric performance. Using GeTe as a prototype, we show that microdomain formation determines the thermal conduction in the polar metal examined by the spatial correlation between the domain structure and the thermal conductivity. In particular, the thermal conductivity decreased by a factor of five following the appearance of the micro-sized antiparallel-aligned domains. Conductive force microscopy shows that the electrical conduction does not change in spite of the presence of domain discontinuities. This is in line with the band gap reduction and the electron–phonon decoupling from density-functional theory calculations. The direct visualization of the association between microdomain formation and thermal/electrical transport suggests the domain and domain wall engineering as a key ingredient in advancing polar-metal-based thermoelectrics.

KFM 9.3 Tue 12:15 H9

Hybrid ferroelectric-antiferroelectric 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 A. Hunnestad[1], Mohsen Sadeqi-Moqadam[1], Julia Glaum[1], Sverre M. Selbach[1], Joachim Hemberger[3], Petra Becker[3], Ladislav Bohaty[3], Amit Kumar[2], Antonius T. J. van Helvoort[1], and Dennis Meier[1] — [1]Norwegian University of Science and Technology — [2]Queen's University Belfast — [3]University of Cologne

Antiferroelectrics are emerging as advanced functional materials and are fertile ground for unusual electric effects. For example, they enhance the recoverable energy density in energy storage applications and give rise to large electromechanical responses. In my talk, I will present noncollinearity in dipolar order as an additional degree of freedom, unlocking physical properties that are symmetry-forbidden in classical antiferroelectrics. I will show that noncollinear order of electric dipole moments in $K_3[Nb_3O_6|(BO_3)_2]$ leads to a coexistence of ferroelectric and antiferroelectric behaviors. Besides the double-hysteresis loop observed in antiferroelectrics, a pronounced piezoresponse and electrically switchable domains are observed, separated by atomically sharp and micrometer-long charged domain walls. Similar hybrid ferroelectric-antiferroelectric responses are expected in a wide range of noncollinear systems, giving a new dimension to the research on antiferroelectrics and multifunctional oxides in general.

KFM 9.4 Tue 12:30 H9

Step sintering process on sol-gel synthetized Bi0.5Na0.5TiO3 for enhanced temperature stability of relaxor ferroelectric state and energy storage properties — •Thomas Fourgassie[1], Cécile Autret-Lambert[1,2], and Pierre-Eymeric Janolin[2] — [1]Laboratoire GREMAN, UMR 7347 Université de Tours, CNRS, INSA CVL, Université de Tours UFR Sciences & Techniques, 37200 Tours, France — [2]Laboratoire SPMS, UMR 8580 Université Paris-Saclay, CNRS, CentraleSupélec, 91190 Gif-sur-Yvette, France

With the ever-growing need for energy in our society, researchers are striving to obtain new materials with better energy storage properties capable of replacing current lead-based materials. Among all lead-free materials that have been synthesized, Bi0.5Na0.5TiO3 (BNT) has attracted the attention of many. The main reasons are his high temperature of maximum permittivity called Tm at 320°C, a huge maximum polarization and relaxor ferroelectric properties making his phase transition very diffuse in temperature. However, the good energy storage properties only apply at a temperature higher than the depolarization temperature Td (200°C). Usually, to reduce Td, researchers either make solid solutions with other perovskite ceramics or use donor dopants. Here we show the results we obtained while keeping the pristine BNT phase by optimizing the sol-gel synthesis process used. The BNT exhibits sub-micrometric grain size thanks to a multi-step sintering process lowering Td (around 160°C). This BNT has enhanced relaxor ferroelectric at lower temperatures. Results about donor dopants reducing dielectric losses on this BNT will also be shown.

KFM 9.5 Tue 12:45 H9

Composite quadrupole order in ferroic and multiferroic materials — •Matthias Geilhufe — Department of Physics, Chalmers University of Technology, 412 96 Göteborg, Sweden

The formalism of composite and intertwined orders has been remarkably successful in discussing the complex phase diagrams of strongly correlated materials and high-Tc superconductors. Here, we propose that composite orders are also realized in ferroelectric and ferromagnetic materials when lattice anisotropy is taken into account. This composite order emerges above the ferroic phase transition, and its type is determined by the easy axis of magnetization or polarization, respectively. In multiferroic materials, where polarization and magnetization are coupled, composites of both orders are possible. This formalism of composite orders naturally accounts for magnetoelectric monopole, toroidal, and quadrupole orders. More broadly, composite orders may explain precursor phenomena in incipient ferroic materials, arising at temperatures above the ferroic phase transition and potentially contributing to the characterization of currently hidden orders.

[1] R Matthias Geilhufe, J. Phys.: Condens. Matter, 37, 05LT01 (2025)

KFM 10: Materials for the Storage and Conversion of Energy (joint session MM/KFM)

Time: Tuesday 14:00–15:15 Location: H22

KFM 10.1 Tue 14:00 H22

Multiscale defective interfaces for realizing Na-CO2 batteries with ultralong lifespan — •changfan xu, tzuchin huang, and yong lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

The cycling capability of Na-CO2 batteries has been impeded by limitations in the kinetics of cathodic CO2 reduction/evolution reaction (CO2RR/CO2ER) as well as the challenging process of depositing/stripping metallic Na during cycling.[1-3] Herein, a "two-in-one" electrode with multiscale defective FeCu interfaces (CP@FeCu) is presented, improving the kinetics of CO2RR/CO2ER and modulating sodium deposition behavior.[4] The enhancement of sodiophilicity and catalytic properties is attributed to multiscale defective FeCu interfaces, as revealed by experimental and theoretical investigations. The defect and valence oscillation effects originate in multiscale defective FeCu interfaces, effectively facilitating reactant adsorption and Na2CO3 decomposition during CO2RR/CO2ER processes, along with exceptional cycling stability of 2400 cycles (4800 h) at 5 μA cm*2. Meanwhile, the CP@FeCu with high sodium affinity creates a uniform electric field and strong Na adsorption, promoting favorable nucleation sites for dendrite-resistant and durable anodes. This work provides scientific insights into the design of "two-in-one" electrodes, which are crucial for addressing challenges in sodium anodes and CO2 cathodes. [1] Small 2023, 2206445 [2] Adv. Funct. Mater. 2023, 2300926 [3] Energy Environ. Mater. 2024, 7, e12626 [4] Adv. Mater. 2024, 2409533

KFM 10.2 Tue 14:15 H22

Electro-chemo-mechanical behavior of a layered cathode material upon cycling — •Robert Löser[1], Yug Joshi[2], Roham Talei[1], and Guido Schmitz[1] — [1]University of Stuttgart, Stuttgart, Germany — [2]Max-Planck-Institut für Nachhaltige Materialien GmbH, Düsseldorf, Germany

The mechanical properties of lithium-ion cathode materials play a critical role in determining battery performance such as cycle life, durability, and safety, especially when the battery is under external pressure which is typical for all-solid-state batteries. This research investigates LiCoO2 (LCO), a prevalent hexagonal layer-structured cathode material, and explores its mechanical responses during de-/lithiation using sputter-deposited thin films and nanoindentation. The values of the experimental Young*s modulus in pure (101) and (003) lattice orientations are quantified to 337.1 * 8.7 GPa and 267.9 * 7.2 GPa, respectively, in the fully lithiated state. Furthermore, a substantial texture-dependent decrease in Young*s modulus upon lithium deintercalation is demonstrated, probably due to modification of the bonding interactions between the cobalt oxide layers. Delithiation also elevates the relative contribution of plastic deformation, indicating that dislocation glide becomes easier in deintercalated states. By extensive cycling, the Young*s modulus in higher lithiated charge-states decreases considerably which is most-likely due to irreversibility of phase transitions. The work provides valuable insight on the dynamic changes of the mechanical properties during electrochemical cycling of LiCoO2, which paves the way for all other layered cathode materials.

KFM 10.3 Tue 14:30 H22

$MnTiO_3$ as a Carbon-Free Cathode for Rechargeable Li-oxygen Batteries — Doaa Ahmed[1,2], Wernfried Mayr-Schmölzer[1], Mustafa Çelik[3,4], Abdulkadir Kizilaslan[3,4], and •Gregor Vonbun-Feldbauer[1,2] — [1]Institute of Advanced Ceramics, TU Hamburg, Germany — [2]Institute of Soft Matter Modeling, TU Hamburg, Germany — [3]Research, Development and Application Center (SARGEM), Sakarya University, Turkey — [4]Department of Metallurgical and Materials Engineering, Engineering Faculty, Sakarya University, Turkey

Lithium-oxygen batteries (LOB) are promising energy storage systems due to their high theoretical energy density. However, their main challenges are the sluggish kinetics of oxygen reduction and evolution reactions (ORR/OER) and high charge overpotentials. To overcome these challenges, the development of a suitable catalyst is crucial. Here, $MnTiO_3$ was investigated as a carbon-free cathode catalyst using density functional theory (DFT) calculations and experimental approaches. DFT calculations revealed the coexistence of Mn and Ti energy levels near the Fermi level of $MnTiO_3$, which facilitates ORR/OER. This feature endows MnTiO3 with a bifunctional role in promoting battery performance. Our DFT-based investigation further elucidates the surface stability and catalytic properties of $MnTiO_3$. In addition, experiments confirm that the electrochemical reactions on $MnTiO_3$ follow a two-electron pathway. LOBs with $MnTiO_3$ exhibit a total overpotential of 1.18 V and 1.55 V from DFT and electrochemical measurements, respectively, and current densities up to 1 A/g.

KFM 10.4 Tue 14:45 H22

Modeling and optical characterization of Lithium deposition on Copper current collectors — •Len Kimms[1], Tjark Ingber[2], Diddo Diddens[1,2], and Andreas Heuer[1] — [1]Institut für physikalische Chemie, Universität Münster — [2]Helmholtz Institute Münster (IEK-12), Forschungszentrum Jülich GmbH

In this contribution, we will present modeling results of the initial deposition of lithium metal on a copper current collector combined with experimental insights. Zero–excess lithium–metal batteries (ZELMBs) may offer higher energy densities, better safety, and reduced cost by reducing the amount of lithium employed in the cell. Instead of an excess of lithium as electrode, the anode is formed in situ during charging. When charging the battery, lithium is plated on the current collector directly. However, the lifespan of ZELBMs in practical applications is still limited by irreversible loss of active lithium. The loss is induced by the high reactivity of lithium which causes parasitic side reactions and dendrite growth during charging cycles. To uncover the mechanisms at play, the initial deposition of lithium metal has been experimentally investigated by plating varying amounts on a copper surface with different current densities. The deposits have been characterized by scanning electron microscopy (SEM) and laser scanning microscopy (LSM) in an automated way. Numerical simulations of a simple geometric model were employed to uncover the relevant mechanisms which govern the growth over different stages. Combining the experimental and numerical results, an effective description of the deposition has been found.

KFM 10.5 Tue 15:00 H22

Preparation of Prussian blue analogue materials and their application to potassium-ion batteries — •Ping Hong, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Prussian blue (PB) and its analogs (PBAs), with their unique open framework structure and chemical stability, have emerged as promising cathode materials for potassium-ion batteries (PIBs). PB and PBAs feature three-dimensional channels, facilitating rapid potassium-ion intercalation and de-intercalation, thus delivering excellent rate performance. Furthermore, its low-cost synthesis and environmentally friendly properties provide a strong foundation for potential commercial applications. Despite these advantages, the practical application of PBAs is hindered by challenges such as their high solubility in electrolytes and limited cycle stability and life. To overcome these limitations, we optimized synthesis techniques (by simple adjustment of the co-precipitation method) and structural design, leading to significant improvements in material performance. In addition, a series of adjustments were made to the binder, electrolyte, and voltage range used in the batteries. The improved PBA cathode exhibited remarkable cycling stability, showing almost no capacity decay after 500 cycles at a current density of 100 mA/g within the voltage range of 2.0-4.0 V. It maintained excellent cycling performance even under high current conditions, providing strong support for the advancement of high-performance PIBs.

KFM 11: (Multi)ferroic States: From Fundamentals to Applications (V)

This focus session explores the intricate properties of (multi)ferroic states, spanning from fundamental understanding to cutting-edge applications. Topics include the design and control of (multi)ferroic states and domain structures at interfaces, domain walls, and in heterostructures. Emphasis will be placed on theoretical models, advanced characterization techniques, and the engineering of emergent properties for use in nano-electronic devices.

Chair: Manuel Zahn (University of Augsburg)

Time: Wednesday 9:30–10:45 Location: H9

Invited Talk KFM 11.1 Wed 9:30 H9

Towards 3D nanoscale chemical mapping with atom probe tomography — •Kasper Hunnestad, Constantinos Hatzoglou, Antonius van Helvoort, and Dennis Meier — Norwegian University of Science and Technology, Trondheim, Norway

The discovery of new physical phenomena in materials is closely linked to the progress in characterization, and is propelled by the ability to observe and study physical processes occurring at the atomic level. Nanoscale structural characterization has been a cornerstone for many discoveries related to ferroic phenomena. Chemical characterization at the atomic level, however, remains a major challenge.

In the first part of this talk, I will present how atom probe tomography (APT) can be incorporated into the toolkit of nanoscale research to study ferroic oxide materials. In the second part of this talk, a special emphasis will be put on various ferroic phenomena, such as ferroelectric domain walls and interface effects. The focus will be on understanding their chemical state and the role of defects in controlling their physical properties.

The presentation will demonstrate that correlations between defect chemistry and ferroic phenomena can be experimentally probed with nanoscale spatial resolution using APT, opening an avenue to obtain a deeper understanding of ferroic materials.

KFM 11.2 Wed 10:00 H9

Tuning of ferroelectric polarization by lattice chemistry — •Ipek Efe[1], Alexander Vogel[2], William S. Huxter[1], Elzbieta Gradauskaite[1], Christian L. Degen[1], Marta D. Rossell[2], Manfred Fiebig[1], and Morgan Trassin[1] — [1]ETH Zurich — [2]Empa, Switzerland

Engineering the lattice chemistry in oxide thin film systems opens up new possibilities for tuning electrostatic boundary conditions beyond the depolarizing-field tuning approaches. Controlling the formation of polarizing charged layers may stabilize highly desired polar textures such as charged domain walls and charge planes, offering great promises for future ultralow-energy-consuming oxide electronics. Here, we demonstrate lattice-chemistry engineering of perovskite oxide ferroelectrics in a heterostructure utilizing Aurivillius-type layering. We insert functional perovskite oxides, including $BiFeO_3$ and $BaTiO_3$, into the layered framework of the Aurivillius phase. By exploiting the characteristic charged interfaces present in the Aurivillius crystal structure and varying the perovskite constituent, we fine-tune the electric-dipole configurations within our composite heterostructures. Using in-situ optical second harmonic generation, we directly resolve the influence of controlled atomic-scale poling of the Aurivillius charged layers on the perovskite constituent. As a result, we achieve new properties while preserving the functionalities of the parent compounds.

KFM 11.3 Wed 10:15 H9

Vector Scanning Electron Microscopy for Domain Imaging in Ferroelectric Polycrystals — •Ellinor Benedikte Anjali Lindström, Ruben Skjelstad Dragland, Jonas Åmli Ingdal, Jan Schultheiss, Jiali He, and Dennis Meier — NTNU Norwegian University of Science and Technology, Norway

Domain imaging in polycrystalline ferroelectrics is challenging due to the non-uniform crystallographic orientation of grains. To gain the full information including the domain polarization and orientational information, imaging techniques such as piezoresponse force microscopy (PFM) and scanning electron microscopy (SEM) are often complimented by electron backscatter diffraction (EBSD) experiments.

