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

chair: Elzbieta Gradauskaite (CNRS/Thales, FR)

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

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

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

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

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

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

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

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

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

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

FM 18.3 Thu 11:15 BEY/0138

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

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

FM 18.4 Thu 11:30 BEY/0138

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

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

FM 18.5 Thu 11:45 BEY/0138

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

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

FM 18.6 Thu 12:00 BEY/0138

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

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

FM 18.7 Thu 12:15 BEY/0138

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

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

FM 18.8 Thu 12:30 BEY/0138

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

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