KFM 27: Polar oxides: Lithium niobate and lithium tantalate

Chair: Manuel Zahn (Uni Augsburg)

Time: Thursday 15:00–16:20 Location: EMH 025

KFM 27.1 Thu 15:00 EMH 025

The role of domain wall conductivity in ferroelectric domain inversion — •Michael Rüsing[1,2], Boris Koppitz[2], Iuliia Kiseleva[2], Laura Padberg[1], Christof Eigner[1], Christine Silberhorn[1], and Lukas M. Eng[2,3] — [1]Paderborn University, Integrated Quantum Optics, Institute for Photonic Quantum Systems (PhoQS), Warburger Str. 100, 33098 Paderborn, Germany — [2]TU Dresden, Institute of Applied Physics, Nöthnitzer Strasse 61, 01187 Dresden, Germany — [3]ct.qmat: Dresden-Würzburg Cluster of Excellence EXC 2147, TU Dresden, 01062 Dresden, Germany

During electric field poling of single-domain, single-crystals, like lithium niobate, it is observed that the nucleation and growth of spike domains predominantly starts from one crystallographic side. This phenomenon is often explained by different surface barriers at the crystal's surface. The conductivity of ferroelectric DWs is suggested to be central to general domain reversal, e.g. by assisting and allowing screening processes [1]. In this work we will discuss how the directionality of DW conductivity, as well as the observed dominance of only sign of charge carrier in conductive DWs [2], can explain the preference of one of the crystal surfaces for initial domain reversal independent of the surface's properties. This work shows that DW conductivity can play a key role when explaining macroscopic ferroelectric material properties. [1] B. Sturman and R. Podivilov, JETP Letters, 116, 246 (2022); [2] H. Beccard et al., ACS Appl. Nano Mater. 5, 8717 (2022).

KFM 27.2 Thu 15:20 EMH 025

Theoretical Modelling of Domains and Domain Walls in Ferroelectric Oxides — •Leonard Verhoff and Simone Sanna — Institut for Theoretical Physics, Justus Liebig University, Giessen, Germany

Ferroelectric domain walls (DW) in lithium niobate (LN) and lithium tantalate (LT), i.e. interfaces between regions of different polarization, present a compelling field of study with diverse emergent functionalities. DW not only exhibit unique electronic and optical properties but also present a rich avenue for tailoring and manipulating the material's behaviour for advanced applications in optoelectronics and information processing.

We employ various methods to model DW parallel to the z-axis in the ferroelectric oxides LN and LT. Beginning with a symmetry-based description, we utilizie Ginzburg-Landau-Devonshire theory for qualitative insights. We delve into specific, high-symmetry DW orientations through density functional theory (DFT) calculations to investigate the ionic structure around the DW and the respective formation energies in detail. These energies, interpreted as interaction strengths of neighboring domains, are then incorporated into a 2D Ising model to simulate the formation of DW on a larger scale lattice, that would be inaccessible through DFT due to the large number of atoms. Special emphasis is placed on understanding the shape of emerging ferroelectric domains, with a focus on the anisotropy of formation energy that leads to hexagonal domain shapes in LN, while LT forms triangular domains.

KFM 27.3 Thu 15:40 EMH 025

Ab initio investigation of the ferroelectric phase transition in $LiNbO_3$ and $LiTaO_3$ — •Alexander Kapp, Wafaa Al Nachwati, and Simone Sanna — Institute for Theoretical Physics, Justus Liebig University, Giessen, Germany

Lithium niobate (LN, $LiNbO_3$) and Lithium tantalate (LT, $LiTaO_3$) are synthetic, isomorph solids. Both crystallize in a trigonal lattice, belonging to the space group R3c for the ferroelectric state and R$\bar{3}$c for the paraelectric states. These materials display several favorable properties such as ferroelectricity, piezoelectricity and the Pockels effect, just to name some examples. For this reason, these crystals are used in many applications e.g., in the telecommunication market for mobile telephones or optical modulators, and also for laser uses like Q-switching or frequency doubling. In this work, we model the transition from the paraelectric to the ferroelectric state and determine the Curie temperature in both crystals using ab initio molecular dynamics, as implemented in the Vienna Ab initio Simulation Package (VASP). Within this approach, atoms in the supercell can move according to existing forces, estimated by density functional theory (DFT). In our calculations, we take into account the expansion of cell volume with increasing temperature. Moreover, very large supercells are used to reduce finite-size effects. Within this approach, we obtain transition temperatures in close agreement with the measured values.

KFM 27.4 Thu 16:00 EMH 025

Vibrational and optical properties of $LiNbO_3$ and $LiTaO_3$ under uniaxial stress — •Mike Pionteck[1], Matthias Roeper[2], Ekta Singh[2], Boris Koppitz[2], Sven Reitzig[2], Michael Lange[2], Sam Seddon[2], Michael Rüsing[2,3], Laura Padberg[3], Simone Sanna[1], and Lukas Eng[2,4] — [1]Institut für Theoretische Physik, Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen, 35392 Gießen, Germany — [2]Institut für Angewandte Physik, Technische Universität Dresden, 01062 Dresden, Germany — [3]Paderborn University, Integrated Quantum Optics, Institute for Photonic Quantum Systems (PhoQS), Warburger Str. 100, 33098 Paderborn, Germany — [4]ct.qmat: Dresden-Würzburg Cluster of Excellence - EXC 2147, TU Dresden, 01062 Dresden, Germany

Our work provides, for the first time, a theoretical description of phonon frequencies of $LiNbO_3$ and $LiTaO_3$ under uniaxial stress along Cartesian axes using density functional theory (DFT). The calculations show a roughly linear dependence of the Raman frequencies on the applied uniaxial stress, which is confirmed by corresponding Raman measurements [1]. Additionally, we model linear and non-linear optical properties of $LiNbO_3$ in dependence on uniaxial stress using time-domain DFT. We find roughly linear changes for all components of the second harmonic generation under uniaxial stress. From the calculated dielectric tensor under stress, the dispersion of the piezo-optic and photoelastic coefficients are obtained. [1] E. Singh *et al.* Phys. Rev. Mat. **7**, 024420 (2023).