Here, we introduce a new SEM-based approach that allows simultaneous mapping of domains and grain orientation information. By performing systematic SEM measurements as a function of the stage rotation angle on the model system $ErMnO_3$, we observe distinct contrast intensity changes within the same grain. Notably, the domain contrasts invert when the stage is rotated by 180°. Complementary PFM and EBSD data confirm that these changes in contrast correlate with both the domain state and the orientation of the polar axis relative to the surface. Our approach offers a contact-free alternative to vector PFM and partially reduces the need for EBSD, giving new opportunities for domain imaging in ferroelectrics.

KFM 11.4 Wed 10:30 H9

Ranges and limits of p-doping in Y:HfO$_2$ - an electronic structure study by HAXPES — •Oliver Rehm[1], Lutz Baumgarten[2], Florian Wunderwald[3], Andrei Gloskovskii[4], Christoph Schlueter[4], Thomas Mikolajick[3,5], Uwe Schroeder[3], and Martina Müller[4] — [1]Universität Konstanz — [2]Forschungszentrum Jülich — [3]NaMLab, Dresden — [4]DESY, Hamburg — [5]TU Dresden

Ferroelectric HfO_2-based thin films exhibit huge potential for the next generation of nonvolatile memory applications, such as FeRAM or FeFET. However, the application of HfO_2-based thin films as active ferroelectrics (FE) in devices still faces reliability issues like wake-up, imprint, and fatigue. A critical concentration of oxygen vacancies (OVs) determines both the stabilization of a FE phase as well as the breakdown during electrical cycling. For p-doped HfO_2, the electronic limits of OV formation remain an experimentally open question.

We investigated Y:HfO_2 samples synthesized via atomic layer deposition (ALD) with Y doping concentrations from 2.1% to 8.6%. TiN/Y:HfO_2 interfaces are investigated regarding the local chemistry and electronic properties by hard X-ray photoelectron spectroscopy (HAXPES). The Hf 4f core level is analyzed to identify Hf^{3+} components and rigid binding energy (BE) shifts, both of which serve as indicators for OVs. We determine the (unexpected) formation of OVs as a function of Y doping, with the conclusion that Y doping above a threshold limit has a detrimental effect on interface stability, thereby promoting increased OV formation at the interface that finally speeds up fatigue and breakdown.

KFM 12: Holistic Structural and Safety Assessment of Lithium-ion and Post-Lithium Cells and their Materials (Modelling of Battery Materials and Degradation)

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.

Chair: Carlos Ziebert (Karlsruhe Institute of Technology)

Time: Wednesday 11:00–12:45 Location: H9

Invited Talk KFM 12.1 Wed 11:00 H9

Model-assisted Insight into Degradation of Li-Ion Batteries during Thermal Abuse — •Ulrike Krewer, Leon Schmidt, and Jorge Valenzuela — Karlsruhe Institute of Technology, Institute for Applied Materials -Electrochemical Technologies, Karlsruhe, Germany

The electrolyte in Li-ion batteries is inherently thermodynamically instable; this leads to formation of the solid-electrolyte interphase and capacity loss. Exposing batteries to high temperatures above ca. 60°C accelerates interphase growth, but also leads to its dissolution and renewed formation. If the related exothermic heat is not sufficiently fast removed, this leads to self-heating and a thermal runaway of the cell. This talk uses modelling to give a deep insight into the processes and properties causing self-heating and thermal runaway of Li-ion batteries. A complex interaction of exothermic and endothermic reactions is revealed, and the effects of evaporative cooling [1], conditions during battery manufacturing and battery age. [2] Gas analysis with online electrochemical mass spectrometry aids in identifying the network and further sensitivities. [3]

[1] Baakes F. et al., J. Power Sources, 2022, 522, 230881 [2] Baakes, F. et al., Chem. Sci, 2023, 14, 13783 [3] Bläubaum, L. et al., Batter. Supercaps 2024, 7, e20230053.

KFM 12.2 Wed 11:30 H9

computational investigation of lignin based anode ma- terials for Li- and post-Li ion batteries* — •jafar azizi[1], Holger Euchner[2], and Axel Gross[1] — [1]Institute of Theoretical Chemistry, Ulm University, 89069 Ulm, Germany — [2]2 Institute of Physical and Theoretical Chemistry, Tübingen University, 72076 Tübingen, Germany

Post-lithium ion batteries have gained a lot of attention as a promising energy storage technology for large-scale grid applications due to their high energy density and low cost. Hard Carbon is one of the most promising anode materials, but is still associated with some performance problems. It is anticipated that improved hard carbon-based cells with a higher energy density and better electrochemical performance will be highly interesting in electrochemical energy storage. Hence, in this work, we propose a novel anode material based on the structure of lignin, one of the most prevalent biomass materials. Based on ab initio molecular dynamic (AIMD) simulations and density functional theory (DFT) calculations we study the formation of lignin-based hard carbon at different temperatures which results show a promising new amorphous structure. We find a noticeable structure stability, and higher energy capacity (AMC$_n$, $n < 6$) compared to the usual graphite system.

KFM 12.3 Wed 11:45 H9

Stability Enhancement of Cubic CsSnCl$_3$ as Solid Electrolyte - A Computational Approach — •Johannes Döhn[1], Martin Uhrin[2], and Axel Gross[1,3] — [1]Institute of Theoretical Chemistry, Ulm University, Germany — [2]Multidisciplinary Institute in Artificial Intelligence, Université Grenoble Alpes, France — [3]Helmholtz Institute Ulm, Germany

For the transition towards renewable energy systems, efficient and reliable technologies for energy storage are needed. Batteries are one of the most widely used storage devices, but current technology based on the transfer of Li-ions faces several challenges including their dependence on critical materials with respect to both, scarcity and toxicity.

In our contribution, we will present atomic-scale investigations of potential future battery materials carried out using a combination of density functional theory (DFT) and machine learning interatomic potential (MLIP) calculations. We employed a high-throughput approach in order to evaluate potential dopants for the well-known Cl-ion conductor CsSnCl$_3$; a solid electrolyte material for chloride ion batteries (CIBs) which is ascribed the capability to fully exploit the potential of this alternative battery type. The investigated dopants where chosen based on a dual doping strategy: Cation doping aims at enhancing the stability of the material while the introduction of mobile species, i.e., Cl vacancies/interstitials, balances the formal charge of the system and aims at improving the Cl-ion conductivity.

KFM 12.4 Wed 12:00 H9

Stability of MgSc$_2$Se$_4$ Surfaces — •Sebastian Utz[1] and Axel Gross[1,2] — [1]Ulm University, Ulm, Germany — [2]Helmholtz Institute Ulm, Ulm, Germany

Magnesium metal anodes are a promising material for post-lithium battery systems because of their high theoretical gravimetric energy density. One issue that hinders their application is the low ionic conductivity of many magnesium electrolytes. One of the few electrolytes that show good magnesium ion conductivity is the solid electrolyte MgSc$_2$Se$_4$ with a spinel structure. While the structural and diffusion properties of the bulk material are already well understood, its surfaces and interfaces are hardly explored. To shed some light on the surface properties of this solid-state electrolyte, first principles calculations within the framework of periodic density functional theory were conducted. The stability of low index {100} and high index {222} surfaces are being compared. Additionally, common structural features of the different surfaces that may lead to a stabilisation or destabilisation will be explored.

KFM 12.5 Wed 12:15 H9

Hybrid Interfaces in Focus – Decoding the Berlinite Surface with a Synergetic NMR-DFT Approach — •Javier Valenzuela Reina[1], Vera Barysch[2], Simone Köcher[2,1], and Christoph Scheurer[1,2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Institute of Energy Technologies (IET-1), Forschungszentrum Jülich GmbH

One of the milestones in the development of the next generation of high-performance lithium batteries is the understanding and improvement of hybrid electrolytes and their interfaces. Nuclear magnetic resonance (NMR) spectroscopy is a non-destructive, powerful technique for unraveling the intricate interface structure and ion dynamics in these materials.

We exploit the synergies between NMR experiments and density-functional theory (DFT) simulations for investigating Berlinite (AlPO$_4$) as a model for the surface of the well-known solid ion conductor Li$_{1+x}$Al$_x$Ti$_{2-x}$P$_3$O$_{12}$ with $0 \leq x \leq 1$ (LATP), a promising candidate for a hybrid electrolyte. By supporting surface-selective NMR techniques such as cross-polarization (CP) and transfer of populations in double resonance (TRAPDOR) on AlPO$_4$ powder with DFT calculations of NMR observables, we study multiple surface models, infere structural characteristics of the sample, and study its interactions with water as well as organic molecules. We demonstrate that the joint experimental-theoretical approach holds future potential for understanding and improving materials whose performance relies on the properties and behavior of complex organic/ceramic interfaces.

KFM 12.6 Wed 12:30 H9

Pits and Traps in the Impedance Analysis of Ionic Conductors — •Janis K. Eckhardt — Center for Materials Research (ZfM), Justus Liebig University, Giessen D-35392, Germany

The development of innovative electrochemical storage systems, such as solid-state batteries, is critical for achieving climate neutrality and sustainability goals. Several hurdles must be overcome before such technologies are ready for the market. Impedance spectroscopy is a powerful method for characterizing the electrical transport properties of new materials and for monitoring systems in operation. Although it is an older measurement technique, the interpretation of data for inhomogeneous solid-state systems lacks established concepts for reliable results. Therefore, we use 3D electrical network models for spatially-resolved transport simulations and systematic investigation of the influence of sample microstructure and solid-solid interface morphology. The material-specific transport quantities derived from 1D models (e.g., brick layer model) sometimes exhibit inaccuracies of several orders of magnitude. In addition, the impedance response of the system exhibits geometric signatures that cannot be adequately represented in physically motivated circuit models, e.g., current constriction phenomena.

KFM 13: Holistic Structural and Safety Assessment of Lithium-ion and Post-Lithium Cells and their Materials (Experimental Characterisation and Safety Testing)

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.

Chair: Philipp Finster (Karlsruhe Institute of Technology)

Time: Wednesday 15:00–16:45 Location: H9

KFM 13.1 Wed 15:00 H9

Are Li-ion batteries safe for 2nd-life applications? - The case of aged cells with SEI growth — •Thomas Waldmann[1,2,4], Gabriela G. Gerosa[1], Jihed Ayari[2,3], Abdelaziz A. Abd-El-Latif[1], Philipp Moosmann[1,5], Max Feinauer[1], Olaf Böse[1], Markus Hölzle[1], and Margret Wohlfahrt-Mehrens[1,2] — [1]Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg (ZSW), Helmholtzstrasse 8, Ulm, 89081, Germany — [2]Helmholtz Institute Ulm (HIU), Helmholtzstrasse 11, Ulm, 89081, Germany — [3]Karlsruhe Institute of Technology (KIT), Karlsruhe, 76021, Germany — [4]Institute of Surface Chemistry and Catalysis, Ulm University, Albert-Einstein-Allee 47, 89081 Ulm, Germany — [5]Porsche AG, Porschestrasse 911, 71287 Weissach, Germany

Re-using aged Li-ion batteries in 2nd-life applications can increase sustainability. However, there is a lack of knowledge on the safety of aged cells with regard to the underlying aging mechanisms. Room temperature and high temperature aging often lead to growth of the solid electrolyte interphase (SEI) on the surface of graphite or Si/graphite anodes as commonly observed by post-mortem analysis of Li-ion battery cells with physico-chemical analysis methods. We show results on the influence of aging of commercial Li-ion cells in the 1st-life on safety in 2nd-life. Our safety tests (ARC, nail penetration, overcharge, overdischarge) reproducibly show similar or better safety levels for cells with SEI growth in contrast to aged cells with the different mechanism of lithium plating. Possibilities are pointed out to avoid critical mechanisms and for early detection of unsafe behavior.

KFM 13.2 Wed 15:15 H9

Diffraction computed tomography for non-destructive analysis of li-ion batteries — •Vladislav Kochetov — Heinz Maier-Leibnitz-Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany

This contribution discusses the application of Diffraction Computed Tomography (DCT), including both X-ray and neutron probes, as a powerful method for non-destructive structural analysis in materials science. DCT uses a pencil-beam scanning technique to yield the reconstructed images of internal structure and chemical gradients of materials, extending the traditional imaging approaches. A notable application of DCT is in the study of commercial lithium-ion batteries, where it has been used to resolve inhomogeneities in lithium distribution and structural evolution during cycling. We apply DCT to various commercial battery types, specifically focusing on cylindrical cells with different diameters, featuring diverse chemistries such as NCA, NMC, and graphite anodes. By employing high-resolution DCT, we map lithiation distributions and investigate electrode degradation mechanisms, providing key insights in battery performance and aging. The efficiency of the method, state-of-the-art resolution capabilities, and technique's extension to neutrons are discussed.

[1] V. Kochetov et al, Powder diffraction computed tomography: a combined synchrotron and neutron study, J Phys Condens Matter 33 (10), 2021. [2] D. Petz et al, Lithium distribution and transfer in high-power 18650-type Li-ion cells at multiple length scales, Energy Storage Materials 41, 2021.

KFM 13.3 Wed 15:30 H9

Optical, structural and electrochemical properties of resynthesized Graphite powder for Anode battery application — •slaheddine Jabri[1], Anna Rollin[2], Sukanya Sukanya[3], René Wilhelm[2], Michael Kurrat[3], Uta Schlickum[1], and Markus Etzkorn[1] — [1]Technische Universität Braunschweig, Institute of Applied Physics, Meldensohn Straße2, 38106 Braunschweig, Germany — [2]Mendelssohnstraße 2 — [3]Technische Universität Clausthal, Institute of Organic Chemistry, Leibnitzstraße 6, 38678 Clausthal-Zellerfeld, Germany

By focusing on preserving the components of Li-Ion battery material through cheaper and envi-ronmental friendly methods, recycling process could introduce scavenged impurities into resyn-thesized material and modify its structural and morphological properties. In this work, we investi-gate the optical, structural and electrochemical properties of recycled Graphite compared to the new material. Our findings reveal that a proper recycling process can remove the Solid Electrolyte Interphase (SEI) layer, which is of significant importance in battery performance. The analysis showed that proper cleaning can significant reduce the amounts of organic and inorganic impuri-ties in the graphite, leading to an improvement in material quality. As a result, the battery perfor-mance can even be enhanced by 89% after 200 charge-discharge cycles compared to the commer-cial base material, demonstrating the potential of recycling methods for improving battery life and efficiency.

KFM 13.4 Wed 15:45 H9

Facilitating Sodium-Ion Diffusion in Fe-Doped Co3O4 for High-Rate Performance — •Yonghuan Fu, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Due to its high theoretical capacity, cobalt oxide (Co3O4) has attracted attention to sodium-ion battery (SIB) anodes. However, its low conductivity and poor rate performance have limited its practical application. This work proposes a co-precipitation doping strategy to synthesize iron-doped Co3O4 nanoparticles (FexCo3-xO4 NPs). Both experimental and theoretical results confirm that iron (Fe) doping at octahedral sites within spinel structures is a critical factor in enhancing rate performance. The decreased band gap and enlarged ion transport spacing originate in Fe doping. This effectively facilitates the electron and Na+ transport during discharge/charge processes, delivering an impressive rate capability of 402.9 mA h g-1 at 3 A g-1. The FexCo3-xO4 NPs demonstrate remarkable cycling stability. They maintain a high specific capacity of 786.2 mA h g-1 even after 500 cycles at 0.5 A g-1, with no noticeable capacity fading. This work provides valuable insights into the functional design of high-rate electrodes, offering a promising approach to addressing the critical challenges faced by sodium anodes.

