Physics Seminar

Tuesday, 3 June 2014 at 11h00
(coffee at 10h45)

Campus Limpertsberg
Room BSC 1.04

Talk by Dr. Patrick Rinke
Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Space-Charge Transfer in Hybrid Inorganic-Organic Systems

Hybrid inorganic-organic systems (HIOS) have opened up new opportunities for the development of (opto)electronic and photovoltaic devices due to their potential of achieving synergy by combining the best features of two distinct material classes. The properties of HIOS can be tuned by inserting dipolar layers at the interface between the two materials. We use quantum mechanical first-principles approaches to study the interface between ZnO and molecular dipole layers. To take the bulk doping concentration of ZnO into account, I here present an approach that introduces excess charge in the unit cell by means of the virtual crystal approximation with fractionally charged nuclei [1] and that includes the energy contribution of space-charge layers and the associated band bending explicitly [1-3].

For the bulk terminated ZnO(0001) surface covered with half a monolayer of hydrogen (2x1-H), I demonstrate that electrons from bulk dopants can stabilize deviations from this half monolayer coverage at low hydrogen pressures [2]. Ambient hydrogen background pressures are therefore more conducive than ultra high vacuum conditions to form the defect free, semiconducting 2x1-H surface, which would be a more controlled substrate in HIOS [2]. For the interface between ZnO(0001) 2x1-H and tetra uoro-tetracyanoquinodimethane (F4TCNQ) monolayers, I show that the adsorption energy and the charge transfer to the molecules depend strongly on the bulk dopant concentration. While the build-up of a space-charge layer is not unexpected, the magnitude of its effect is astounding: the adsorption energy of F4TCNQ changes by more than 2 eV and more than doubles from low to high doping [3]. In the limit of low bulk doping concentrations, charge transfer becomes vanishingly small in agreement with photoemission data [3], while the F4TCNQ induced work function increase remains unaffected and large. The bulk doping concentration and the associated build-up of a space-charge layer therefore provide an additional way to tune the interface properties in HIOS and might generally affect interface properties.


Next Seminars

- Tuesday, 10 June 2014
  Limpertsberg, 16h00
  **Françoise Cornu**
  *Thermal contact in stochastic thermodynamics*

- Wednesday, 18 June 2014
  Limpertsberg, 16h00
  **Anja Kuhnhold**
  *Passive and active microrheology of an unentangled polymer melt studied by molecular dynamics simulation*