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

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

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

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

Invited Talk FM 12.1 Wed 9:30 BEY/0138

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

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

FM 12.2 Wed 10:00 BEY/0138

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

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

FM 12.3 Wed 10:15 BEY/0138

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

The uniaxial ferroelectric lithium niobate ($LiNbO_3$) can exhibit significantly enhanced domain wall (DW) conductivity, rendering it an interesting system for DW-based nanoelectronics. Specifically, head-to-head (h2h) DWs exhibit conductivities several orders of magnitude higher than that of the surrounding bulk. We create h2h DWs with a near-90° inclination angle by using the diffusion annealing technique, followed by chemical treatment to change the functional properties. The characterization of the structure and morphology is conducted by piezoresponse force microscopy and transmission electron microscopy. To characterize electronic transport, we use resistivity measurements under varying temperatures in dark or under UV light illumination, complemented by conductive atomic force microscopy. Our findings indicate only transient conductivity at the DWs, but substantial differences in photoconductivity between monodomain and bidomain crystals, with persistent photoconductivity in crystals with DWs. Furthermore, we report a drastic drop in domain wall photoconductivity upon heating above 80°C, which can be explained by the emptying of charge carrier traps in the DW as the system gains higher thermal energy.

FM 12.4 Wed 10:30 BEY/0138

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

In reservoir computing, input data are mapped into higher dimensional space, translating non-linear problems into linearly solvable ones. In general, any physical system that possesses non-linearity, complexity, short-term memory, and reproducibility can serve as reservoir. Here, we investigate the ferroelectric semiconductor $ErMnO_3$ as a potential candidate material for reservoir computing. We show that the system displays pronounced non-linear changes in photocurrent under varying light intensity. The response can be tuned by changing the metal-semiconductor contacts (Schottky- or Ohmic-like behavior) used for readout, determining the timescale on which the photocurrent vanishes after illumination. This relaxation behavior in the OFF state gives fading memory. We perform training on variations in the output (photocurrent), which allows for recognition in time-series tasks. Interestingly, ferroelectric domain walls can also be used as reservoirs with characteristic photocurrent signals, giving new opportunities to down-scale or enhance the complexity of physical reservoirs.

Coffee break

FM 12.5 Wed 11:00 BEY/0138

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

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

FM 12.6 Wed 11:15 BEY/0138

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

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

FM 12.7 Wed 11:30 BEY/0138

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

Ferroelectric heterostructures offer a platform to realize topological patterns with functionalities relevant to future electronic devices.[1] While short-range machine-learned interatomic potentials can capture ferroelectric instabilities in pure materials, long-range dipole interactions remain essential for heterostructures, where depolarizing field plays a role.[2] We address this challenge by combining MACE message-passing networks with a latent Ewald-summation scheme[3] capable of learning long-range interactions and inferring Born effective charges without explicit training on response properties. The model predicts transition temperature and spontaneous polarization of $BaTiO_3$ in close agreement with experiments. It further captures the multidomain formed in heterostructures, consistent with coarse-grained effective-Hamiltonian results, and generalizes well to untrained configurations, including those containing oxygen vacancies.

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

FM 12.8 Wed 11:45 BEY/0138

From Stacking Faults to Field-Stabilized Polarity: Connecting RP Phases and the MFP Phase in $SrTiO_3$ — •Christian Ludt[1,2], Hartmut Stöcker[1,2], Matthias Zschornak[1,2,3], and Dirk C. Meyer[1,2] — [1]TU Bergakademie Freiberg, 09599 Freiberg, Germany — [2]Zentrum für Effiziente Hochtemperatur-Stoffwandlung, 09599 Freiberg, Germany — [3]Hochschule für Technik und Wirtschaft Dresden, 01069 Dresden, Germany

Polar functionalities in perovskites often arise from a subtle interplay between lattice distortions, defect chemistry, and stacking faults. In this work, particular attention is given to the migration-induced field-stabilized polar (MFP) phase in $SrTiO_3$, a recently identified polar state that arises from field-driven oxygen mobility and picometer-scale cation displacements. To provide a structural framework for understanding and enhancing this phenomenon, the electronic properties of Ruddlesden-Popper-type (RP) stacking faults in $SrO(SrTiO_3)_n$ are analyzed using density functional theory. These faults introduce symmetry breaking, modified lattice environments and characteristic changes in the electronic structure that closely resemble the local conditions required to form the MFP phase. By combining insights from RP-layered configurations with the field- and defect-driven mechanisms underlying MFP formation, a unified perspective emerges in which stacking faults act as natural templates that support, amplify, or localize MFP-like polar distortions. This connection highlights new pathways for engineering polar responses and optoelectronic functionalities in complex perovskite oxides.

Coffee Break

FM 12.9 Wed 12:15 BEY/0138

Integration of imprint-free and low coercivity ferroelectric $BaTiO_3$ thin films on silicon — Jingtian Zhao[1,2], Majid Ahmadi[1,2], Beatriz Noheda[1,2], and •Martin F. Sarott[1,2] — [1]Zernike Institute for Advanced Materials, University of Groningen, The Netherlands — [2]Groningen Cognitive Systems and Materials Center (CogniGron), University of Groningen, The Netherlands

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

FM 12.10 Wed 12:30 BEY/0138

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

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

FM 12.11 Wed 12:45 BEY/0138

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

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

by scanning probe techniques, microscopy imaging and 4-probe resistivity measurements.