KFM 13.5 Wed 16:00 H9

Reversible Structural Evolution of 3D Vanadium Sulfide Anodes in Sodium-Ion Battery Applications — •Osamah Ali Fayyadh, Yulian Dong, Huaping Zhao, and Yong Lei — Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau

Sodium-ion batteries (SIBs) are a promising alternative to lithium-ion batteries due to sodium's abundance and wide distribution. However, SIBs face challenges such as low capacity, poor cycling, and sluggish ion diffusion, due to the large ionic radius of Na+. Thus, extensive research has focused on advanced anode materials, among which vanadium sulfides (VSx) have gained significant attention due to their large interlayer spacing, high theoretical capacities, and versatile electrochemical mechanisms. However,VSx suffer from mechanical pulverization, severe volume changes, and limiting their practical application. Here, we demonstrate a 3D micro/nanostructured VSx anode fabricated, achieving a remarkable reversible capacity of 961.4 mAh g-1 after 1500 cycles at 2 A g-1. The sodiation-driven reconfiguration of 3D-VSx into a stable structure mitigates volume changes, enhances ion diffusion, and improves structural stability.[1] The sodiation-driven reconfiguration enhances ion diffusion, mitigates volume changes, and stabilizes the structure. Electrochemical studies and density functional theory calculations reveal significantly improved Na+ storage capabilities, offering a pioneering strategy for developing high-performance SIB anodes with excellent capacity and stability. [1] Y. Dong, Y. Lei et.al. Adv. Energy Mater. 2023, 13, 2204324.

KFM 13.6 Wed 16:15 H9

synergizing nickel (II) oxide-based catalyst for sodium-carbon dioxide battery — •Tzu-Chin Huang, Changfan Xu, Huaping Zhao, and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Na-CO2 battery is a novel and environmentally friendly green energy device. Conceptually, it demonstrates excellent capabilities. However, during the operation of batteries, undecomposed discharge products, sodium carbonate, accumulate continuously, which is highly insulating, thermodynamically stable, and difficult to decompose. This increases the ohmic resistance within the battery, resulting in high charging potential and excessive polarization, which leads to serious side reactions, such as the decomposition of the electrolyte and cathode material, reducing the battery's reversibility. Herein three Ni oxide-based catalysts, NiO, NiCoO, and CuNiCoO, attached to carbon clothe cathode were synthesized and employed in Na-CO2 batteries. Electrochemical testing demonstrated that CuNiCoO exhibits the best battery stability and long-term performance. This superior performance is driven by the ability of CuNiCoO catalyst to effectively promote the generation and decomposition of discharge products. Cyclic voltammetry (CV) analysis revealed strong redox peaks, underscoring the outstanding catalytic activity of CuNiCoO catalyst. Furthermore, XRD and Raman characterizations confirmed this by showing the appearance and gradual disappearance of sodium carbonate peaks during charge and discharge cycles, indicating remarkable reversibility.

KFM 13.7 Wed 16:30 H9

A Solar Battolyzer Approach: On-Demand Hydrogen Production and Energy Storage in a 2D Niobium-Tungstate Material — Yang Wang[1], •Yu-Te Chan[2], Takayoshi OshimaViola[1], Viola Duppel[1], Sebastian Bette[1], Kathrin Küster[1], Andreas Gouder[1], Christoph Scheurer[2,3], and Bettina Lotsch[1,4] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]Fritz-Haber-Institut der MPG, Berlin — [3]IEK-9 Forschungszentrum, Jülich — [4]Ludwig-Maximilians-Universität, Munich

In the quest to overcome the limitations of solar intermittency, materials that can simultaneously capture and store solar energy offer promising avenues for clean energy solutions. Here, we introduce the 2D niobium-tungstate $\mathrm{TBA^{+}NbWO_6^{-}}$ as a novel solution capable of harnessing light energy and storing it either for direct grid integration or as fuel through on-demand hydrogen production. This dual-functionality is central to the emerging concept of "battolyzers," devices that combine battery and electrolyzer capabilities to provide both energy storage and fuel generation. Exposure to light triggers ion intercalation and stable polaron formation within the material, reducing resistance and allowing electron storage for extended durations. Introducing Pt as the catalyst allows the stored electrons to be released to generate hydrogen, demonstrating the material's capability for efficient, on-demand solar energy conversion. Our findings on optoionic processes in $\mathrm{NbWO_6}$ lay the groundwork for future solar battolyzers, bridging solar energy storage and hydrogen fuel generation in a single system. [1] Y. Wang et al., J. Am. Chem. Soc. **146**, 25467 (2024)

KFM 14: Poster

Chairs: Jan Schultheiß (NTNU, Norway) Anna Grünebohm (RUB)

Time: Wednesday 17:00–18:30 Location: P1

KFM 14.1 Wed 17:00 P1

Stability of Machine-Learned Interatomic Potentials in Molecular Dynamics Simulations for Organic Semiconductors and Metal-Organic Frameworks — •Martin Tritthart and Egbert Zojer — Institute for Solid State Physics, Graz, Austria

Organic semiconductors (OSCs) and metal-organic frameworks (MOFs) are two classes of materials that have garnered significant interest in materials science. To optimize their performance, it is crucial to understand the physical properties of these crystalline polymer materials, such as heat transport and mechanical stability. This understanding can lead to improvements in properties like thermal stability. Molecular dynamics (MD) simulations are commonly used for this purpose, as they are orders of magnitude less computationally expensive than first-principles calculations. While machine learning interatomic potentials (MLIPs) are much faster than ab initio methods, they approximate the true potential energy surface, which can result in significant errors for atomic configurations outside the training data space. Such shortcomings lead to incorrect predictions of forces and energies in MD simulations, potentially causing molecular instability during simulations. To address this issue and improve the robustness of MLIPs, a reliable estimation of their uncertainty is necessary. This enables the identification of uncertain structures, which can then be incorporated into the training set to enhance accuracy. With this iterative approach, larger and more complex molecules can be simulated with relatively efficient computational effort.

KFM 14.2 Wed 17:00 P1

Assessment of new cocrystals of amphotericin B and miltefosine (leishmanicidal pharmaceuticals) via powder X-ray diffraction analysis. — •Memoona Bibi, muhammad Iqbal Choudhary, and Sammer Yousuf — H.E.J. Research Institute of Chemistry, ICCBS, University of Karachi, Pakistan.

Cocrystals and other cutting-edge technologies offer substantial opportunities for patents that present multiple strategies for managing the life cycle of existing and novel drugs. The creation of cocrystals by employing suitable coformers represents a valuable approach toward stability, enhancement, and bio availability of pharmaceutical medications. The focal point of current study was co-crystallization of well-known commercially available anti-leishmanial drugs i.e. Amphotericin B and Miltefosine. Multiple cocrystals of amphotericin B and miltefosine were successfully synthesized. To prepare the co-crystals neat grinding method via mixer mill was applied. The characterization was conducted through powder X-ray diffraction revealing unique crystallinity and significant variation in 2θ values of cocrystals. DSC/TGA, UV, FTIR and melting point were also proceeded for further evaluation. The solubility studies of amphotericin B at pH 6.8, 7.4 and in distilled H2O in comparison with their co-crystals revealed promising results. Invitro testing of all co-crystals against L. major, L. donovani, and L. tropica demonstrated potent anti-leishmanial activity in comparison with reference standard drugs i.e. amphotericin B and miltefosine. However, cytotoxicity results revealed none of them exhibited cytotoxic effect against MTT (3T3) cell line.

KFM 14.3 Wed 17:00 P1

High-temperature properties of $\mathbf{LiNbO_3}$ and $\mathbf{LiTaO_3}$ — •Eva Westenferlder Gil, Felix Bernhardt, and Simone Sanna — Institut für Theoretische Physik and Center for Materials Research, Justus-Liebig-Universität Gießen, Germany

Lithium niobate (LN) and lithium tantalate (LT) are ferroelectric crystals with a wide range of applications, extending from piezoelectric sensors [1] to integrated photonics [2]. Both, LN and LT, undergo a phase transition towards a paraelectric (PE) phase at around 1400K and 870K, respectively. Since devices employing LN and LT as functional materials are often operated at high temperatures, extensive research has been conducted in order to describe the materials high-temperature properties [3,4]. Here, we show that the high symmetry PE structure for both LN and LT is energetically favoured, which is in contrast to previously suggested models representing the PE phase as a superposition of differently oriented ferroelectric phases [5]. The electronic band structures indicate that both crystals remain electronic insulators in the PE phase. Furthermore, we provide thermal expansion coefficients and elastic constants, calculated from machine-learned potentials. Our results show a good agreement to recent experimental measurements.

[1] M. Xu *et al*, ACS Appl. Mater. Interfaces **9**, 40, (2017)
[2] W. Sohler *et al*, Optics & Photonics News **19**, 1, (2008)
[3] P. Gaczyński *et al*, Phys. Status Solidi A, 2300972, (2024)
[4] C. Kofahl *et al*, Solid State Ionics **409**, 116514 (2024)
[5] F. Bernhardt *et al*, Phys. Rev. Mat. **8**, 054406 (2024).

KFM 14.4 Wed 17:00 P1

Optimizing pre-annealing growth for obtaining pattern fidelity of highly ordered GaAs nanowires — •Juliane Koch[1], Jiajia Qiu[2], Chris Bohlemann[1], David Ostheimer[1], Peter Kleinschmidt[1], Huaping Zhao[2], Yong Lei[2], and Thomas Hannappel[1] — [1]TU Ilmenau, Institute for Physics, Fundamentals of Energy Materials, Ilmenau, Germany — [2]TU Ilmenau, Institute for Physics, Applied Nanophysics, Ilmenau, Germany

Bottom-up grown III-V semiconductor nanowires (NWs) offer significant potential for advanced electrical and optoelectronic device applications. This study presents a fabrication strategy for highly ordered GaAs NW arrays by combining a non-lithographic nanostructuring technique with metalorganic vapor phase epitaxy (MOVPE). Uniform Au nano-disk arrays, created using anodic aluminum oxide templates, act as catalysts for the subsequent NW growth. The special fabrication process of the Au nano-disks prevents undesired substrate imprinting, which leads to a different behavior than previously utilized methods, namely to an Au particle diffusion during the MOVPE process. The nucleation duration, optimized in terms of the Au particle volume, is crucial for maintaining array uniformity. A short nucleation period fails to anchor particles, resulting in undesired diffusion. To resolve this, pre-annealing nucleation is extended to initiate III-V growth of a pedestal structure that secures the array's highly ordered geometry. A detailed analysis of MOVPE sub-processes supports the development of a refined growth model.

KFM 14.5 Wed 17:00 P1

Synthesis, Properties, and Phase Transitions analysis of ferroelectric TMCM-MnCl3 hybrid halide — •Chithra Kandappanthodi, Sobhan Fathabad, Doru C.Lupascu, and Vladimir V.Shvartsman — Institute for material science, Essen, Germany

Organic-inorganic hybrid halides have gained significant attention in material science due to their environmentally friendly, cost-effective fabrication and exceptional piezoelectric or optoelectronic properties. In this study, we synthesized trimethyl chloromethyl ammonium manganese trichloride (TMCM-MnCl3) and Fe-doped TMCM-MnCl3 crystals. We demonstrate that TMCM-MnCl3 exhibits a monoclinic crystal structure at room temperature, which transforms into a hexagonal structure upon heating, as confirmed by temperature-dependent x-ray diffraction. The phase transitions at 408 K for TMCM-MnCl3 and 404 K for TMCM-Mn0.95Fe0.05Cl3 were further corroborated by differential scanning calorimetry. The step-like anomaly in the temperature dependence of dielectric permittivity observed in TMCM-MnCl3 indicates an improper ferroelectric transition. Piezoresponse force microscopy revealed regular ferroelectric domains. Additionally, Raman spectroscopy identify the vibrational modes of the crystal. Through UV-vis spectroscopy, we observed that the bandgap is tunable through moderate Fe doping. This comprehensive characterization highlights the potential of TMCM-MnCl3 for advanced applications.

KFM 14.6 Wed 17:00 P1

Investigation of hydrogen diffusion in $\mathbf{LiNbO_3}$ and $\mathbf{LiTaO_3}$ from density-functional theory — •Christa Fink and Simone Sanna — Institute for Theoretical Physics, Justus-Liebig-University, Heinrich-Buff-Ring 16, 35392 Giessen, Germany

Hydrogen is always present in $LiNbO_3$ and $LiTaO_3$ crystals. Therefore, the lattice locations of hydrogen within the crystal as well as its diffusion and mobility have been a matter of research for many years. While the energetically most favorable positions of hydrogen within the atomic lattice have been investigated intensely, there exist less investigations of diffusion paths and energy barriers. To fully understand the diffusion of hydrogen in $LiNbO_3$, $LiTaO_3$ and their solid solutions, we calculate energy barriers and three-dimensional minimum energy paths for hydrogen diffusion using the nudged elastic band method based on density-functional theory as implemented in VASP [1, 2]. Starting from the energetically most favorable position, we calculate minimum energy paths through the crystal towards the next equivalent position. We extend our calculations from the stoichiometric material to crystals with Lithium vacancies, which are the most common defects in LN and LT, for a better comparison to experimental results [3, 4].

[1] G. Kresse, J. Furthmüller, Computational Materials Science 6, 15 (1996). [2] G. Kresse, J. Furthmüller, Phys. Rev. B 54, 11169 (1996). [3] Kofahl, C. et al., Defect and Diffusion Forum, 429, 136-143 (2023). [4] Kofahl, C. et al., Solid State Ionics 403, 116383 (2023).

KFM 14.7 Wed 17:00 P1

Epitaxial Growth of Phase-Pure LiNbO3 Thin Films on LiTaO3 by Pulsed Laser Deposition (PLD) — •Hyeyeon Cho, Steffen Ganschow, René Bararugurika, and Jutta Schwarzkopf — Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, 12489 Berlin, Germany

Lithium niobate (LiNbO3) is a widely used material in electro-optical and electroacoustic devices due to its outstanding ferroelectric, piezoelectric, electro-optical, and nonlinear optical properties. Thin-film LiNbO3 offers significant advantages, including component miniaturization, broader bandwidths at higher frequencies, and reduced operational voltages. However, achieving these benefits requires the growth of phase-pure films with excellent crystalline quality, stoichiometric composition, and low surface roughness. Pulsed Laser Deposition (PLD) is a reliable method for growing LiNbO3 thin films, providing precise control over stoichiometry and the ability to produce high-quality epitaxial layers. However, high volatility of Li2O at enhanced temperatures during deposition often leads to Li-poor secondary phase formation. In this study, we investigated the effects of various deposition parameters to optimize the growth of phase-pure LiNbO3 films on LiTaO3. Key parameters, including substrate temperature, oxygen partial pressure, laser fluence, laser frequency, and target-substrate distance, were systematically varied. We also explored the use of lithium-rich targets to address lithium loss at high temperatures. X-ray diffraction (XRD) and atomic force microscopy (AFM) analyses confirmed the epitaxial growth of high-quality films with smooth surfaces.

