KFM 18: Materials Research in Polar Oxides: Perspectives for Optics & Electronics

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. The goal is to improve the mutual understanding of each other research goals and necessities. Examples for topics could be improved or novel techniques for domain engineering, which are relevant for (nonlinear) optical applications, the growth of novel polar oxides with improved properties over traditional materials, such as higher temperature stability or improved nonlinear characteristics, or the discussion of novel emergent properties in this context, like conductive domain walls in opto-electronical applications.

Chairs: Michael Rüsing (Paderborn University), Christof Eigner (Paderborn University)

Time: Thursday 15:30–17:45 Location: H9

Invited Talk KFM 18.1 Thu 15:30 H9

Domain gratings of sub-micrometer period for quantum technologies — •Carlota Canalias — KTH-Royal Institute of Technology, Stockholm Sweden

This talk explores the challenges and advancements in developing submicron ferroelectric domain gratings, which are vital for nonlinear optical devices capable of generating counter-propagating photons. Conventional materials and poling methods have proven insufficient to support these cutting-edge optical interactions, thereby constraining their applications in both classical and quantum technologies. The presentation showcases a breakthrough in periodic poling techniques for KTP isomorphs, enabling the fabrication of bulk structures with domain sizes as small as 200 nm. This achievement leverages coercive-field gratings formed via ion exchange, which play a pivotal role in domain formation. Our results demonstrate that the creation of sub-micron domains is governed by the characteristics of the ion-exchanged region, rather than the poling period, opening new possibilities for designing smaller and more intricate domain-engineered devices.

KFM 18.2 Thu 16:00 H9

Gray tracks in $KTiOPO_4$ from DFT calculations — •Adriana Bocchini, Uwe Gerstmann, and Wolf Gero Schmidt — Department Physik, Universität Paderborn, 33095 Paderborn, Germany

Ferroelectric $KTiOPO_4$ (KTP) is commonly applied in (nonlinear) optical devices. However, the irradiation with high-intensity laser light or the application of strong electric fields triggers the formation of detrimental gray tracks [1], the microscopic origin of which is usually attributed to Ti^{3+} centers (i.e., reduced titanium atoms) charge compensating for oxygen vacancies [2]. In this study, we use DFT routines to further clarify the gray-tracking mechanisms by systematically model oxygen-vacancy related Ti^{3+} centers in application-relevant environments, i.e., potassium vacancies and rubidium dopants. We find that the only thermally stable [2] Ti^{3+} center forms close, but not adjacent the oxygen vacancy itself. In addition, displaced potassium ions provide the stabilizing forces, whereas potassium interstitials rather than oxygen vacancies alone appear to be directly related to gray tracks. For this we suggest that the current gray-tracking model has to be partially revised. [3]

[1] M. Roth, in Springer Handbook of Crystal Growth, Chap 20, 691 (2010, Berlin, Heidelberg)

[2] S. D. Setzler, et al., J. Condens. Matter Phys. 15, 3969 (2003)

[3] A. Bocchini, et al., submitted to Phys. Rev. B

KFM 18.3 Thu 16:15 H9

Interaction between small electron-polaron and neutral domain wall in $PbTiO_3$: A DFT+U study — •Mohammad Amirabbasi, Jochen Rohrer, and Karsten Albe — Technical University of Darmstadt, Materials Modelling Division, Otto-Berndt-Straße 3, Darmstadt D-64287, Germany

$PbTiO_3$ is a widely studied ferroelectric material that often requires doping to tailor its electronic structure for specific applications. Understanding charge compensation mechanisms, particularly those mediated by local lattice distortions such as small polarons, is crucial for optimizing these modifications. This research investigates the formation and stability of a small electron polaron in $PbTiO_3$, focusing on its interaction with the neutral 180° Pb-centered domain wall using density functional theory with Hubbard corrections (DFT+U). We begin by calculating the formation energy of the 180° Pb-centered domain wall. Next, we determine the Born effective charges for various ions and compute the polarization profile across the domain wall. Our results show that the polarization in the bulk region reaches a saturation value, which is in good agreement with experimental measurements. Finally, we calculate the trapping energy of a small electron polaron at Ti centers in both bulk and domain wall regions. The results reveal that the trapping energy is negative in both cases, indicating that small electron polaron formation is energetically favorable. Furthermore, the similarity in trapping energy values suggests that the 180° Pb-centered domain wall in $PbTiO_3$ has a minimal impact on this type of small electron polaron formation.

