Modeling of Defects and Surfaces in Perovskite Ferroelectrics

Gunnar Borstel

Department of Physics, University of Osnabrueck, D-49069 Osnabrueck, Germany

Thin ferroelectric films are important for the development of optical waveguides and integrated optics applications. The $SrTiO_3$ (110) surface is also widely used as a substrate for the cuprate superconductor growth. It is well known that the efficiency of ferroelectric devices is strongly affected by the presence of point defects, first of all, vacancies which are always present in non-stoichiometric crystals. In this talk, we present the state-of-the art of computer modeling of perfect and defective bulk perovskites and their surfaces, combining quite different theoretical approaches ranging from first principles to semi-empirical quantum mechanical and classical shell-model methods. Among the topics treated are: F-type electron centers (O vacancy which trapped one or two electrons), hole polarons bound to a K vacancy, self-ordering effects, and surface relaxation for $SrTiO_3$ surfaces with different terminations