KFM 14.8 Wed 17:00 P1

PALS of Hot-Rolled and Subsequently T4-Treated AlCuMgAg — •Lucian Mathes[1], Leon Heinl[2], Andreas Wagner[3], Maik Butterling[3], and Christoph Hugenschmidt[1] — [1]Heinz Maier-Leibnitz Zentrum, TU München — [2]Institute of Casting Research, Montanuniversität Leoben, Austria — [3]Helmholtz-Zentrum Dresden-Rossendorf, Institute of Radiation Physics

Positron annihilation lifetime spectroscopy (PALS) is a unique tool for studying the concentration and types of open-volume defects. We performed depth-resolved PALS to investigate such defects and the properties of precipitates in differently (heat) treated AlCuMgAg samples. Alloying AlCu with Ag has been shown to leverage the formation of the so-called Ω(Al$_2$Cu) phase, known for its high strength and thermal stability. We present PALS measurements of Al-4Cu-0.3Mg-0.7Ag containing Ω phase precipitation after hot-rolling and subsequent T4-treatment. Our findings showcase the high thermal stability of the Ω phase and that positron annihilation studies help in understading and optimizing the process of strength hardening AlCuMgAg alloys.

KFM 14.9 Wed 17:00 P1

Polycrystalline FeS as ultra-fast charging sodium-ion battery anode — •Zidong Wang and Yong Lei — Fachgebiet Angewandte Nanophysik, Institut für Physik & IMN MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Fast charging is considered a key development trend and a competitive advantage for sodium-ion battery (SIB) technology. Achieving fast-charging SIBs relies on developing electrode materials that combine high rate performance with excellent capacity retention. While iron sulfide, known for its high theoretical capacity, has shown potential, its fast-charging performance is hindered by poor rate performance due to volume expansion. Conventional approaches, such as compositing with carbon materials or adjusting the cut-off voltage, come with drawbacks*carbon composites reduce volumetric energy density, while cut-off voltage adjustments compromise capacity. Neither approach aligns well with practical applications. To address these challenges, we capitalized on the crystalline structural diversity of iron sulfides and successfully synthesized carbon-free polymorphic FeS. This material achieves high rate performance without relying on carbon additives or cut-off voltage adjustments, marking a significant step forward in SIB development. Impressively, anode demonstrates the best rate performance reported to date at an exceptionally high current density, achieving 236 mAh/g at 50 A/g.

KFM 14.10 Wed 17:00 P1

Nanoscale Thermal Expansion in Crystals Probed by Echo-Resolved Terahertz Spectroscopy — •Nicolas Sylvester Beermann, Andreas Gebauer, Wentao Zhang, Tomoki Hiraoka, Savio Fabretti, Hassan Hafez, and Dmitry Turchinovich — Fakultät für Physik, Universität Bielefeld, Universitätsstraße 25, 33615 Bielefeld, Germany

Thermal expansion of solids is a ubiquitous phenomenon in condensed matter physics [1]. However, its observation was out of limits for terahertz time-domain spectroscopy (THz-TDS) due to the relatively long sub-millimeter wavelength of THz radiation. To address this, we introduce echo-resolved THz spectroscopy (ERTS) that utilizes THz main and echo pulses in time-domain measurements to simultaneously determine frequency-dependent complex optical constants and material thickness [2]. By numerically solving complex transcendental transmission equations, ERTS allows for sample thickness measurements with deep-subwavelength precision on the order of $\lambda/1000$. We used the ERTS to analyze the THz-TDS data of magnesium oxide, sapphire, and gallium arsenide crystals measured in the temperature range of 10-300 K. The thermal expansion of the crystals on a sub-micrometer scale was measured, and the simple phonon model was applied to determine the material-specific Grüneisen parameters.

[1] K. Takenaka, Sci. Technol. Adv. Mater. 13, 13001 (2012)

[2] N. S. Beermann et al., Terahertz Time-Domain Spectroscopy for Simultaneous Measurement of Optical Constants, and Material Thickness with Deep-Subwavelength Precision, submitted manuscript

KFM 14.11 Wed 17:00 P1

Two Photon Absorption in Lithium niobate tantalate inspected via *z*-scan technique — •Niklas Dömer[1], Anton Pfannstiel[1], Steffen Ganschow[2], Mike Pionteck[2], Simone Sanna[3], and Mirco Imlau[1] — [1]Inst. Physics, Barbarastr. 7, Osnabrück Univ., Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, Berlin, Germany — [3]Center for Materials Research J.L.-Univ. Giessen, Heinrich-Buff-Ring 16 , Giessen, Germany

The knowledge of the nonlinear optical properties of polar oxide crystals, such as the two-photon absorption (TPA) coefficient β in lithium niobate (LN), is of significant importance for tailoring technological applications in (integrated) photonics. Here, we present the results of our studies on the dispersion properties $\beta(\lambda)$, i.e. the imaginary part of the third-order susceptibility $\chi^{(3)}_{\mathrm{Im}}$, in the model system lithium niobate tantalate (LNT, LiNb$_x$Ta$_{1-x}$O$_3$ with 0≤x≤1). Experimentally, an open-aperture z-scan experiment pumped by fs-pulses in the spectral range of 330 - 600 nm from an optical parametric amplifier (OPA) is used. The obtained results are compared with literature data for LN ($x = 0$) and LT ($x = 1$) and the non-vegard-like behavior of the band gap. In extension, the study is applied for the determination of the density of states with LN as an example. We discuss our findings with ab-initio calculations for LN and in the framework of transient absorption phenomena induced by TPA in LNT [N. Dömer, J. Koelmann *et al.*, New J. Phys. **26** (2024) 083027]. This work is financially supported by the DFG (projects IM37/13-1, GA 2403/7-1 and SA1948/3-1 within the research unit FOR 5044, ID: 426703838).

KFM 14.12 Wed 17:00 P1

Refractive Indices and Birefringence Behavior of Lithium Niobate Tantalate Solid Solutions — •Tobias Hehemann[1], Anton Pfannstiel[1], Steffen Ganschow[2], and Mirco Imlau[1] — [1]Institute of Physics, Osnabrueck University — [2]Leibniz-Institut für Kristallzüchtung, IKZ, Berlin

Lithium niobate tantalate solid solutions (LNT, LiNb$_{1-x}$Ta$_x$O$_3$ with $0 \leq x \leq 1$) exhibit a wide range of linear and nonlinear optical properties, that can be tuned by composition x. A unique feature is the disappearance of the birefringence Δn for x between $0.93 \leq x \leq 0.96$ [Wood *et al.*, J. Phys.: Condens. Matter **20** 235237 (2008)] enabling customized applications in photonics. While the dispersive behavior of the ordinary $n_o(\lambda)$ and extra-ordinary $n_e(\lambda)$ indices are well documented for the edge compositions LiNbO$_3$ (LN, x=0) and LiTaO$_3$ (LT, x=1), there remains a lack for LNT along x. In particular, nearly nothing is known about the structural relation between the index of refraction and composition. We here present our results for the dispersion behavior of n_o and n_e of LNT for several x, measured using an interferometric technique at specific wavelengths in the visible spectrum. Our data allow for a more detailed inspection of the birefringence $\Delta n = n_o - n_e$ of LNT at room temperature. The obtained data are analyzed and discussed in the context of existing literature, providing deeper insights into the relation between structure and optical properties of LNT. Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 426703838 (IM 37/13-1, GA 2403/7-1 of the FOR 5044).

KFM 14.13 Wed 17:00 P1

Surface and near-surface positron annihilation spectroscopy at very low positron energy — •Maximilian Suhr[1], Lucian Mathes[1,2], Vassily V. Burwitz[2], Danny R. Russell[1], and Christoph Hugenschmidt[1] — [1]Heinz Maier-Leibnitz Zentrum, TU München — [2]School of Natural Sciences, Physics Department, TU München

Positron annihilation spectroscopy is a highly sensitive tool for defect characterization in solids. We present the Setup for Low-Energy Positron Experiments (SLOPE) at TUM. This monoenergetic positron beam is realized via a high-activity ^{22}Na source, a W moderator, a sophisticated electromagnetic beam guidance system and two high purity Ge detectors. Our instrument features a state-of-the-art range of implantation energy, namely 3 eV to 40 keV, enabling bulk measurements as well as investigations of surfaces. With three different measurements we showcase the versatile applications of SLOPE: a full range depth profile of a W monocrystal, coincidence ratio curves of H-loaded Ni, and a valley-to-peak (positronium formation) scan of Cu and Kapton at very low implantation energies.

KFM 14.14 Wed 17:00 P1

Microscopic view into non-volatile resistive switching in Au/Prussian blue/Ag layer stacks — •Mohammed Fayis Kalady[1], Daniel Wolf[1], Michael Pohlitz[2], Christian Mueller[2], and Axel Lubk[1,3] — [1]Leibniz Institute for Solid State and Materials Research (IFW) Dresden, Helmholtzstraße 20, 01069 Dresden — [2]University of Applied Sciences Zwickau, 08056 Zwickau, Germany — [3]Institute of Solid State and Materials Physics, TU Dresden, Haeckelstraße 3, 01069 Dresden, Germany

Due to their distinct electrochemical properties, Prussian blue (PB) and its analogs (PBA) are emerging materials for memristor applications. This study uses transmission electron microscopy (TEM) techniques to explore resistive switching in PB-based memristors. Our work will utilize in-situ TEM to apply electrical bias, correlating nanoscale structural changes with electronic properties and employing methods like high-resolution TEM, electron energy-loss spectroscopy, and energy-filtered TEM. By changing the polarity of the external voltage, the Au/PB(A)/Ag is switched between two stable resistance states, the high resistance state and the low resistance state. The experimental technique seeks to elucidate the resistive switching mechanism, contributing to designing efficient and reliable memristor devices for advanced memory applications.

KFM 14.15 Wed 17:00 P1

Phonon Properties of perovskite oxides and halides — •Mwanaidi Mauwa Namisi and Benyao Sun — Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-University Bochum, Germany

Perovskite materials, which have proven useful in many areas including photovoltaics and ferroelectrics [1], are highly structurally unstable due to the dynamic nature of the metal-halide octahedra and cation off-centering. It is therefore evident that understanding the vibrational properties of these materials is crucial in their modelling and applications. Meanwhile, there is considerable research value in developing high-performance, environmentally friendly, and health-conscious lead-free ferroelectric materials [2, 3]. Particularly, BaTiO3- based lead-free perovskites have become a major research focus. However, systematic studies on BaTiO3-based superlattices combined with BaSnO3 remain scarce. Here, we investigate the phonon properties of perovskite oxides (BaSnO3) and halides (CsPbX3, (X=I, Br, Cl) and discuss the distortions, do- main structures by the anharmonicity. We also investigate how these instabilities couple with an external field and discuss the differences in the ferroelectric nature between perovskite oxides and halides. Additionally, structural optimization was performed on BaTiO3/BaSnO3 superlattices with varying Sn concentration gradients. References (1) Bergenti, I. Appl. Phys. 2022, 55, 033001. (2) Grunebohm, A., Madhura, M., Claude, E. Appl. Phys. Lett. 2015, 107,102901. (3) Grunebohm, A.; Marathe, M. Phys. Rev. Mat. 2020, 4,4417.

KFM 14.16 Wed 17:00 P1

Thermodynamics of Barium Boranate using DFT — •Markus Mehlhorn[1], Konrad Burkmann[2], Angus Demmer[2], Jakob Kraus[1], Franziska Habermann[2], Jürgen Seidel[2], Klaus Bohmhammel[2], Jens Kortus[1], and Florian Mertens[2] — [1]Institut für Theoretische Physik, TU Bergakademie Freiberg — [2]Institut für Physikalische Chemie, TU Bergakademie Freiberg

Materials containing high hydrogen content are interesting candidates for solid hydrogen storage. However, there are well-known fundamental challenges to address like the reversibility of the (de)-hydrogenation and sufficiently fast kinetics for these processes before possible applications. Here we present results on thermodynamic properties of $Ba(BH_4)_2$. Unfortunately, the isobaric heat capacity function of this material is not accessible experimentally. $Ba(BH_4)_2$ could not be synthesized in sufficient purity. Therefore we attempt to fill this gap by means of computations based on density functional theory using the PBEsol functional. The quasi harmonic approximation is used to describe volume expansion due to thermal effects assuming that for each fixed volume the harmonic approximation can be employed. For each volume the phonon density of states has been calculated via density functional perturbation theory. This procedure allows to calculate the Gibbs free energy and therefore gives access to thermodynamic properties like entropy and isobaric heat capacity. Comparing the heat capacity to other metal boranates, which have been synthesized and measured, one finds very similar behavior.

KFM 14.17 Wed 17:00 P1

3D nanoscale chemical analysis of WO_3 using Atom Probe Tomography — •Katharina Wolk[1], Jack T. Eckstein[2], Kasper A. Hunnestad[1], Constantinos A. Hatzoglou[1], Gustau Catalán[3], Ekhard K. H. Salje[2], Julia Glaum[1], and Dennis Meier[1] — [1]Department of Materials Science and Engineering, NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]Department of Earth Sciences, University of Cambridge, Cambridge, UK — [3]Institut Català de Nanociència i Nanotecnologia, Campus Universitat Autònoma de Barcelona, Bellaterra, Catalonia

The functional properties of oxides are closely linked to their chemical composition. The transition metal oxide WO_3 is notable for its structural versatility and unusual physical properties, such as the formation of superconducting ferroelastic domain walls. To understand the relation between local variations in chemical composition and material properties, we apply atom probe tomography (APT). APT offers compositional mapping in 3D with sub-nanometer spatial resolution and chemical sensitivity of 100 ppm. Using scanning electron microscopy, we image the ferroelastic domain structure in WO_3 single crystals and extract specimens from different regions of interest with a focused ion beam for the APT analysis. Based on 3D reconstructions, we investigate site-specific variations in chemical composition, exploring the oxidation state and potential formation of oxygen defects. Varying experimental APT parameters, such as laser energy, enables insights into optimizing compositional accuracy.

KFM 14.18 Wed 17:00 P1

Isovalent exchange of Al, Mg and Zr in strontium hexagallate (SrGa12O19) — •Finn. H. Bietz[1], Ch. Rhode[2], and S. 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

$SrGa_{12}O_{19}$ can be used as a substrate for the growth of barium hexaferrite, a ferrimagnetic and 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 lattice-matched growth and strain engineering of barium hexaferrite. A microscopic picture of the doping mechanisms and their effect on the lattice parameters is 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.

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 the $Ga^{(4)}$ site. While the results are in very good agreement with the experimental results in the case of Mg and Al doping, the experimentally determined lattice site of Zr differs from the theoretical predictions, suggesting the formation of defect complexes or co-doping related effects.

KFM 14.19 Wed 17:00 P1

Tailoring ferroelectric and magnetic properties in polycrystalline hexagonal manganites — Jonas Åmli Ingdal[1], •Ruben Skjelstad Dragland[1], Catalina Salazar[2], Ellinor Benedikte Anjali Lindström[1], Katharina Wolk[1], Tino Gottschall[2], Jiali He[1], Jan Schultheiss[1], and Dennis Meier[1] — [1]Norwegian University of Science and Technology (NTNU), Trondheim, Norway — [2]Dresden High Magnetic Field Laboratory, Dresden, Germany

Rare-earth hexagonal manganites are extensively studied for their diverse physical phenomena, including tunable electronic behavior at ferroelectric domain walls, pronounced magnetocaloric effects, and significant thermal Hall conductivity, which make them highly interesting as advanced multi-functional materials. The intriguing effects arise from the unique combination of improper ferroelectricity and antiferromagnetic ordering, which are intimately linked to the rare-earth ions.

