DF 16: Dielectric surfaces and interfaces

Time: Thursday 11:40–12:20 Location: EB 107

DF 16.1 Thu 11:40 EB 107

Resistive switching of Nb-doped $SrTiO_3$ single crystals — •Christian Rodenbücher, Krzysztof Szot, and Rainer Waser — Peter-Grünberg-Institut 7, Forschungszentrum Jülich, 52425 Jülich

The resistive switching effect in $SrTiO_3$ can be understood as an insulator to metal transition where a d-electron plays an important role which can be generated by creation of oxygen vacancies, electrodegradation or donor doping. In this talk we present the very surprising fact that Nb-doped $SrTiO_3$, although it is commonly regarded as a metallic material, can be switched. To clarify the nature of this phenomenon we investigated the crystallographic structure, the stoichiometry, the electronic structure and the transport by electrical measurements as well as by surface sensitive measurements like XPS, AFM and LEED which unquestionable reveal that switching occurs in a semiconducting surface layer which has greatly different properties than the metallic bulk. The stoichiometry and electronic structure of this surface layer can be dramatically altered by different preparation techniques like etching, leaching, heating in different atmospheres or Ar-bombardment. To get an insight in the nanoscopic origin of the switching, local conductivity AFM measurements were performed uncovering the highly local nature of the resistive switching which takes place in 10-30 nm big clusters which are present in the single crystal.

DF 16.2 Thu 12:00 EB 107

Water adsorption on $LiNbO_3$ Z-cut surfaces calculated from first principles — •Rebecca Hölscher, Simone Sanna, and Wolf Gero Schmidt — University of Paderborn

$LiNbO_3$ (LN) is a frequently used material for optical and acoustic applications due to its unusual but useful piezoelectric, pyroelectric, and photorefractive properties. As for other ferroelectric materials the surface reactivity can be changed by manipulating the polarization. This opens the possibility for the realization of molecular detectors and other devices[1]. Unfortunately only few data about the structure of the surface are available. Most studies do not refer to clean surfaces in UHV conditions, but are rather performed in ambient conditions, where the adsorption of foreign species like water will modify the the LN surface properties. Here we present ab initio calculations on the adsorption of H_2O molecules and thin water films on the positive (0001) and negative $(000\overline{1})$ surface of LN. The adsorption is modelled by means of density functional theory within the generalized gradient approximation[2,3]. The adsorption site and energy are determined as a function of the H_2O coverage. Different adsorption patterns are found depending on the surface polarity. The occuring water reconstruction is shown in phase diagrams as a function of temperature and pressure which reveal that at ambient conditions a H_2O film is present at the LN Z-cut.

[1] D. Li, M.H. Zhao, J. Garra, et al., Nature Materials ***7*** *(2008) 473. [2] W.G. Schmidt, M. Albrecht, S. Wippermann, S. Blankenburg, E. Rauls, et al., Phys. Rev. B* ***77*** *(2008), 035106. [3] S. Sanna, A.V. Gavrilenko, W.G. Schmidt, Phys. Stat. Sol. C* ***7*** *(2010) 145.*