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.