KFM 4: (Multi)ferroic States: From Fundamentals to Applications (II)

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: Nives Strkalj (Institute of Physics, Zagreb)

Time: Monday 11:30–13:00 Location: H9

KFM 4.1 Mon 11:30 H9

Oersted Mapping of Current Flow in Ferroelectric Domain Walls with a Single-spin Magnetometer — •James Dalzell, Conor McCluskey, Marty Gregg, and Amit Kumar — Queen's University Belfast

Nitrogen vacancy (NV) [1] based magnetometers offer outstanding sensitivity for detecting static or dynamic magnetic fields at the nanoscale. As a result, this technique can be employed to evaluate current flow in materials with complex topologies and microstructures through direct measurement of the Oersted fields generated along any current pathways [2]. This creates an opportunity to evaluate fundamental aspects of electron transport in conducting ferroelectric domain walls, employed recently in lab-level ephemeral transistors and neuromorphic domain-wall based computing. We exploit the capability of the NV-AFM system to measure the current density along conducting domain walls in erbium manganite. By integrating high field sensitivity with exceptional spatial resolution, NV-based Oersted mapping has been shown to potentially offer a non-invasive approach to characterizing current flow in ferroelectrics. This advancement paves the way for a deeper understanding of electron transport phenomena in ferroelectric systems with current densities >1x104A/cm2, with improvements capable of being achieved by following pulse probe methods.

[1] Rondin, L. et al, Rep.Prog.Phys. 77 056503,(2014) [2] Tetienne, Jean-Philippe. et al, Sci. Adv. 3, e1602429 (2017). [3] Broadway,D.A, et al, Physics Review Applied 14(2) (2020).

KFM 4.2 Mon 11:45 H9

Transport behavior at domain walls in a depleted ferroelectric semiconductor — •Jiali He[1], Ruben Dragland[1], Leonie Richarz[1], Zewu Yan[2,3], Edith Bourret[3], Gustau Catalan[4,5], and Dennis Meier[1] — [1]NTNU Norwegian University of Science and Technology — [2]ETH Zurich, Switzerland — [3]Lawrence Berkeley National Laboratory, USA — [4]Institut Català de Nanociencia i Nanotecnologia (ICN2), Spain — [5]Institucio Catalana de Recerca i Estudis Avançats (ICREA), Spain

Electronic depletion regions naturally form at metal-semiconductor interface, which enables control of electrical currents in pn-junctions and is widely used in CMOS technology. Here, we expand the research towards ferroelectric domain walls, studying their functional properties under electronic depletion. Using ferroelectric p-type semiconductor $ErMnO_3$ as the model system, we deposit W electrodes and systematically investigate changes in the local transport behavior as the material is thinned down to the sub-10 nm range. Combined imaging experiments in terms of scanning electron microscopy (SEM) and scanning probe microscopy (SPM) reveal that for a critical thickness, t_c, a step-like drop occurs in the electronic conduction, which we associate with the width of the depletion region at the $W/ErMnO_3$ interface. Interestingly, ferroelectric domain walls within the depletion region exhibit qualitatively different transport behavior than in the p-type regions. Our results give new insight into the physics of domain walls and demonstrate additional opportunities for controlling their electronic responses, which is of interest for domain-wall-based electronics.

KFM 4.3 Mon 12:00 H9

Domain and domain wall conductance in the vicinity of metal-semiconductor contacts — •Ruben Dragland[1], Leonie Richarz[1], Ingvild Hansen[1], Manuel Zahn[1], Jiali He[1], Zewu Yan[2], Edith Bourret[2], Mario Hentschel[3], and Dennis Meier[1] — [1]NTNU Norwegian University of Science and Technology, Trondheim, Norway — [2]Lawrence Berkeley National Laboratory, Berkeley, CA,USA — [3]University of Stuttgart, Stuttgart, Germany

Ferroelectric domain walls hold promise as functional quasi-2D systems and are intensively studied as key electronic elements for next-generation nanotechnology. Despite their outstanding application potential, however, little is known about the performance in actual device geometries and the contact phenomena that co-determine the current injection. In this study, we perform a systematic analysis of the local transport behavior of the ferroelectric semiconductor $ErMnO_3$ in the vicinity of different electrode materials. By applying electron beam lithography and evaporation, we design metal-semiconductor contacts with varying work functions and investigate the impact on the electronic conductance and respective barrier formation. Combining conductive atomic force microscopy (cAFM), Kelvin probe force microscopy (KPFM), as well as mesoscopic probe techniques, we correlate the band bending at the interface to the measured conductance of domains and domain walls. Our results are relevant for the integration of ferroelectric domain walls and the understanding of the nanoscale physics at metal-semiconductor junctions in ferroelectrics in general.

