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

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

Chair: Johanna Nordlander (University of Zurich)

Time: Monday 9:30–11:15 Location: H9

Invited Talk KFM 1.1 Mon 9:30 H9

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

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

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

KFM 1.2 Mon 10:00 H9

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

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

KFM 1.3 Mon 10:15 H9

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

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

KFM 1.4 Mon 10:30 H9

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

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

KFM 1.5 Mon 10:45 H9

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

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

KFM 1.6 Mon 11:00 H9

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

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

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