DF 3: Nonlinear dielectrics, phase transitions, relaxors

Time: Monday 15:00–16:00 Location: EB 107

DF 3.1 Mon 15:00 EB 107

Ferroelectric transition in $LiNbO_3$ calculated from first principles — •Simone Sanna and Wolf Gero Schmidt — Lehrstuhl für Theoretische Physik, Universität Paderborn

Lithium niobate ($LiNbO_3$, LN) belongs to the most important ferroelectric materials. It is furthermore one of the most important optic materials, being the equivalent in the field of non-linear optics and optoelectronics to silicon in electronics [1]. Despite the extensive technological usage, the knowledge of the mechanisms underlying the ferroelectric phase transition is rather poor. The nature of the phase transition itself (displacive or order-disorder) is still argument of debate [2]. In this contribution we report on our first-principles theoretical studies of the ferroelectric transition, which is described in detail at the microscopic level. Total energy calculations as well as long-run molecular dynamics simulations are used to understand the driving forces and mechanisms of the phase transition. Our calculations show that the structural phase transition is not an abrupt event, but rather a continuous process occurring over about 100 K and involving different ionic species at different temperatures. Because of the different behavior of the Li and Nb sublattice, the ferroelectric transition displays both displacive and order-disorder character. In addition to pure materials, the role of the widely used dopant Ti is investigated, and the results of existing experiments explained in the light of our theoretical models. [1] A. Räuber, Chemistry and Physics of Lithium Niobate (North-Holland Publ. Company, Current Topics in Mat. Sci., 1978). [2] I. Inbar and R. E. Cohen, Phys. Rev. B 53, 1193 (1996).

DF 3.2 Mon 15:20 EB 107

Comparison of hydrostatic and chemical pressure in lead-free $Na_{0.5}Bi_{0.5}TiO_3$-based materials studied by first-principles methods — •Melanie Gröting[1], Silke Hayn[1], Igor Kornev[2], Brahim Dkhil[2], and Karsten Albe[1] — [1]Materialwissenschaft, TU Darmstadt, Darmstadt, Germany — [2]Laboratoire SPMS, Ecole Centrale Paris, Chatenay-Malabry, France

$Na_{0.5}Bi_{0.5}TiO_3$-based materials show extraordinarily high strains and are thus promising environmentally friendly alternatives to the toxic lead-containing standard piezoelectric materials. $Na_{0.5}Bi_{0.5}TiO_3$ is considered as a model relaxor ferroelectric with a complex perovskite structure having two different cations (Na^+ and Bi^{3+}) on the A-site.

In this contribution, the influence of hydrostatic pressure and chemical substitution on ferroelectric instabilities and octahedral tilting in $Na_{0.5}Bi_{0.5}TiO_3$-based solid solutions is studied by first-principles methods. In pure $Na_{0.5}Bi_{0.5}TiO_3$ under positive pressure an orthorhombic Pbnm phase is stabilized above few GPa in good agreement with experimental data. While the polarization is "killed" leaving only tilts under positive pressure, for negative pressure the polarization survives whereas the tilts are suppressed leading to a tetragonal P4mm phase. We find that solid solutions of $Na_{0.5}Bi_{0.5}TiO_3$ with $CaTiO_3$ or $BaTiO_3$ show the same sequence of phase transitions as pure $Na_{0.5}Bi_{0.5}TiO_3$ under hydrostatic pressure and identify the origin of chemical pressure. Chemical substitution leads to a combination of both misfit and modulus effects due to differences in ionic sizes and chemical bonding properties of the different A-cations, respectively.

DF 3.3 Mon 15:40 EB 107

Investigation of the ferroelectric phase transition at silver sodium nitrite using noise measurements — •Jumna Mehlis, Ulrich Straube, and Martin Diestelhorst — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle

The thermal current noise in the vicinity of the ferroelectric-paraelectric phase transition was studied. For this purpose silver sodium nitrite is well-suited, because of its low relaxation frequencies. The current noise density of a short-circuited single crystal was amplified by a low noise operational amplifier. The noise spectra were measured as a function of the temperature by using a spectrum analyzer. The results are in agreement to the Nyquist theorem. That means the noise density is proportional to the temperature and the losses. Contrary to ohmic resistors the thermal noise density of ferroelectrics depends on the frequency. Moreover, the measured spectra show a characteristical change of the shape in dependence on the temperature. This change is strongly correlated with the ferroelectric phase transition temperature, which was determined by the simultaneously measured dielectric function.