SYMM 1 Multiferroic Materials - Theory

Time: Tuesday 14:30–16:00 Room: HSZ 04

Invited Talk SYMM 1.1 Tue 14:30 HSZ 04

Magnetoelectric Multiferroics from First Principles — •C. Ederer and N. Spaldin — Materials Department, University of California, Santa Barbara

The combination of magnetic and ferroelectric properties in a single material is appealing both because of the interesting coupling effects that emerge as well as due to a variety of technological applications that can be envisaged. Computational methods based on density functional theory have made invaluable contributions to the present understanding of such magnetoelectric multiferroics. In this talk I will present an overview over current research activities in the field of multiferroic materials and illustrate how first principles methods can be used in various ways to investigate these systems. In particular, I will discuss the application of first principles methods to explain the confusing and sometimes contradictory experimental observations for the room-temperature multiferroic $BiFeO_3$, to predict novel effects like electric-field induced switching of magnetic order parameters in $BaNiF_4$, and to design new multiferroic materials with improved properties.

Invited Talk SYMM 1.2 Tue 15:00 HSZ 04

Electrostatic Interface Tuning in Superconducting Oxide Heterostructures — •N. Pavlenko — Institute of Physics, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany

In oxide heterostructures consisting of high-temperature superconducting films and ferroelectric/dielectric layers, electric fields can be used to switch between superconducting and insulating states by electrostatically tuning the free carrier density. Analyzing the superconducting pairing in a cuprate film in terms of a developed microscopic model model, we show that a coupling to electric dipoles and phonons at the interface of film and dielectric/ferroelectric gate localizes the injected charge and leads to a superconductor-insulator transition [N. Pavlenko et al., Phys. Rev. B, 72 (2005) 174516]. We find that in the correlated oxide films, the strong interface polaron effect is inherently connected to the stabilization of interface charge orderings and inhomogeneous states. This leads to a dramatic modification of the doping dependent phase diagrams which is expected to shed light on recent electric field-effect experiments with HTSC cuprates. Based on these results, we consider several novel design concepts for superconducting field-effect devices [N. Pavlenko, Phys. Rev. B 70 (2004) 094519; N. Pavlenko et al., Appl. Phys. Lett. 70 (2005) 012507] and discuss the ways to amplify the electric field effect.

Invited Talk SYMM 1.3 Tue 15:30 HSZ 04

Modelling realistic ferroic materials - multiscale approaches — •S. Gemming, I. I. Chaplygin, W. Alsheimer, and G. Seifert — Institut für Physikalische Chemie, TU Dresden, D-01069 Dresden

The complex coupling of electronic and structural degrees of freedom in ferroic materials makes it necessary to treat different physical properties on a different theoretical level. First-principles calculations based on the density-functional theory yield electronic and atomistic structure, potential and field distribution, as well as dielectric properties. Pure bulk or composite compounds, but also nanostructured species and systems including defects such as grain boundaries and vacancies can thus be investigated at the microscopic scale. Beyond this, the calculations provide a database for mesoscopic approaches, for instance for the conductivity mediated by both electronic and ionic contributions. Also the coupling between different spin subsystems in correlated systems is much better described by a modified Heisenberg approach, whose parameters can be based on first-principles data. In this way the phase sequence and transition temperatures in ferroic oxides have been accessed. Examples for bridging the microscopic and macroscopic length scales are provided by finite-element modelling of the elastic properties of realistic compounds, which contain microscopic defects, or by mean-field approaches to derive the long-range potential or field distribution of nanostructured matter.