In this study, we systematically investigate the role of the rare-earth atom on the ferroelectric and magnetic properties of h-RMnO3. Polycrystalline samples with R = Tm, Er, Y, Ho, and Dy are synthesized using a solid-state approach. Ferroelectric order is verified across all compositions using piezoresponse force microscopy. Direct adiabatic temperature change measurements in the cryogenic regime reveal a strong correlation between rare-earth magnetism and the caloric response. Our results highlight the possibility to tune both the ferroelectric order and magnetic responses, offering new opportunities for optimizing the system for envisioned applications.

KFM 14.20 Wed 17:00 P1

Characterizing Domains in GeTe using Atom Probe Tomography — •Jan Köttgen[1], Maria Häser[1], Lina Jäckering[1], Julian Pries[1], Carl-Friedrich Schön[1], Pengfei Cao[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]Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons ER-C, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

The thermoelectric GeTe undergoes a solid-state phase transition from its cubic to its rhombohedral crystal structure when cooled from the melt to room temperature. This phase transformation results in domains. In this study a polycrystalline GeTe bulk sample was investigated using atom probe tomography (APT), which enables the determination of the sample*s stoichiometry with atomic resolution. The

APT analysis revealed that different domains evaporate with different probabilities of multiple events (PME). Metavalent solids such as GeTe are known generally to exhibit a high PME in APT. Our experiments additionally show an anisotropy between different grains as observed in the PME. Using a correlative approach involving TEM, EBSD, AFM, SNOM, and DFT calculations, this effect can be attributed to an expansion of the unit cell and a concomitant change of the dielectric function. Our experiments open new avenues for atom probe tomography as a tool to investigate domains and the atomic distribution simultaneously crucial to improve the performance of thermoelectrics.

KFM 14.21 Wed 17:00 P1

Long-lived, pulse-induced transient absorption in LiNb$_{1-x}$Ta$_x$O$_3$ ($0 \leq x \leq 1$) solid solutions — •Julian Koelmann[1], Niklas Dömer[1], Mira Hesselink[1], Tobias Hehemann[1], Anton Pfannstiel[1], Felix Sauerwein[1,2], Laura Vittadello[1,2], Steffen Ganschow[3], and Mirco Imlau[1] — [1]Institute of Physics, Barbarastr. 7, Osnabrück University, Osnabrück, Germany — [2]Research Center for Cellular Nanoanalytics, Osnabrueck (CellNanOs), Osnabrueck University, Barbarastr. 11, Osnabrueck, 49076, Germany — [3]Leibniz-Institut für Kristallzüchtung, Max-Born-Straße 2, Berlin, Germany

Femto-/nanosecond pulse-induced, red and near-infrared absorption is studied in LiNb$_{1-x}$Ta$_x$O$_3$ (LNT) solid solutions with the aim of studying transient optical nonlinearities associated with optically generated small bound electron polarons. As a result, a long-lived transient absorption is uncovered for LNT which exceeds lifetimes and starting amplitudes of LiNbO$_3$ (LN) and LiTaO$_3$ (LT) by a significant factor. The transients provide strong evidence for an underlying hopping transport mechanism of small bound polarons. All findings are discussed in comparison to the model systems LN and LT within the framework of appropriate band models and optical generation of polarons via two-photon excitation. To explain the significant differences, the simultaneous presence of Nb$^{5+}_{\mathrm{Li}}$, Ta$^{5+}_{\mathrm{Li}}$ antisites, and Ta$^{5+}_{\mathrm{V}}$ interstitial defects is assumed for LNT. Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) * Project-ID 426703838 (IM 37/13-1, GA 2403/7-1 of the FOR 5044).

KFM 14.22 Wed 17:00 P1

Investigation of Pressure-Induced Dimerization in a Pyrene-based Dyad Crystal: Associated with Auxiliary exhibition of thermally Induced Intramolecular Charge Transfer — •Argha Barman[1], Agniezska Huć[2], and Krishnayan Basuroy[1] — [1]DESY, Hamburg, Germany — [2]University of Warsaw, Poland

We present the design and photophysical properties of a D-B-A dyad with N, N-dimethylaniline (DMA) as the electron donor and pyrene (Py) as the acceptor, linked by a -CH=CH- chain. The molecule crystallizes in the triclinic space group P-1, undergoing a reversible phase transition with solvent-dependent transition temperatures (e.g., 200K in cyclohexane, 198K in toluene, 209K in dichloromethane). Structural changes include variations in bond lengths and pyramidalization at the tertiary nitrogen atom, with persistent strong π***π stacking. Photophysical analysis reveals a small HOMO-LUMO gap (3.06 eV) and temperature-dependent dual fluorescence from locally excited (LE) and intramolecular charge transfer/excimer (ICT) states, with ICT emission diminishing above 220K. Under hydrostatic pressure (0.5*2.0 GPa), the crystals exhibit piezochromic behavior with emission redshift and quenching. These multifunctional properties make Py-CH=CH-DMA crystals promising for optoelectronics and pressure sensors.

KFM 14.23 Wed 17:00 P1

Multiscale modeling of intergranular corrosion in iron — •Vahid Jamebozorgi[1], Karsten Rasim[2], and Christian Schröder[1] — [1]Bielefeld Institute for Applied Materials Research, Bielefeld University of Applied Sciences and Arts, Interaktion 1, 33619 Bielefeld, Germany — [2]Faculty of Physics, Bielefeld University, Universitätsstraße 4, 33615 Bielefeld, Germany

Localized corrosion, particularly intergranular corrosion, causes a significant economical and structural challenge across various industries. An accurate predictive intergranular corrosion modeling should incorporate atomic scale details, including crystallographic aspects of grain boundaries, and their evolution by time increment. However, the size and scale limitations imposed by atomistic methods hinder the development of realistic models. To overcome these limitations, we propose a novel multiscale modeling approach that combines the detailed atomistic insights provided by reactive molecular dynamics with the computationally tractable finite element method. This multiscale strategy not only ensures the preservation of crucial atomistic details but also enables the simulation of larger spatial and temporal scales, thereby offering a comprehensive view on the microstructure*s evolution during the intergranular corrosion process.

KFM 14.24 Wed 17:00 P1

Theoretical Investigation of [100] Edge Dislocations in Ferroelectric Perovskites — •Himal Wijekoon[1], Pierre Hirel[2], and Anna Grünebohm[1] — [1]Interdisciplinary Center for Advanced Materials Simulation (ICAMS) and Center for Interface-Dominated High-performance Materials (ZGH), Ruhr Universität Bochum, Germany — [2]Université de Lille, CNRS, INRAE, Centrale Lille, UMET, F-59000 Lille, France

Ferroelectric switching is critically influenced by nucleation and pinning at defects within the material. Despite their significance particularly at strained interfaces, the role of dislocations on switching is however largely unexplored. We employ atomistic core-shell potentials [1] to demonstrate that edge dislocations can facilitate domain nucleation and reduce the coercive field. These findings suggest that a more comprehensive understanding of these defects could lead to improved material performance.

[1] M. Sepliarsky, A. Asthagiri, S.R. Phillpot, M.G. Stachiotti, and R.L. Migoni, Atomic-level simulation of ferroelectricity in oxide materials, Current Opinion in Solid State and Materials Science, 9(3):107-113, June 2005.

KFM 14.25 Wed 17:00 P1

Interaction of NaYF$_4$:Yb:Er Upconversion Nanoparticles with ultrashort laser pulses — •Leon Siemon[1], Felix Sauerwein[1], Thibault Mengis[1], Leonie Birk[2], Eike Wienbeuker[2], Markus Haase[2], Jacob Piehler[2], and Mirco Imlau[1] — [1]Institute of Physics, Osnabrück University, Germany — [2]Dept. of Biology/Chemistry, Osnabrück University

Lanthanide-doped upconversion nanoparticles (ucNP), such as NaYF$_4$:Yb:Er, play a significant role for future all-optical interrogation techniques of cellular systems due to their ability to convert infrared excitation light (980 nm/Yb-absorption) into green/red luminescence (520, 540, 660 nm/Er-emission). The corresponding conversion characteristics and energy transfer mechanisms have been studied extensively under continuous-wave illumination - however, so far, the interaction of ucNPs with ultrashort laser pulses has not been studied. We have adressed this question via diffuse fs-pulse reflectometry [C. Kijatkin *et al.*, Photonics **4** (2017) 11] of NaYF$_4$:Yb:Er nanoparticles ($d \approx 18\,nm$) exposed to 980 nm sub-ps-pulses ($\tau_{\mathrm{pulse}} > 40$ fs) at peak intensities up to 10^{14}W/m^2 and repetition rates down to 50 Hz. We observe severe differences in the intensity dependence, quantum yield and average power density that are attributed to modified population pathways in the energy diagram if the pulse duration falls below the resonant energy transfer time between Yb and Er ions. The impact of our findings for ucNP applications in cellular environments, particularly to reduce laser-induced cell damages, is discussed. Financial support DFG/RTG2900, 'nanomaterials@biomembranes'.

KFM 14.26 Wed 17:00 P1

Harmonic Nanoparticles: State-of-the-knowledge and future applications — •Moritz Domack[1], Jan Klenen[1], Mirco Imlau[1], and Laura Vittadello[2] — [1]Inst. Physics, Barbarastr. 7, Osnabrück Univ., Germany — [2]Laboratoire SYMME, 7 Chemin de Bellevue, Université Savoie Mont Blanc, France

Harmonic nanoparticles (HNPs) are receiving growing attention in anorganic chemistry, nanophotonics and life sciences due to their potential for upcoming imaging techniques. For instance, HNPs are successfully used as nanophotonics markers in the near-infrared (NIR) bio-optical windows (III) and (IV), so-called NIR-to-NIR imaging [L. Vittadello *et al.*, Nanomaterials **11** (2021) 3193], as well as for destruction free in-vivo imaging [L. Vittadello *et al.*, Opt. Mater. Express **11.7** (2021) 1953-1969]. HNPs are based on polar oxide nanocrystals with pronounced nonlinear optical response, such as sodium niobate (NaNbO$_3$) or potassium niobate (KNbO$_3$) and can already be synthesized at the nanometer scale (<100 nm), e.g. via hydrothermal synthesis [N. Kohlenbach *et al.*, Nanoscale **12** (2020) 19223], but also surface-functionalized. Nonlinear Diffuse femtosecond-pulse reflectometry of powder-pressed-HNP-samples has been established as major tool for characterization of the nonlinear optical properties [C. Kijatkin *et al.*, Photonics **4.1** (2017) 11]. We here give insight to the state-of-the-art processing routine of HNPs from synthesis, via characterization to applications and highlight upcoming fields, particularly in the framework of all-optical interrogation of cellular environments. Financial support by the DFG/RTG2900, 'nanomaterials@biomembranes'.

KFM 15: Crystal Structure Defects / Real Structure / Microstructure

Chair: Theo Scherer (Karlsruhe Institute of Technology)

Time: Thursday 9:30–13:15 Location: H9

Invited Talk KFM 15.1 Thu 9:30 H9

Is CVD diamond now ready to become an electronic material? — •Philippe Bergonzo — University College London UK — Seki Diamond System, San Jose CA, USA

CVD Diamond is an exceptional material combining superlative properties like electronic properties, thermal conductivity, biocompatibility, radiation resistance, and optical properties. These advantages make diamond an excellent material for a broad range of applications, including radiation detectors, high transparency windows, electronic devices, quantum devices, sensors, etc. Remarkable devices have been fabricated and are still respected as a reference. But still, can diamond come out of the lab to become a competitive device material? Although diamond synthesis is a pretty well-established technique, there are still more than 80% of the machines growing diamond on the planet that grow it to make gemstones. And this has always inhibited the progress this material deserved. Only very recently, and with the recent huge downturn that affects the gem business, one can consider that we may have reached an inflection point where CVD diamond may soon benefit from being something else than a gemstone. Potentially, innovative developments for physics may not be kept secret because they could be more valuable for the gem market, if this latter one is collapsing. In this context, how can we facilitate this progress? Drawing from typical cases where diamond-based devices are used for specific applications, examples will be used to illustrate material opportunities and challenges towards diamond to become a standard for device applications.

KFM 15.2 Thu 10:00 H9

Numerical analyses and loss tangent measurements for the W7-X ECRH gyrotron diamond output windows — •Gaetano Aiello[1], Andreas Meier[1], Heinrich Peter Laqua[2], Theo Scherer[1], Sabine Schreck[1], and Dirk Strauss[1] — [1]KIT, Karlsruhe, Germany — [2]IPP, Greifswald, Germany

The 140 GHz 1 MW gyrotron for the electron cyclotron resonance heating (ECRH) system at the stellarator Wendelstein 7-X (W7-X) is being upgraded to 1.5 MW continuous wave operation to increase the total heating power for achieving operating regimes with high plasma beta and low collisionality. The gyrotron features a chemical vapor deposition (CVD) polycrystalline diamond window with an aperture of 88 mm and a disk of 1.8 mm thickness and 106 mm diameter. In this work, numerical analyses of the window are shown with loss tangent values provided by experimental measurements on 25 bare diamond disks. Computational fluid dynamics (CFD) conjugated heat transfer and structural analyses were carried out to check the window performance at 1.5 MW operation, when cooled by water and silicon oil Dow Corning 200(R) 5cSt.

KFM 15.3 Thu 10:15 H9

Single- and polycrystalline diamond characterization with superconducting microresonators — •Francesco Mazzocchi[1], Martin Neidig[2], Sebastian Kempf[2], Dirk Strauss[1], and Theo Scherer[1] — [1]Karlsruhe Institute Of Technology IAM-AWP — [2]Karlsruhe Institute Of Technology IMS

The development of high optical quality, ultra-low-loss single-crystal diamond windows is essential for the realization of future nuclear fusion facilities, such as DEMO, due to the anticipated increase in power for microwave ECRH systems. So far, accurate measurement of the dielectric properties (ϵr and tanδ) of these materials has primarily relied on Fabry-Perot microwave resonators in different setups, with a resolution limit around 1E-5 in the determination of the loss tangent. Superconducting thin-film resonators, capable of reach Q factors in excess of 1E6, have the potential to assess the dielectric characteristics of ultra-low-loss materials like single- and polycrystalline diamond while offering a significant boost in resolution when compared to the state-of-the-art Fabry-Perot resonance cavities. We hereby report measurements performed at low (4 - 9 K) an ultra-low (10 - 700 mK) temperatures of several samples including single and poly-crystalline diamond. The samples have been grown with different techniques, including CVD, cloning and HPHT processes.

KFM 15.4 Thu 10:30 H9

Simulated nano-extrusion of graphene hyperbolic pseudosphere surfaces — •Peter Klaver[1], Alfredo Iorio[2], Ruggero Gabbrielli[3], and Dominik Legut[1] — [1]VSB Technical University of Ostrava, Ostrava, Czech Republic — [2]Charles University, Prague, Czech Republic — [3]Independent researcher

We produce curved graphene hyperbolic pseudosphere surfaces in molecular dynamics (MD) simulation of a nano-scale extrusion process. During the extrusion process the carbon atoms form pentagons, hexagons and heptagons and such a mixture is unrealistically less stable than pure graphite or diamond. During relaxation and lengthy high temperature annealing after the extrusion process, polycrystalline curved graphene with a limited number of point defects is formed. The point defects cause bending of the graphene and the pseudosphere edges even more. When these free edges are removed from the simulations by attaching periodic flat graphene sheets to the pseudosphere edges, the carbon atoms assume positions with a root mean square deviation of some tenths of Å from the mathematical hyperbolic pseudosphere surface. The hyperbolic pseudospheres proved to be mechanically stable against large shearing and elongation deformations as well as against annealing at 1500 K. Our methodology is easy to use, employing the REBO2 carbon interaction potential within the open source MD code LAMMPS. Our method offers a practical way to create simulated stable, curved graphene surfaces with a wide variety of desired shapes. It allows for the testing in advance of the stability of graphene shapes that are to be produced experimentally.

