FM 11: Poster Session Functional Materials

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

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

FM 11.1 Tue 18:00 P4

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

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

FM 11.2 Tue 18:00 P4

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

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

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

FM 11.3 Tue 18:00 P4

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

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

FM 11.4 Tue 18:00 P4

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

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

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

FM 11.5 Tue 18:00 P4

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

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

FM 11.6 Tue 18:00 P4

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

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

FM 11.7 Tue 18:00 P4

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

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

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

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

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

FM 11.8 Tue 18:00 P4

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

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

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

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

FM 11.9 Tue 18:00 P4

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

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

FM 11.10 Tue 18:00 P4

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

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

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

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

FM 11.11 Tue 18:00 P4

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

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

FM 11.12 Tue 18:00 P4

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

Metal-organic frameworks (MOFs) are emerging as tunable platforms for sensing, photocatalysis, and energy conversion, where charge transfer, spin interactions, and defect states play key roles. Here, we identify and characterize a native NH· radical defect intrinsic to the aminoterephthalate linker in UiO-66-NH_2 MOF. Combining density functional theory (DFT) modeling with multi-frequency electron spin resonance (ESR) spectroscopy, we elucidate the radical's electronic structure, spin density distribution, formation pathway, and spin-coherence properties. Our findings reveal the radical's exceptional stability and highlight its relevance for both photocatalytic charge separation and quantum-enhanced sensing in MOFs.

FM 11.13 Tue 18:00 P4

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

Proton-conducting solid-oxide fuel cells (H-SOFCs) are promising for direct ammonia-fed SOFC applications, as they eliminate NO_x emissions compared to conventional oxide-ion-conducting solid-oxide fuel cells. However, current proton-conducting electrolytes operate at high temperatures and suffer from leakage currents. Known suitable materials remain rare, calling for systematic investigations into novel proton conductor classes. We present a framework that combines machine-learning techniques with high-throughput computation to screen and design efficient proton conductors at intermediate temperatures. Through an ion-exchange strategy applied to known alkaline-ion conductor classes, we identify a database of potential proton-conducting materials. Machine learning molecular dynamics simulations are employed to assess stability and diffusion barriers, enabling the selection of top-performing candidates. The screened proton conductors contain cations that span from monovalent to pentavalent, including Rb^+, Ba^{2+}, Ca^{2+}, B^{3+}, Zr^{4+}, and Nb^{5+}, and predominantly feature ${SO_4}^{2-}$ and ${PO_4}^{3-}$ polyanion groups. Proton transport in these materials follows the Grotthuss mechanism. The strength of hydrogen bonds increases after ion-exchange engineering, thereby enhancing proton transfer.

FM 11.14 Tue 18:00 P4

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

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

FM 11.15 Tue 18:00 P4

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

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

FM 11.16 Tue 18:00 P4

Correlated Imaging of Thermal Conductivity and Ferroelectric Domains in $PbTiO_3$ Using Scanning Probe Microscopy — •Ciara Ward, Lindsey Lynch, and Raymond McQuaid — Queen's University Belfast, Belfast, UK

Perovskite ferroelectrics are an attractive platform for realising thermal conductivity switching through voltage configuration of domain microstructure. Reported mechanisms involve thermal conductivity modulation through structural re-orientation (anisotropy) [1,2] or phonon scattering by domain wall defects [3-5], both of which can be controlled through sample geometry and applied fields. Heat flow measurements and thermoreflectance investigations have quantitatively benchmarked thermal switching ratios but, in some cases, a lack of direct thermal mapping introduces ambiguity as to the relative role played by the two mechanisms. We are using Scanning Thermal Microscopy to explicitly map the local thermal conductance in samples of archetypal ferroelectric $PbTiO_3$ to clarify the underlying mechanisms that enable modulation of thermal transport. In tandem, we are using domain engineering and electric-field poling techniques to demonstrate the maximum achievable contrast in thermal conductance in this system.

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

FM 11.17 Tue 18:00 P4

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

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

FM 11.18 Tue 18:00 P4

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

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

FM 11.19 Tue 18:00 P4

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

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

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

[1] H.-J. Lunk and H. Hartl, ChemTexts 9, 5 (2023).

[2] H. Hamdi et al., Phys. Rev. B 94, 245124 (2016).

FM 11.20 Tue 18:00 P4

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

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

FM 11.21 Tue 18:00 P4

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

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

FM 11.22 Tue 18:00 P4

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

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

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

[1] D. A. Scrymgeour et al., Phys. Rev. B 71, 184110 (2005)

[2] D. Lee et al., Aplied Physics Letter 98, 092903 (2011)

FM 11.23 Tue 18:00 P4

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

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

FM 11.24 Tue 18:00 P4

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

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

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

FM 11.25 Tue 18:00 P4

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

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

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

FM 11.26 Tue 18:00 P4

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

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

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

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

FM 11.27 Tue 18:00 P4

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

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

FM 11.28 Tue 18:00 P4

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

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

FM 11.29 Tue 18:00 P4

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

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

FM 11.30 Tue 18:00 P4

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

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

FM 11.31 Tue 18:00 P4

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

This work aims to establish time-resolved Extended X-ray Absorption Fine Structure (tr-EXAFS) spectroscopy as a methodology for solids where the structural information of the EXAFS is combined with a pump-probe setup to study local dynamic lattice processes in the time domain.

As a proof of concept, we analyze the structural cubic-to-tetragonal phase-transition in the ferroelectric perovskite $BaTiO_3$. The coexistence of displacive and order-disorder phenomena accompanying this transition is a topic of debate in the literature on this extensively studied material.Difference-EXAFS scans at the Ti K-edge and the Ba L_3-edge between the pumped and unpumped state provide a direct way to investigate changes in lattice-structure and thermal-induced disorder in the vicinity of the absorbing atom. We correlate our spectroscopic findings with *ab initio* multiple-scattering calculations using the FEFF10 code to quantify structural dynamics.

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FM 11.32 Tue 18:00 P4

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

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

FM 11.33 Tue 18:00 P4

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

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

FM 11.34 Tue 18:00 P4

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

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

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

FM 11.35 Tue 18:00 P4

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

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

FM 11.36 Tue 18:00 P4

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

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

FM 11.37 Tue 18:00 P4

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

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

FM 11.38 Tue 18:00 P4

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

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

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

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