15 min. break

KFM 18.4 Thu 16:45 H9

Atomistic Modelling of Ferroelectric Bonded Structures — •Nils Andre Schäfer and Simone Sanna — Institute for Theoretical Physics, Justus Liebig University Giessen, Germany

Direct bonding in ferroelectric materials, such as lithium niobate (LN), provides a method to create both head-to-head (H2H) and tail-to-tail (T2T) domain walls (DWs). These DW configurations are particularly interesting due to their ability to exhibit (semi-)metallic behavior by the formation of a two-dimensional electron or hole gas. This phenomenon enables the creation of localized conducting areas within an otherwise wide-gap semiconductor material.

In this work, we model H2H and T2T bonded structures within DFT. Therefore, we start with the thermodynamically stable z-cut surfaces of LN. Simulations were conducted on slabs with varying film thickness to minimize the surface interactions before constructing the bonded structures. The energy landscape of the interface was mapped by systematically translating the films relative to each other and analyzing various quantities, such as free charge carrier densities, the film distance, and the surface energy. In conclusion, H2H and T2T bonded structures exhibit distinct morphological and electronic interfaces, resulting in variations in their expected conductivities.

KFM 18.5 Thu 17:00 H9

Influence of different organic molecules on dielectric response in halide perovskites — •Doru Lupascu[1], Youn Un Jin[1], Witchitaya Arpavate[1], Andre Karabanov[1], Lars Leander Schaberg[1], Niels Benson[1], Bernd Marler[2], and Andre Salak[3] — [1]Universität Duisburg-Essen — [2]Ruhr-Universität Bochum — [3]Universidade de Aveiro

The charge carrier mobility in halid perovskites is still not fully understood. We have been discussing dielectric effects as one fundamental piece in the explanation of the large screening of defects and the polaron mobility. In this presentation we compare different organic molecules for their influence on the dielectric response. The interrelation of molecule mobility and dielectric screening will be discussed.

KFM 18.6 Thu 17:15 H9

Piezoresponse force microscopy study of local polarization dynamics in uniaxial relaxors — •Vladimir Shvartsman[1], Boris Slautin[1], Jan Dec[2], Sergei Kalinin[3], and Doru Lupascu[1] — [1]Institute for Materials Science, University Duisburg-Essen, Essen, Germany — [2]University of Silesia, Katowice, Poland — [3]University of Tennessee-Knoxville, USA

The unusual properties of relaxor ferroelectrics are related to their particular polar structure. In these materials, the polarization is correlated only on the nanometer scale within the so called polar nanoregions (PNRs). The dynamics of PNRs strongly affects the dielectric properties of relaxors. Here, we report about piezoresponse force microscopy study of local polarization dynamics in SrxBa1-xNb2O6 single crystals. In these materials having uniaxial polarization, the cross-over

from ferroelectric to relaxor behavior occurs with increasing Sr content making SBN a good model system. We use time-resolved piezoresponse force spectroscopy. This technique measures temporal decay of the piezoresponse induced by a locally applied electric field over a dense spatial grid. The analysis of the time dependences of the piezoresponse allows to estimate the local relaxation time. Spatial maps of relaxation parameters are constructed, giving information on the spatial heterogeneity of polarization dynamics for different compositions and temperatures. Temperature dependences of local relaxation time are analyzed.

KFM 18.7 Thu 17:30 H9

Surface-near domain engineering in multi-domain x-cut lithium niobate tantalate mixed crystals — Laura Bollmers[1,2], Tobias Babai-Hemati[2], Boris Koppitz[3], Christof Eigner[1], Laura Padberg[1,2], •Michael Rüsing[1,2], Lukas M. Eng[3,4], and Christine Silberhorn[1,2] — [1]Paderborn University, Institute for Photonic Quantum Systems (PhoQS), 33098 Paderborn, Germany — [2]Paderborn University, Integrated Quantum Optics, 33098 Paderborn, Germany — [3]Institut für Angewandte Physik, Technische Universität Dresden, 01062 Dresden, Germany — [4]ct.qmat: Dresden-Würzburg Cluster of Excellence|EXC 2147, TU Dresden, 01062 Dresden, Germany

Lithium niobate tantalate mixed crystals present a novel material platform, which offer new possibilities over pure lithium niobate or lithium tantalate, such as improved thermal stability or the possibility to tune the birefringence. A key requisite for application in nonlinear optics, electronics and piezotronic is the possibility of domain engineering. So far, this proved difficult for mixed crystals due to stoichiometric inhomogeneities, which stabilizes the random as-grown domain structure. In this work, we investigate surface-near periodic poling of x-cut mixed crystals and demonstrate microscopically how the random domain structure in the as-grown crystals can inhibit large scale poling. If monodomain areas are poled, however, periodic poling becomes possible. Our work lays the foundation for future applications of lithium niobate tantalate mixed crystals.