KFM 15.5 Thu 10:45 H9

Inverted Designs of Dielectric Metasurfaces Based on TiO$_2$.: A Study on Quasi-Bound States in Continuum (qBIC) — •Justin Schulz[1], Jack Dobie[1,2], Oisin McCormack[1,2], Yongliang Zhang[1], Hodjat Hajian[1], Owen Moynihan[2], Brian Corbett[2], and A. Louise Bradley[1,2] — [1]School of Physics, Trinity College Dublin, Dublin 2, Ireland — [2]IPIC, Tyndall, University College Cork, Cork, Ireland

Dielectric metasurfaces, engineered to manipulate light primarily by controlling the phase and amplitude of the scattered light, have garnered significant interest in recent years, particularly due to their ability to support quasi-Bound States in Continuum (qBIC).

Building upon previous work on slotted disk metasurfaces fabricated in Si$_3$N$_4$, we investigate inverted TiO$_2$-based designs. TiO$_2$, with its high refractive index, offers distinct advantages in enhancing the resonance properties of dielectric metasurfaces, enabling more efficient light-matter interactions. A key objective of this work is to perform a comparative analysis between slotted disk structures and their inverted counterparts, with a focus on their respective lattice and qBIC modes. Future prospects of TiO$_2$-based dielectric metasurfaces and the potential applications in low-energy switching and polariton lasing are discussed, with a particular focus on their integration with transition-metal dichalcogenide (TMDC) monolayers or quantum dots. This project is funded through; Taighde Éireann/Research Ireland Frontiers for the Future Award - SFI-21/FFP-P/10187, 12/RC/2278_2, and 12/RC/2276_P2.

15 Minutes Break

KFM 15.6 Thu 11:15 H9

Phase modifications in Beta-Gallium Oxide via Focus ion beam irradiations — •Umutcan Bektas, Nico Klingner, Paul Chekhonin, Fabian Ganss, Rene Hübner, Maciej Oskar Liedke, and Gregor Hlawacek — Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Gallium oxide (Ga2O3) is a highly versatile material with power electronics, optoelectronics, and battery technologies applications. Among its polymorphs, monoclinic β-Ga2O3 is the most chemically and thermally stable phase. However, managing the metastable polymorph phases remains challenging, and the fabrication technology for nanoscale structures is still under development. We aim better to understand the polymorph conversion mechanisms under ion irradiation. In this study, we investigate the β-Ga2O3 samples irradiated with different ions and fluences, together with α- and κ-Ga2O3 thin films. Focused ion beam (FIB) irradiation was used to locally modify the samples under controlled conditions by varying the ion beam current, size, spacing, scan type, and ion species. The irradiated regions were characterized using electron backscatter diffraction and transmission electron microscopy to analyze structural changes. Broad beam irradiation experiments were complemented by positron annihilation spectroscopy methods to determine defect types and concentrations. Initial results indicate that spatially resolved polymorph transitions can be achieved using FIB irradiation. In addition, the defect size and concentration were found to depend on the polymorph and the implanted ion species, providing critical into defect engineering in Ga2O3.

KFM 15.7 Thu 11:30 H9

An EXAFS analysis of the laser-driven tetragonal to cubic phase-transition in BaTiO$_3$ — •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 first step along this road, the information contained in a difference-EXAFS scan between the pumped and unpumped state is analyzed.

As proof of concept, the structural cubic to tetragonal phase transition in ferroelectric BaTiO$_3$ is analyzed. The coexistence of displacive and order-disorder phenomena accompanying this transition is debated in the literature of this widely investigated material. Difference-EXAFS scans at the Ti-K and Ba-L$_3$ edge between the tetragonal and cubic phase provide a direct way to investigate changes in 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 thermal and structural contributions.

We thank the Deutsche Forschungsgemeinschaft (in the framework of the Collaborative Research Center 1242) for financial support.

KFM 15.8 Thu 11:45 H9

Dislocation correlations in GaN epitaxial films revealed by EBSD and XRD — •Domenik Spallek, Vladimir M. Kaganer, Philipp John, Oliver Brandt, and Jonas Lähnemann — Paul-Drude-Institut für Festkörperelektronik, Berlin, Germany

Threading dislocations in group-III nitrides are omnipresent and are a challenge especially in heteroepitaxial growth for device applications. However, the correlation of individual dislocations with each other and the resulting screening of the strain is often disregarded although it is a necessity to describe elastic energies in an extended crystal.

In this study, two GaN epitaxial layers with threading dislocation densities (TDD) of 5×10^8 cm^{-2} and 1.8×10^{10} cm^{-2} are investigated by x-ray diffraction (XRD) and high-resolution electron backscatter diffraction (HR-EBSD), complemented by Monte Carlo simulations to model and interpret the experimental results.

While the XRD measurement directly gives quantitative results about the average strain in the illuminated area, a cross-correlation analysis of Kikuchi patterns results in spatially-resolved maps for the components of the strain and rotation tensors. Through an analysis of the strain-strain correlation functions for the measured and simulated maps, it is found that the spatial resolution in the HR-EBSD maps is highly anisotropic. Furthermore, we discover that the strain is significantly underestimated for higher dislocation densities. As main result, the screening distances for dislocations were determined as 2 μm and 0.3 μm for the sample with the lower and higher TDD, respectively.

KFM 15.9 Thu 12:00 H9

Multiscale modeling of intergranular corrosion in iron — •Vahid Jamebozorgi[1], Karsten Rasim[2], and Christian Schröder[3] — [1]Bielefeld Institute for Applied Materials Research, Bielefeld University of Applied Sciences and Arts, Interaktion 1, 33619 Bielefeld, Germany — [2]Faculty of Physics, Bielefeld University, Universitätsstraße 4, 33615 Bielefeld, Germany — [3]Bielefeld Institute for Applied Materials Research, Bielefeld University of Applied Sciences and Arts, Interaktion 1, 33619 Bielefeld, Germany

Localized corrosion, particularly intergranular corrosion, causes a significant economical and structural challenge across various industries. An accurate predictive intergranular corrosion modeling should incorporate atomic scale details, including crystallographic aspects of grain boundaries, and their evolution by time increment. However, the size and scale limitations imposed by atomistic methods hinder the development of realistic models. To overcome these limitations, we propose a novel multiscale modeling approach that combines the detailed atomistic insights provided by reactive molecular dynamics with the computationally tractable finite element method. This multiscale strategy not only ensures the preservation of crucial atomistic details but also enables the simulation of larger spatial and temporal scales, thereby offering a comprehensive view on the microstructure*s evolution during the intergranular corrosion process.

15 Minutes Break

KFM 15.10 Thu 12:30 H9

Landau Theory for Quasicrystals at the Mesoscale — •Marcello De Donno[1], Luiza Angheluta[2], Ken R. Elder[3], and Marco Salvalaglio[1,4] — [1]Institute of Scientific Computing, TU Dresden, 01062 Dresden, Germany — [2]Njord Centre, Department of Physics, University of Oslo, 0371 Oslo, Norway — [3]Department of Physics, Oakland University, Rochester, Michigan 48309, USA — [4]Dresden Center for Computational Materials Science (DCMS), TU Dresden, 01062 Dresden, Germany

Quasicrystals challenge traditional concepts of crystallinity by exhibiting ordered yet aperiodic atomic structures. Their peculiar atomic arrangements give rise to exceptional physical properties, including high hardness, low friction, and remarkable wear resistance, making them worth exploring for high-performance engineering applications. Additionally, their slow dislocation creep leads to high-temperature strength and stability in plastic regimes. We present a mesoscale field theory that unifies the modeling of growth, elasticity, and dislocations in quasicrystals. Using the amplitude formulation of the density-wave representation, our approach models the dynamics of quasicrystals through a free energy functional for complex amplitudes, with non-conserved dissipative dynamics describing their evolution. By specifying only the lattice structure in reciprocal space, our theory self-consistently captures elasticity-including phononic and phasonic deformations-along with defect nucleation and motion. Predictions include the kinematics of dislocations and the formation of semi-coherent interfaces, offering new insights into the mechanics of quasicrystals.

KFM 15.11 Thu 12:45 H9

An all-order phonon approach to thermal diffuse scattering — •Benjamin Fahl and Arkadiy Simonov — ETH,Zurich,Switzerland

Phonons play a role in various phenomena, from superconductivity through phonon-electron coupling and spintronics via phonon-spin interactions, to dynamical stability of solids, and are fundamental to elastic properties. They can be probed by measuring Thermal Diffuse Scattering (TDS) from single crystals. However, modelling of the TDS, is a computational challenge due to the number of intensities in the experiment. With existing software, like AB2TDS, the full experiment can be calculated only in one- or two-phonon approximations. Approximations of higher order are possible, but are computationally expensive and can be performed only on small portions of reciprocal space. In this work, we propose a new method for modeling and fitting TDS signals using joint atomic displacement parameters in YELL. This approach uses the crystal's dynamical matrix as input, which is derived by various methods including universal potentials, DFT, or approximated from elastic constants. By using a Fast-Fourier Transform, our method can quickly calculate large volumes of TDS in infinite phonon approximation. This development will enhance the 3D-ΔPDF suite, enabling extraction of elastic constants from various materials and extending to the analysis of high-amplitude soft phonons, which are relevant in negative thermal expansion materials like ScF$_3$. The softwares capability to handle higher-order phonon contributions makes it particularly valuable for systems where these effects are significant, addressing a current gap in available tools.

KFM 15.12 Thu 13:00 H9

Solving the phase problem: retrieving complex structure factors using Large-Angle Rocking-Beam Electron Diffraction — •Sam Fairman[1], Grigory Kornilov[2], Benedikt Haas[2], Zbignew Galazka[3], Adnan Hammud[4], Niklas Delby[5], and Christoph T. Koch[2] — [1]Physikalisch Technische Bundesanstalt, Berlin, Germany — [2]Humboldt Universität zu Berlin, Berlin, Germany — [3]Leibniz-Institut für Kristallzüchtung, Berlin, Germany — [4]Fritz-Haber-Institut, Berlin, Germany — [5]Nion Company, Kirkland, WA, USA

X-ray crystallography phasing methods have previously been successfully applied to electron diffraction experiments. However, dynamical scattering, caused by the electron's much larger scattering cross section, is normally viewed as a hindrance to structural determination and is mitigated, e.g. by continuous rotation or precession. Presented here is an ab-initio method that makes use of dynamical scattering to solve the phase problem directly from experimental data. A custom weighting scheme is combined with the ADAM optimizer to directly fit the complex structure factors in the Bloch-wave formalism to Large-Angle Rocking-Beam Electron Diffraction data. Our method allows for an approximate 5−fold increase in spatial resolution compared to the largest spatial frequency directly measured. This recovery of resolution is ideal for beam sensitive materials where high order diffraction data is impossible to measure. Simulated and experimental results are presented for non-centrosymmetric GaN and centrosymmetric $\beta-\mathrm{Ga_2O_3}$.

KFM 16: Perovskite and Photovoltaics II (joint session HL/KFM)

Time: Thursday 9:30–13:00 Location: H13

KFM 16.1 Thu 9:30 H13

Optical Simulations of Nanophotonic Back Contacts for Light Management in Ultrathin CIGSe Solar Cells — •Daniel Jiménez Tejero[1], Merve Demir[1], Bodo Fuhrmann[2], Roland Scheer[1], Ralf Wehrspohn[1], and Alexander Sprafke[1,2] — [1]Martin-Luther-Universität Halle-Wittenberg, Institut für Physik, Von-Danckelmann-Platz 3, 06120 Halle (Saale) — [2]MLU, Interdisziplinäres Zentrum für Materialwissenschaften, Nanotechnikum Weinberg, Heinrich-Damerow-Str. 4, 06120 Halle (Saale)

The development of ultrathin-film Cu(In,Ga)$\mathrm{Se_2}$ (CIGSe) solar cells aims to reduce material usage and expand applications such as bifacial or tandem solar cells. However, CIGSe absorber layers with thicknesses below 1 μm exhibit diminished light absorption, particularly for wavelengths near the bandgap, leading to decreased power conversion efficiency. This can be counteracted by utilising functional back contacts that effectively increase the optical path length within the absorber layer through scattering, reflection, and nanophotonic mechanisms.

This work employs nano-optical simulations to investigate the potential of $\mathrm{SiO_2}$ nanostructures on a flat gold back contact for enhancing the performance of CIGSe solar cells. By solving the Maxwell equations using the finite element method, the quantum efficiency and photocurrent under ideal charge carrier collection conditions are computed, enabling a comparison of various nanostructure geometries viable for fabrication. We find photocurrents higher than those of conventional CIGSe solar cells with an absorber thickness of 4 μm, indicating the potential of our light management approach.

KFM 16.2 Thu 9:45 H13

Stabilizing Perovskite Solar Cells by Organic Salts Under One Full Sun and Maximum Power Point Tracking — •Zekarias Teklu Gebremichael[1,2], Niklas Manikowsky[2,3], Chikezie Williams Ugokwe[1,2], Bashudev Bhandari[2,3], Ulrich S. Schubert[1,2], and Harald Hoppe[1,2] — [1]Laboratory of Organic and Macromolecular Chemistry (IOMC Jena), Friedrich-Schiller- University Jena, Jena, Germany — [2]Center for Energy and Environmental Chemistry Jena (CEEC Jena), Friedrich-Schiller-University Jena, Jena, Germany — [3]Faculty of Physics and Astronomy, Friedrich-Schiller- University Jena, Jena, Germany

The use of organic halide salts to passivate metal halide perovskite (MHP) surfaces have been studied extensively. Passivating the surface defects of the MHP is of critical importance for realizing high-efficiency and stability of perovskite solar cells (PSCs). Here we discuss the success of a multifunctional organic salt used as passivation material for grain boundary defects and as molecular sealing layer in terms of stabilization. To assess the stability of PSCs, maximum power point tracking is seemingly the most realistic condition for the ageing test. Here, PSCs made from the four cation RbCsMAFA based perovskite absorber layer were aged under full light with maximum power point tracking and in addition they were tested periodically by IV-characterization, in order to yield all photovoltaic parameters for improved understanding of the ageing process.

KFM 16.3 Thu 10:00 H13

Hyperuniform discordered structures for Light Management in Ultrathin CIGSe Solar Cells — •Katharina Trockel[1], Merve Demir[1], Frank Syrowatka[2], Ralf Wehrspohn[1], Roland Scheer[1], and Alexander Sprafke[1,2] — [1]Martin Luther University Halle-Wittenberg, Institute of Physics, 06120 Halle, Germany — [2]Martin Luther University Halle-Wittenberg, Interdisciplinary Center of Materials Science, 06120 Halle, Germany

Ultrathinfilm Cu(In,Ga)Se2 (CIGSe) solar cells are highly attractive due to their reduced material consumption and low manufacturing costs. While conventional CIGSe solar cells can achieve efficiencies of up to 21 %, increasing the efficiency of ultrathin solar cells remains a key research objective to enhance their competitiveness. A promising approach involves extending the optical path length in the absorber layer by integrating textured structures at the back or front contact of the solar cell. Most studies focus on periodic textures.

In this work, we investigate hyperuniform disordered (HuD) structures for light management in ultrathin CIGSe solar cells. The HuD structures are fabricated using polymethyl methacrylate (PMMA) particles deposited onto the back contact of the solar cells. These particles are covered with an indium tin oxide (ITO) layer and subsequently removed via a calcination process. The resulting ITO layer functions as a textured back contact, improving both light scattering and electrical performance.