KFM 4.4 Mon 12:15 H9

Exploring ferroelectric oxides for reservoir computing — •Yan Meng Chong[1], Atreya Majumdar[2], Ingvild Hansen[1], Karin Everschor-Sitte[2], and Dennis Meier[1] — [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

In reservoir computing, input data is 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 or fading memory, and reproducibility can serve as reservoir. Here, we investigate ferroelectric semiconductor $ErMnO_3$ as 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) used for read-out, determining the timescale on which photocurrents vanish after illumination. This relaxation behavior in the OFF state gives the fading memory. We perform training for recognition on variations in the output (photocurrent), which allows for reconstructing the sequential input (light pulses). Interestingly, both ferroelectric domains and domain walls can be used as reservoirs with characteristic photocurrent signals, giving new opportunities for downscaling or enhancing the complexity of physical reservoirs.

KFM 4.5 Mon 12:30 H9

Coupling between small polarons and ferroelectricity in $BaTiO_3$ — •Darin Joseph[1] and Cesare Franchini[1,2] — [1]Dipartimento di Fisica e Astronomia, Università di Bologna, 40127 Bologna, Italy — [2]University of Vienna, Faculty of Physics, Center for Computational Materials Science, Vienna, Austria

Ferroelectric properties of materials are found to be modified upon polaron formation. In this study, we investigate the formation of electron and hole small polarons in the prototypical ferroelectric material barium titanate ($BaTiO_3$), with a focus on their interaction with ferroelectric distortive fields. To accurately describe the ferroelectric phase in $BaTiO_3$, we employ the HSE06 hybrid functional, which addresses the limitations of conventional DFT and DFT+U models, providing a more precise depiction of both ferroelectric and polaronic behaviours. Our analysis spans three structural phases of $BaTiO_3$: cubic, tetragonal, and rhombohedral. We uncover a phase-dependent trend in electron polaron stability, which progressively increases across the structural phases, peaking in the rhombohedral phase due to the constructive coupling between the polaron and ferroelectric phonon fields. In contrast, hole polarons exhibit a stability pattern largely unaffected by the phase transitions. Furthermore, we observe that polaron self-trapping significantly alters the local ferroelectric distortive pattern,

which propagates to neighbouring sites but has a minimal effect on the long-range macroscopic spontaneous polarization. Charge trapping is also associated with localized spin formation, opening new possibilities for enhanced functionalities in multiferroic materials.

KFM 4.6 Mon 12:45 H9

Energy barriers for small electron polaron hopping in bismuth ferrite from first principles — •Sabine Körbel[1,2] and Harini Priyanka Shanmugasundharam Swaminathan[2,3] — [1]Institute of Physical Chemistry, Friedrich Schiller University Jena — [2]Institute of Condensed Matter Theory and Optics, Friedrich Schiller University, Fürstengraben 1, 07743 Jena, Germany — [3]University of Applied Sciences Jena, Carl-Zeiss-Promenade 2, 07745 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 transport could occur by hopping of small electron polarons rather than by band-like transport. Here, by means of first-principles calculations, small electron polaron hopping in $BiFeO_3$ was investigated. Both bulk $BiFeO_3$ and a typical ferroelectric domain wall, the neutral 71° domain wall, were considered. The latter was included to account for experimental observations of currents that appear to be localized within domain-wall planes. The object of this study is to shed light on the intrinsic n-type conduction mechanism in rhombohedral $BiFeO_3$ and the role of the ferroelectric domain walls in electrical conductivity. Based on the computed energy barriers for small electron polaron hopping, the intrinsic n-type mobility in bulk $BiFeO_3$ and at 71° domain walls is estimated.