DF 5: Invited Talk - Simone Sanna

Time: Tuesday 9:30–10:15 Location: GER 37

Invited Talk DF 5.1 Tue 9:30 GER 37

Understanding the puzzling behavior of $LiNbO_3$ surfaces form *first-principles* — •Simone Sanna — Lehrstuhl für Theoretische Physik, Universität Paderborn, 33098 Paderborn, Germany

The hallmark of ferroelectric surfaces is the possibility to switch their surface chemistry and physics by switching the bulk polarization. This is a unique feature, successfully exploited in modern applications, such as molecular self-assembly or molecular detectors. At the same time, however, the polarization charge gives rise to many exciting surface phenomena such as reconstructions and relaxations, which are not fully understood. Striking differences in the evaporation rates, work functions, chemical reactivity, etching rates and water freezing temperatures at differently polarized $LiNbO_3$ (0001) surfaces are further puzzling examples of a peculiar behavior, whose origin is still unclear. Unfortunately, the atomic structure of the $LiNbO_3$ surfaces remained for a long time experimentally inaccessible, as the unscreened surface charges hinder atomic force microscopy (AFM). In this work we present theoretical models of the technologically relevant (0001) and $(2\overline{1}\overline{1}0)$ lithium niobate surfaces, commonly referred to as Z-cut and X-cut. In a first step, the microscopic structure of the stable surface terminations is determined by ab initio thermodynamics. In a second step, the outcome of available experiments is explained on the basis of our density functional theory models. Particular emphasis is given to the interpretation of available AFM-images and to the explanation of several uncommon properties.