First experimental results on the implementation of CIGSe solar cells with integrated HuD structures will be presented.

KFM 16.4 Thu 10:15 H13

A Theoretical study of charge transport properties in perovskite analogues for high performance solar cells. — •Prerna Prerna[1,2] and Harald Oberhofer[1,2] — [1]University of Bayreuth — [2]Bavarian Center for Battery Technology, Bayreuth, Germany

Perovskite materials have emerged as promising candidates in solar cell technology, offering exceptional efficiency and affordability. Their remarkable performance, surpassing that of conventional inorganic materials, has placed them at the forefront of next-generation solar cell research, attracting significant attention from both academic and industry.

To harness their potential, we are investigating their charge transport properties using first-principles calculations (DFT) within the band transport regime. Our focus includes the calculation of carrier mobility, scattering rates and relaxation time through a detailed analysis of effective mass, deformation potential, and elastic properties. Our studies also incorporate the effects of structural deformations, aiming to align theoretical predictions with experimental results, providing deeper insights into the transport mechanisms in perovskites.

Furthermore, we are exploring the anisotropic nature of perovskites to understand directional dependencies in their electronic and mechanical properties. This anisotropy analysis is crucial for optimizing their performance and tailoring their application in advanced solar technologies. Together, these studies offer a comprehensive approach to enhancing the functionality of perovskites for cutting-edge solar energy solutions.

KFM 16.5 Thu 10:30 H13

THz-Driven Phonon Fingerprints of Hidden Symmetry Breaking in 2D Layered Hybrid Perovskites — •Joanna M. Urban[1], Michael S. Spencer[1], Maximilian Frenzel[1], Gaëlle Trippé- Allard[2], Marie Cherasse[1,3], Charlotte Berrezueta Palacios[4], Olga Minakova[1], Luca Perfetti[3], Stephanie Reich[4], Martin Wolf[1], Emmanuelle Deleporte[2], and Sebastian F. Maehrlein[1,5,6] — [1]FHI Berlin — [2]LuMIn, Université

Paris-Saclay, ENS Paris-Saclay, CentraleSupélec, CNRS — [3]LSI, CEA/DRF/IRAMIS, CNRS, École Polytechnique, Institut Polytechnique de Paris — [4]FU Berlin — [5]HZDR — [6]TU Dresden

Metal halide perovskites (MHPs) are emerging as promising candidates for spintronic applications. In MHPs which lack inversion symmetry, strong spin-orbit coupling induces the Rashba-Dresselhaus effect, allowing spin current control. Here we use intense THz fields to coherently drive lattice dynamics in Ruddlesden-Popper 2D layered perovskites. We identify simultaneous IR and Raman activity of specific inorganic cage modes, suggesting the presence of inversion symmetry breaking despite the globally centrosymmetric crystal structure. By exploring the driving pathways of coherent phonons bearing the signatures of broken inversion symmetry, we lay the groundwork for simultaneous ultrafast control of optoelectronic and spintronic properties in 2D MHPs.

KFM 16.6 Thu 10:45 H13

Analysis of real-space transport channels in halide perovskites — •Frederik Vonhoff[1], Maximilian J. Schilcher[1], David R. Reichman[2], and David A. Egger[1] — [1]Physics Department, TUM School of Natural Sciences, Technical University of Munich, James-Franck-Straße 1, 85748 Garching, Germany — [2]Department of Chemistry, Columbia University, New York, NY 10027, USA

The charge carrier transport is a crucial factor for the performance of halide perovskites as solar energy conversion material. However, standard semiconductor transport theories fail to model the transport properties of halide perovskites because of their unusual transport behavior triggered by the anharmonic nuclear dynamics and its dynamic disorder [1]. For an accurate prediction of electron and hole mobilities of $MAPbI_3$ and $MAPbBr_3$, we capture the anharmonicity with molecular dynamics trajectories as a backbone for a time-dependent real-space hopping model [2,3] parametrized with hybrid density functional theory. With our transport model, we trace back the transport behavior of $MAPbI_3$ and $MAPbBr_3$ to their band structures via the projected density of states and the dynamics in the orbital occupation configurations. The real-space nature of our model allows us to determine the microscopic transport mechanisms which are driven by three transport channels.

[1] M. J. Schilcher et al, ACS Energy Lett. 6, 2162 (2021)
[2] M. Z. Mayers et al, Nano Lett. 18, 8041 (2018)
[3] M. J. Schilcher et al, Phys. Rev. Mater. 7, L081601 (2023)

15 min. break

KFM 16.7 Thu 11:15 H13

Unravelling how solvated PbI_2 Crystallites precede the Crystallization of Lead Halide Perovskites by UV/VIS In-Situ measurements — •Maximilian Spies[1], Simon Biberger[1], Fabian Eller[2], Eva M. Herzig[2], and Anna Köhler[1] — [1]Soft Matter Optoelectronics, University of Bayreuth, Bayreuth, Germany — [2]Dynamics and Structure Formation, University of Bayreuth, Bayreuth, Germany

The fabrication of reproducible, high-quality lead iodide perovskite films via solution-based methods requires a comprehensive understanding of crystallization dynamics. The formation of perovskite films is primarily dictated by the composition of the precursor solution and its processing conditions. In this study, we present an in-situ absorption study, i.e. during spin-coating, of the critical pre-nucleation stage to unravel the formation mechanisms of lead iodide perovskite films. We tracked the evolution of iodoplumbate complexes within the precursor solution and identified a distinctive absorption feature at 3.15 eV, emerging prior to film formation. We attribute this feature to the development of a crystalline PbI_2-DMF solvated (PDS) phase. In particular, we propose that PDS crystallites serve as precursors to the crystalline perovskite phase, acting as nucleation sites within the precursor solution. Notably, the amount of this PDS phase correlates closely with the concentration of the solution layer during spin coating, suggesting that increasing concentration promotes PDS formation. These findings provide valuable insights into the early stages of perovskite crystallization.

KFM 16.8 Thu 11:30 H13

Effect of a 2D/3D Heterostructure on Contact Formation of the Double Perovskite $Cs_2AgBiBr_6$ with Hole Transport Layers Revealed by In-Situ KPFM Growth Studies — •Tim P. Schneider and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

The application of a 2D perovskite interlayer caused by surface modification with organic amines between the absorber and contact layers is widely known to significantly improve the performance of perovskite solar cells. This has already been approved as well for the lead-free double perovskite absorber $Cs_2AgBiBr_6$. To better understand the interaction of the contact layer with the 2D/3D heterostructure, in this work, film growth of Copper Phthalocyanine (CuPc), used as a model hole conductor, onto $Cs_2AgBiBr_6$ modified by different 2D phases was investigated and compared to bare $Cs_2AgBiBr_6$. Employing solar cell geometry, the morphology and work function were inspected intermittently to the evaporation of CuPc by Kelvin Probe Force Microscopy at different average film thickness. The energy alignment was revealed to be more confined on the 2D/3D heterostructures and the growth of CuPc was improved: a more homogenous growth led to formation of closed films even at early stages of deposition. These changes in growth and energy alignment are accompanied by preferential formation of different crystal phases in the CuPc.

KFM 16.9 Thu 11:45 H13

The influence of oxygen and water on $MAPbI_3$ absorber materials measured with in-situ TRPL and PES — •P. Stötzner[1], M. Müller[1], T. Schulz[1], P. Pistor[2], R. Scheer[1], and S. Förster[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Germany — [2]Universidad Pablo de Olavide Sevilla, Spain

Methylammonium lead halide perovskites ($MAPbI_3$) are promising thin-film solar cell absorber materials, but their response to environmental conditions like moisture and oxygen is not well understood. Here, we present a combined photoelectron spectroscopy (PES) and in-situ time-resolved photoluminescence (TRPL) study conducted in one ultrahigh vacuum system, which allows for studying changes in the chemical composition, the electronic structure and charge carrier lifetime. The setup is completed by a high-pressure gas cell enabling for controlled exposure to specific environments.

For $MAPbI_3$, we observe a significant reduction of the charge carrier lifetime compared to ex-situ TRPL measurements. To bridge between the different measurement environments, we conducted additional TRPL measurements in a closed cell having the as-grown sample in nitrogen atmosphere, which is pumped to high vacuum. These results show a decreased lifetime in vacuum but an increased lifetime linked to air contact. Consequently, we exposed $MAPbI_3$ samples to water vapor to mimic air contact, resulting in increased lifetime but also in a decomposition of $MAPbI_3$. Pure oxygen exposure did not affect the lifetime. Surprisingly, the simultaneous exposure to both gases did not show the detrimental effect of water.

KFM 16.10 Thu 12:00 H13

On the Nature of Light Induced Defects in MAPI Thin Films: Long Pulses in TrPL — •Maxim Simmonds and Eva Unger — Kekuléstraße 5, 12489 Berlin, Germany

Metal-halide perovskite (MHP) semiconductors are highly relevant candidates for the fabrication of next generation solar cells but suffer from instability under continuous irradiation. This has been shown with a non-constant steady state PL during illumination. In order to better understand the evolution of recombination mechanisms at play, we usetime resolved photoluminescence (trPL) and differential lifetime plots.

Therefore, in this presentation, we will focus on methylammonium-lead-iodide (MAPI) thin films and the (ir)reversible introduction of traps triggered by quasi-continuous illumination. For this, we develop a method that uses long pulses of light in combination with trPL counting schemes, calling it long pulsed trPL (LP-trPL). From the method, we observe the inclusion of long lived and non-deep trapping sites due to continuous illumination. The data also suggests a highly asymmetric mechanism of trap formation, where trap annihilation is much slower than observed formation. We conclude that previously described mechanisms of iodine outgassing is compatible with the observed shallow nature of traps introduced as well as the asymmetric process of formation/annihilation.

KFM 16.11 Thu 12:15 H13

Phase evolution of sequential evaporated $(FA/Cs)SnI_3$ halide perovskite thin films via in situ X-ray diffraction — •Pu-Chou Lin[1], Josha Damm[1], Roland Scheer[1], and Paul Pistor[2] — [1]Institute of Physics, Photovoltaics Group, Martin-Luther-University, 06120 Halle, Germany — [2]Departamento de Sistemas Físicos, Universidad Pablo de Olavide, 41013 Sevilla, Spain

Tin-based halide perovskites, particularly $FASnI_3$ and $CsSnI_3$, offer promising potential for photovoltaic applications. This study employs in situ X-ray diffraction to investigate these materials' real-time growth mechanisms and thermal stability during sequential vapor deposition and annealing. Our results demonstrate that the deposition sequence significantly impacts the resulting perovskite film quality. For $FASnI_3$, the SnI_2-FAI stack yields superior, cavity-free films compared to the FAI-SnI_2 stack. This suggests that FAI is the primary diffusing species, with $FASnI_3$ forming at interfaces and completing its formation around 160°C. In contrast, the $CsSnI_3$ system exhibits more complex behavior. The SnI_2-CsI sequence leads to the formation of the intermediate phase Cs_2SnI_6, while the CsI-SnI_2 sequence directly forms $CsSnI_3$ with minimal defect formation. This suggests that SnI_2 is the dominant diffusing species in the Cs-based system. $FASnI_3$ and $CsSnI_3$ undergo thermal degradation at 200°C and 240°C, respectively, through co-desorption of their constituent elements. These findings provide valuable insights into tin-based perovskites' growth mechanisms and thermal stability, which can guide future efforts to improve their performance and long-term stability.

KFM 16.12 Thu 12:30 H13

Determining the key parameters of 3C-SiC photoelectrodes for water splitting application — •Marius Wasem[1,2], Sebastian Benz[1,3], Philip Klement[1,2], Joachim Sann[1,3], Jürgen Janek[1,3], Sangam Chatterjee[1,2], and Matthias T. Elm[1,2,3] — [1]Center for Materials Research, Heinrich-Buff-Ring 16, 35392 Giessen — [2]Institute of Experimental Physics I, Heinrich-Buff-Ring 16, 35392 Giessen — [3]Institute of Physical Chemistry, Heinrich-Buff-Ring 17, 35392 Giessen

We investigated the photoelectrochemical properties of n- and p-doped 3C-SiC thin films on n- or p-doped Si substrates, respectively, in a phosphate buffer solution. Key parameters such as the flat band potential and open-circuit potential were determined using various electrochemical methods. The combination of ultraviolet photoelectron spectroscopy and low energy inverse photoelectron spectroscopy measurements yields the estimation of the positions of the Fermi level, as well as the positions of the valence and conduction bands of the differently doped 3C-SiC thin films. Impedance spectroscopy characterized the interfacial processes in more detail. The flat band potential was derived from the space-charge layer capacitance using Mott-Schottky analysis. The determination of these key parameters enabled the construction of an energy level diagram, which explains the electrochemical behavior of n- and p-type 3C-SiC thin films under both dark conditions and illumination.

KFM 16.13 Thu 12:45 H13

Circular Dichroism Engineering via Bismuth Doping and Cation Substitution in 2D Lead-Halide Perovskites — •Jan-Heinrich Littmann[1], Keito Mizukami[1,2], Henrik Spielvogel[1], Philip Klement[1], Satoko Fukumori[2], Hirokazu Tada[2], and Sangam Chatterjee[1] — [1]Institute of Experimental Physics I and Center for Materials Research (ZfM), Justus Liebig University Giessen, Giessen, Germany — [2]Graduate School of Engineering Science, Osaka University, Japan

Hybrid lead halide perovskites have garnered significant attention for their remarkable semiconductor properties. Their building blocks allows for tuneable features such as the crystal structure and the electronic bandgap. Introducing chiral cations into these materials endows them with chiroptical properties, such as circularly polarized luminescence (CPL) and spin-polarized charge transport, promising applications in optoelectronics and spintronics. However, the mechanism of chirality transfer remains poorly understood due to complex structure-property relationships. This study delves into the impact of heterovalent Bi^{3+} doping on the genuine circular dichroism (CD) of 2D lead iodide perovskites incorporating methylbenzylamine (MBA) and (pyridyl)ethylamine (PyEA) cations. Bi^{3+} doping, while preserving the band gap, significantly influences the genuine CD, suggesting a doping-dependent chirality transfer mechanism. Our findings provide valuable insights into the structure-property relationships in chiral perovskites and pave the way for the rational design of advanced chiroptical materials.

KFM 17: Functional Materials: Performance, Reliability and Degradation; and Complex Materials (joint session MM/KFM)

Time: Thursday 11:45–13:00 Location: H23

KFM 17.1 Thu 11:45 H23

Untersuchungen des Bruchverhaltens im Bereich der Ultra-Langzeitfestigkeit von Federstählen — •Jörg Gollnick — THM, FB ME, Wiesenstr. 14, 35390 Gießen

In einer hochfrequenten resonanten Anwendung als Spiegel für Laserscanner werden Federstähle des Typs Ck101 im Grenzbereich belastet. Im Rahmen eines Forschungsvorhabens wurden die spezifischen Möglichkeiten untersucht, die Lebensdauer dieser Bauteile zu steigern. Bislang wurden nur unzureichende Lebensdauern erreicht.

Bemerkenswert war die Ausprägung des Versagensverhaltens, dass in Zusammenhang mit der Fertigungstechnologie einem Sprödbruch unter Mode III nach den bruchmechanischen Ansätzen gemäß Griffith entspricht. Aus der Erklärung der Schädigungen wurden weitere Möglichkeiten untersucht, die Lebensdauer nicht nur zu steigern sondern weiterhin die nach Paris-Erdogan zu erwartende Dauerfestigkeit genau zu bestimmen.

