O 36: Methods: Atomic and electronic structure

Time: Tuesday 15:00–16:00 Location: H34

O 36.1 Tue 15:00 H34

Constructing fully numerical optimum atomic basis-sets — •Björn Lange, Christoph Freysoldt, and Jörg Neugebauer — Max-Planck Institut für Eisenforschung GmbH, 40237 Düsseldorf, Deutschland

Minimum atomic basis-sets as used e.g. for tight-binding calculations are commonly constructed by fitting them or even only their matrix elements to experimental or theoretical data. The resulting models are often optimized only for a specific environment, making a systematic analysis of their transferability impossible. In order to achieve systematically analyzable atom-centered basis-sets, we start from a plane-wave density-functional theory (DFT) calculation where the basis-set convergence is well controlled. The optimum radial shape for each angular momentum channel is determined by maximizing the overlap of the orbitals with the Bloch-states of the underlying plane-wave calculation. While previous approaches employ auxiliary radial basis functions, our orbitals are fully numerical. An analysis of the Bloch state residues shows that part which is not covered by the atomic orbitals and reveals transferability issues and improvement opportunities. To demonstrate the performance of this approach we provide results of an extensive analysis of the transferability characteristics for a wide array of materials such as molecules, semiconductors and metals. Furthermore, we demonstrate the advantages of our basis-sets compared to atomic orbitals obtained from the free atom. For example, detailed convergence checks show that they provide a much better starting point for iterative diagonalization approaches in DFT.

O 36.2 Tue 15:15 H34

Atomic structure of monolayer silica studied by new ion scattering techniques — •Jan Seifert, David Blauth, Andreas Schüller, Stephan Wethekam, and Helmut Winter — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin, Germany

The structure of ultrathin silica (SiO_2) films grown on a Mo(112) substrate is investigated by three recent experimental techniques using grazing scattering of fast atoms (keV energies) from the film surface: (1) Ion beam triangulation (IBT) where electron emission is recorded for scattering of hydrogen atoms as function of azimuthal orientation of the target. From directions of axial surface channels the position of surface atoms is deduced [1]. (2) Rainbow scattering under axial surface channeling conditions [2]. (3) Fast atom diffraction (FAD). For sufficiently small angles of incidence and projectile energies (2 keV), diffraction patterns can be observed in the angular distribution of scattered atoms and molecules. From the Bragg relation, the periodicity of the interaction potential and from the intensity modulation of the diffraction spots the corrugation of the potential and vertical positions of surface atoms can be determined [3]. Our examples demonstrate the attractive features of grazing fast atom scattering as a powerful tool for structure analysis in surface science.

[1] J. Seifert, D. Blauth, and H. Winter, PRL 103, 017601 (2009)
[2] J. Seifert and H. Winter, Surf. Sci. 603, L109 (2009)
[3] J. Seifert, A. Schüller, H. Winter, R. Włodarczyk, M. Sierka, and J. Sauer, to be published

O 36.3 Tue 15:30 H34

Modeling of interfaces and nanostructures: Effects of structure mismatch, bond polarity and interface charges — •Roman Leitsmann — GWT-TUD mbH, Material Calculations, Chemnitz, Germany

The characterization of interface and nanostructure properties versus dimension is of increasing importance [1]. Combinations of strongly ionic semiconductors such as PbTe and CdTe crystallizing in different structures may serve as prototypical systems. However, the theoretical ab initio description of interfaces between polar materials is controversially discussed in the literature [1].

We use ab initio methods to investigate structural and electronic properties of PbTe/CdTe interfaces and nanostructures. For this purpose 4 supercell schemes have been developed to treat internal electric fields, stoichiometry, orientation and thereby to model different experimental situations. The advantages and disadvantages of these models will be discussed at the prototypical example of PbTe/CdTe systems. The obtained interface energies are applied to PbTe nanodots embedded in a CdTe semiconductor matrix. For this system we predict an equilibrium rhombo-cubo-octahedron shape. It is used to show that the special arrangement of polar dot-matrix interfaces induces an electrostatic field, which strongly influences the geometrical and electronic properties and reduces the symmetry of the system [3].

[1] APL 88, 192109 (2006), NJP 8, 317 (2006); [2] PRB 79, 235331 (2009); [3] PRB 78, 205324 (2008), PRB accepted (2009)

O 36.4 Tue 15:45 H34

Characterization of the angular resolution of an inverse-photoemission experiment — •Anna Zumbülte, Kathrin Wulff, Anke B. Schmidt, and Markus Donath — Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Inverse photoemission (IPE) is an experimental method to investigate the unoccupied part of the electronic structure above the Fermi level with **k** resolution within a wide range of the Brillouin zone. The setup consists of a detection system for photons and an electron gun, whose beam divergence determines the angular resolution of the IPE experiment. While the improvement of the energy resolution has been addressed before [1], the improvement of the angular resolution was often neglected so far.

We present a quantitative approach to investigate the electron-beam divergence based on angle-resolved IPE spectra for dispersing sp-derived surface states on Cu(111). The simulation of spectra with different beam divergences shows a strong sensitivity of the peak intensities on the angular resolution. We discuss different criteria, which can be used to evaluate the beam divergence by comparing the simulated with the measured spectra. We apply these criteria to spectra measured with a high-resolution electron gun and compare the results with beam-profile measurements.

[1] M. Budke et al., Rev. Sci. Instrum. **78**, 113909 (2007)