

Colloquium on Solid-State Physics

Date: Thursday, May 26, 2011

Time: 17.15 h
Coffee, tea and cookies at 17.00h in front of the lecture hall

Place: Hörsaal HS 3
Physik - Department
Technische Universität München



Seminar of the Collaborative Research Centre/Transregio TRR 80:

Multifunctional oxides - Influence of defects on the ferroic properties

PD Dr. Sibylle Gemming
Institute of Ion Beam Physics and Materials Research
Helmholtz-Zentrum Dresden-Rossendorf e.V. (www.hzdr.de)
P.O. Box 51 01 19, D-01314 Dresden

Transition metal oxides exhibit a wealth of physical phenomena, among them ferroic properties such as ferroelasticity, ferroelectricity and ferromagnetism, or their combination in multiferroics. In addition, transition metal oxides are sensitive to the chemical environment via the external partial pressure of oxygen; changes induce stoichiometry deviations, which cause conductivity changes and modify the ferroic characteristics.

Ternary and quaternary compounds from the perovskite family will be discussed as examples, which correlate local changes due to point and planar defects with changes of the elastic, polarization and magnetic properties. The microscopic interactions are determined by density functional calculations, which yield the basis for more large-scale simulations with effective Hamiltonian approaches.

Under oxygen-poor conditions, oxygen vacancies in SrTiO_3 accumulate in an external electric field and reduce the hardness. In an Sr/O-rich environment the phases $\text{SrO}(\text{SrTiO}_3)_n$ are formed, which yield a distinct change of the X-Ray reflectivity due to the regular arrangement of extrinsic $\text{SrO}(001)$ stacking faults. YMn_2O_5 has a series of complex antiferromagnetic phases in coexistence with ferroelectricity. In YFeMnO_5 , only one commensurable ferrimagnetic phase was found and ferroelectricity is absent. Based on spin-polarized DFT calculations a Heisenberg model yields the coupling constants of the Fe-substituted and the manganese-only compounds and relates them to crystal-field interactions. BiFeO_3 is a rhombohedral multiferroic with several domain wall configurations. Among them, the 109 degrees and 180 degrees walls have a significant change in the component of their polarization perpendicular to the wall; the corresponding step in the electrostatic potential is consistent with a recent report of electrical conductivity at the domain walls. Changes in the Fe-O-Fe bond angles at the walls change the canting of the Fe magnetic moments which can enhance the local magnetization.