Mit hohen Frequenzen im Bereich bis zu 10000kHz werden Bauteile bis zu 10 Milliarden Schwingungen im Grenzbereich betrieben. Eine mehrstufige Auswertung nach dem Treppenstufenverfahren zeigt, dass eine Auswertung in diesem Segment nicht nur möglich ist, sondern als geeignete Strategie angesehen werden darf, die Erkenntnisse der Ultra-Langzeitfestigkeit diesbezüglich zu erweitern.

Weitergehende Versuche werden vorgestellt.

Falls gewünscht kann der Vortrag und Beitrag gerne auch auf englisch abgefasst werden.

KFM 17.2 Thu 12:00 H23

Searching for ferroelectric porous metal organic frameworks using machine-learning and Monte-Carlo-simulations — •Thomas Bergler[1,2], Harald Oberhofer[1,2], and Dirk Volkmer[3] — [1]University of Bayreuth, Germany — [2]Bavarian Center for Battery Technologies — [3]University of Augsburg, Germany

Metal organic frameworks (MOFs) have so far found a number of successful applications, among them as storage for gasses and filter for gas mixtures. So far these mostly incorporated them as passive materials, but recent research points the way towards a more active role, possibly through the external manipulation of the materials' internal properties. One recent example for such a property is the susceptibility of the lattice parameters of a number of MOFs towards electric fields. Inspired by this, the aim of our project is to further investigate this behavior and potentially design ferroelectric MOFs. Using a hierarchy of Monte-Carlo-simulations aided by Machine-Learning (ML) we sample the design space MOFs augmented by rotatable polar groups. In succession, we first sample a huge space of rotors in a simplified point-dipole model. A selection of thus uncovered MOF geometries is then investigated with a specially parameterized atomistic model to confirm earlier predictions. Using this data, an ML model is trained to predict the dielectric properties of such polar rotor-augmented MOFs. The best candidates extracted with this procedure are finally evaluated with density functional theory. MOF geometries surviving this funnel-like approach can finally be checked experimentally for a variety of applications, ranging from data-storage to gas nano-funnelling.

KFM 17.3 Thu 12:15 H23

Atomic Scale Insights into A-site Deficient Perovskite Catalysts:$La_{0.7}Fe_{0.7}Mn_{0.3}O_3$ — •Roham Talei Jeid — Institute for Material Physics, University of Stuttgart, Deutschland

This study investigates the atomic-scale properties of the A-site-deficient perovskite catalyst $La_{0.7}Fe_{0.7}Mn_{0.3}O_3$ (La07FM), emphasizing the role of iron oxide (FeO) in redox reactions. Advanced techniques, including scanning transmission electron microscopy (STEM), energy-dispersive X-ray spectroscopy (EDXS), and a custom Python-based strain mapping tool linked to chemical analysis reveal nanoscale La deficiencies and Fe enrichments at grain boundaries as key for catalytic activity. Post-catalysis studies identify Fe-rich, FeO-like nanoparticles at strained, defective grain boundaries, underscoring the impact of A-site deficiencies on performance in NOx denitrification (DeNOx). These findings highlight how A-site deficiencies and Fe-rich nanostructures enhance catalytic efficiency, offering broader insights into electrochemistry and heterogeneous catalysis.

KFM 17.4 Thu 12:30 H23

Use of LiMn2O4 for switching applications in silicon waveguide circuits — •Vinit Agarwalla[1], Yug Joshi[2], and Guido Schmitz[1] — [1]Insitut für Materialwissenschaft, Universität Stuttgart, Heisenbergstr.3, 70569 Stuttgart — [2]Max-Planck-Institut für Nachhaltige Materialien, Max-Planck-Straße 1, 40237, Düsseldorf

Lithium ion intercalation and deintercalation play an important role in determining the storage performance of cathode materials for lithium ion batteries. However, intercalation of ions also regularly modifies electron structure and optical properties of the materials. This study explores the possibility of exploiting the optical properties of the cathode material LiMn2O4 (LMO) for optical switching applications in silicon waveguide circuits. For this, LMO is coated as a cladding around Si waveguides suitable for the 1550 nm wavelength of optical telecommunication. To stabilize the interface a thin intermediate Si oxide film is tested as an optical transparent reaction barrier. Our TEM images and the EDX mapping show that the Si does not react with LMO for oxide layer thickness as low as 10 nm. Previous work has explored the change in resonance wavelength of reflectance spectra with lithiation/ delithiation in the visible region[1]. In extension, we have measured FTIR reflectance spectra in the near IR region. They show a fairly continuous spectrum between visible and IR region with reflectance going to 100 % and a gradual shift in resonance wavelength in the IR region with Li intercalation. The optical response on light transmission along the wave guides has been determined in dependence on the degree of lithiation. [1]. DOI:10.1002/adom.201701362

KFM 17.5 Thu 12:45 H23

Chemical short-range order and local lattice distortions in High-Entropy Alloys: state of the art — •Andrea Fantin, Anna Maria Manzoni, Reza Darvishi Kamachali, and Robert Maass — Bundesanstalt fuer Materialforschung und -pruefung, Unter den Eichen 87, 12205 Berlin, Germany

Understanding the intricate atomic-scale structures within High-Entropy Alloys (HEAs) is crucial for tailoring their properties for diverse applications. This contribution tries to provide a brief overview of the state-of-the-art experimental techniques employed to probe local lattice distortions and chemical short-range order in HEAs, with specific focus on X-ray absorption spectroscopy and total scattering. The main problem to overcome in multi-component alloys is the intrinsic reduced scattering contrast between nearest neighbors in the periodic table, which limits the amount of information that can be extracted from the data. This statement remains valid when employing transmission electron microscopy, as well. Specific examples such as the Al-Co-Cr-Cu-Fe-Ni fcc system [Small Science 4(2), 2300225 (2024); Nature Communications 15(1), 7815 (2024)] and the MoNbTaW bcc system [Materials Research Letters 12(5), 346-354 (2024)] will be outlined. It comes clear that rather than specific techniques, it is only the combination of several experiments, supported by simulations and multi-technique simultaneous structural refinements, that can help in disentangling the different contributions to performances of each element within the alloy solid solution, with strength and weaknesses depending on the specific experimental measurements.

KFM 18: Materials Research in Polar Oxides: Perspectives for Optics & Electronics

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. The goal is to improve the mutual understanding of each other research goals and necessities. Examples for topics could be improved or novel techniques for domain engineering, which are relevant for (nonlinear) optical applications, the growth of novel polar oxides with improved properties over traditional materials, such as higher temperature stability or improved nonlinear characteristics, or the discussion of novel emergent properties in this context, like conductive domain walls in opto-electronical applications.

Chairs: Michael Rüsing (Paderborn University), Christof Eigner (Paderborn University)

Time: Thursday 15:30–17:45 Location: H9

Invited Talk KFM 18.1 Thu 15:30 H9

Domain gratings of sub-micrometer period for quantum technologies — •Carlota Canalias — KTH-Royal Institute of Technology, Stockholm Sweden

This talk explores the challenges and advancements in developing submicron ferroelectric domain gratings, which are vital for nonlinear optical devices capable of generating counter-propagating photons. Conventional materials and poling methods have proven insufficient to support these cutting-edge optical interactions, thereby constraining their applications in both classical and quantum technologies. The presentation showcases a breakthrough in periodic poling techniques for KTP isomorphs, enabling the fabrication of bulk structures with domain sizes as small as 200 nm. This achievement leverages coercive-field gratings formed via ion exchange, which play a pivotal role in domain formation. Our results demonstrate that the creation of sub-micron domains is governed by the characteristics of the ion-exchanged region, rather than the poling period, opening new possibilities for designing smaller and more intricate domain-engineered devices.

KFM 18.2 Thu 16:00 H9

Gray tracks in $KTiOPO_4$ from DFT calculations — •Adriana Bocchini, Uwe Gerstmann, and Wolf Gero Schmidt — Department Physik, Universität Paderborn, 33095 Paderborn, Germany

Ferroelectric $KTiOPO_4$ (KTP) is commonly applied in (nonlinear) optical devices. However, the irradiation with high-intensity laser light or the application of strong electric fields triggers the formation of detrimental gray tracks [1], the microscopic origin of which is usually attributed to Ti^{3+} centers (i.e., reduced titanium atoms) charge compensating for oxygen vacancies [2]. In this study, we use DFT routines to further clarify the gray-tracking mechanisms by systematically model oxygen-vacancy related Ti^{3+} centers in application-relevant environments, i.e., potassium vacancies and rubidium dopants. We find that the only thermally stable [2] Ti^{3+} center forms close, but not adjacent the oxygen vacancy itself. In addition, displaced potassium ions provide the stabilizing forces, whereas potassium interstitials rather than oxygen vacancies alone appear to be directly related to gray tracks. For this we suggest that the current gray-tracking model has to be partially revised. [3]

[1] M. Roth, in Springer Handbook of Crystal Growth, Chap 20, 691 (2010, Berlin, Heidelberg)

[2] S. D. Setzler, et al., J. Condens. Matter Phys. 15, 3969 (2003)

[3] A. Bocchini, et al., submitted to Phys. Rev. B

KFM 18.3 Thu 16:15 H9

Interaction between small electron-polaron and neutral domain wall in $PbTiO_3$: A DFT+U study — •Mohammad Amirabbasi, Jochen Rohrer, and Karsten Albe — Technical University of Darmstadt, Materials Modelling Division, Otto-Berndt-Straße 3, Darmstadt D-64287, Germany

$PbTiO_3$ is a widely studied ferroelectric material that often requires doping to tailor its electronic structure for specific applications. Understanding charge compensation mechanisms, particularly those mediated by local lattice distortions such as small polarons, is crucial for optimizing these modifications. This research investigates the formation and stability of a small electron polaron in $PbTiO_3$, focusing on its interaction with the neutral 180° Pb-centered domain wall using density functional theory with Hubbard corrections (DFT+U). We begin by calculating the formation energy of the 180° Pb-centered domain wall. Next, we determine the Born effective charges for various ions and compute the polarization profile across the domain wall. Our results show that the polarization in the bulk region reaches a saturation value, which is in good agreement with experimental measurements. Finally, we calculate the trapping energy of a small electron polaron at Ti centers in both bulk and domain wall regions. The results reveal that the trapping energy is negative in both cases, indicating that small electron polaron formation is energetically favorable. Furthermore, the similarity in trapping energy values suggests that the 180° Pb-centered domain wall in $PbTiO_3$ has a minimal impact on this type of small electron polaron formation.

15 min. break

KFM 18.4 Thu 16:45 H9

Atomistic Modelling of Ferroelectric Bonded Structures — •Nils Andre Schäfer and Simone Sanna — Institute for Theoretical Physics, Justus Liebig University Giessen, Germany

Direct bonding in ferroelectric materials, such as lithium niobate (LN), provides a method to create both head-to-head (H2H) and tail-to-tail (T2T) domain walls (DWs). These DW configurations are particularly interesting due to their ability to exhibit (semi-)metallic behavior by the formation of a two-dimensional electron or hole gas. This phenomenon enables the creation of localized conducting areas within an otherwise wide-gap semiconductor material.

In this work, we model H2H and T2T bonded structures within DFT. Therefore, we start with the thermodynamically stable z-cut surfaces of LN. Simulations were conducted on slabs with varying film thickness to minimize the surface interactions before constructing the bonded structures. The energy landscape of the interface was mapped by systematically translating the films relative to each other and analyzing various quantities, such as free charge carrier densities, the film distance, and the surface energy. In conclusion, H2H and T2T bonded structures exhibit distinct morphological and electronic interfaces, resulting in variations in their expected conductivities.

KFM 18.5 Thu 17:00 H9

Influence of different organic molecules on dielectric response in halide perovskites — •Doru Lupascu[1], Youn Un Jin[1], Witchitaya Arpavate[1], Andre Karabanov[1], Lars Leander Schaberg[1], Niels Benson[1], Bernd Marler[2], and Andre Salak[3] — [1]Universität Duisburg-Essen — [2]Ruhr-Universität Bochum — [3]Universidade de Aveiro

The charge carrier mobility in halid perovskites is still not fully understood. We have been discussing dielectric effects as one fundamental piece in the explanation of the large screening of defects and the polaron mobility. In this presentation we compare different organic molecules for their influence on the dielectric response. The interrelation of molecule mobility and dielectric screening will be discussed.

KFM 18.6 Thu 17:15 H9

Piezoresponse force microscopy study of local polarization dynamics in uniaxial relaxors — •Vladimir Shvartsman[1], Boris Slautin[1], Jan Dec[2], Sergei Kalinin[3], and Doru Lupascu[1] — [1]Institute for Materials Science, University Duisburg-Essen, Essen, Germany — [2]University of Silesia, Katowice, Poland — [3]University of Tennessee-Knoxville, USA

The unusual properties of relaxor ferroelectrics are related to their particular polar structure. In these materials, the polarization is correlated only on the nanometer scale within the so called polar nanoregions (PNRs). The dynamics of PNRs strongly affects the dielectric properties of relaxors. Here, we report about piezoresponse force microscopy study of local polarization dynamics in SrxBa1-xNb2O6 single crystals. In these materials having uniaxial polarization, the cross-over from ferroelectric to relaxor behavior occurs with increasing Sr content making SBN a good model system. We use time-resolved piezoresponse force spectroscopy. This technique measures temporal decay of the piezoresponse induced by a locally applied electric field over a dense spatial grid. The analysis of the time dependences of the piezoresponse allows to estimate the local relaxation time. Spatial maps of relaxation parameters are constructed, giving information on the spatial heterogeneity of polarization dynamics for different compositions and temperatures. Temperature dependences of local relaxation time are analyzed.

KFM 18.7 Thu 17:30 H9

Surface-near domain engineering in multi-domain x-cut lithium niobate tantalate mixed crystals — Laura Bollmers[1,2], Tobias Babai-Hemati[2], Boris Koppitz[3], Christof Eigner[1], Laura Padberg[1,2], •Michael Rüsing[1,2], Lukas M. Eng[3,4], and Christine Silberhorn[1,2] — [1]Paderborn University, Institute for Photonic Quantum Systems (PhoQS), 33098 Paderborn, Germany — [2]Paderborn University, Integrated Quantum Optics, 33098 Paderborn, Germany — [3]Institut für Angewandte Physik, Technische Universität Dresden, 01062 Dresden, Germany — [4]ct.qmat: Dresden-Würzburg Cluster of Excellence|EXC 2147, TU Dresden, 01062 Dresden, Germany

Lithium niobate tantalate mixed crystals present a novel material plattform, which offer new possibilities over pure lithium niobate or lithium tantalate, such as improved thermal stability or the possibility to tune the birefringence. A key requisite for application in nonlinear optics, electronics and piezotronic is the possibility of domain engineering. So far, this proved difficult for mixed crystals due to stoichiometric inhomogeneities, which stabilizes the random as-grown domain structure. In this work, we investigate surface-near periodic poling of x-cut mixed crystals and demonstrate microscopically how the random domain structure in the as-grown crystals can inhibit large scale poling. If monodomain areas are poled, however, periodic poling becomes possible. Our work lays the foundation for future applications of lithium niobate tantalate mixed crystals.

KFM 19: Members' Assembly

We will elect our spokespersons, plan the programme for the next years, and award the poster prize.

Chair: Anna Grünebohm (Ruhr University Bochum), KFM spokesperson

Time: Thursday 18:00–19:00 Location: H9

All members of the Crystalline Solids and their Microstructure Division are invited to participate.