O 70: Methods: Atomic and Electronic Structure III

Time: Friday 10:15–12:00 Location: H42

O 70.1 Fri 10:15 H42

Positron annihilation induced Auger electron spectroscopy (PAES) of thin metal layers on Cu and Si — •Jakob Mayer[1], Christoph Hugenschmidt[1,2], Philip Pikart[1], and Klaus Schreckenbach[1,2] — [1]Technische Universität München, Physikdepartment E21, James-Franck-Str., 85748 Garching — [2]Technische Universität München, ZWE FRM-II, Lichtenbergstr. 1, 85748 Garching

The high intense positron source NEPOMUC at the FRM-II in Munich provides an intensity of $\geq 10^7$ moderated (15 eV) positrons/s. This facility enables measurement times for positron annihilation induced Auger electron spectroscopy (PAES) of a few hours/spectrum. In contrast to the usual ^{22}Na based lab beams with a measurement time of several days, at NEPOMUC a spectrum can be obtained after only three hours. Compared with conventional EAES, PAES has a much higher surface sensitivity and due to the low positron energy even weakly bound atoms/molecules at the surfaces are not destroyed by the incident positron beam. Another advantage of PAES is the low background in the energy region of the Auger peaks.

The primarily high electron background due to surrounding experiments in the experimental hall of the FRM-II has been eliminated and hence background free experiments have become possible. Measurements of single crystalline silicon, polycrystalline copper and Cu coated Si are presented and compared with EAES respectively. The results reveal the advantages and the surface sensitivity of PAES.

O 70.2 Fri 10:30 H42

Electronic band structure of the layered dichalcogenide β-$MoTe_2$ — •Robert Heimburger, Thorsten Zandt, Christoph Janowitz, and Recardo Manzke — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstraße 21, 12489 Berlin

The transition metal dichalcogenide β-$MoTe_2$ grown by chemical vapour transport (CVT) at temperatures above 1175 K and cooled to room temperature shows a layered structure that can be described as stacked sandwiches of the tree layers Te-Mo-Te. One molybdenium atom is surrounded by six tellurium atoms forming an octahedron which is slightly distorted because of the molybdenium atom beeing displaced from the centre. Therefore strong metal-metal bonds are found which form zigzag chains along the crystallographic b-direction. Upon cooling below 250 K the material undergoes a structural phase transition where the β phase (monoclinic) changes to an orthorhombic Td-structure.
In this contribution we present a detailed temperature dependent study of electronic band structure and Fermi-surface of β-$MoTe_2$ performed by angle-resolved photoemission spectroscopy (ARPES). The measurements were carried out at BESSY II. It results that the dispersion of the valence bands along the different high-symmetric directions of the Brillouin zone are extremely weak. These bands reveal close insight into the low temperature and phase transition behaviour of quasi-two dimensional materials like β-$MoTe_2$. Fermi level crossings are studied by Fermi-surface maps. The experimental findings will be compared with tight-binding band structure calculations.

O 70.3 Fri 10:45 H42

Exploiting "local" in local orbital based all-electron electronic structure theory: How near can we get? — •Paula Havu, Ville Havu, Patrick Rinke, Volker Blum, and Matthias Scheffler — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin, Germany

Numeric atom-centered local orbitals (NAO) are efficient basis sets for all-electron electronic structure theory. A strict localization of NAOs can be exploited to render (in principle) all operations of the self-consistency cycle $O(N)$. This is straightforward for 3D integrals using domain decomposition into spatially close subsets ("domains") of integration points, enabling critical computational savings that are effective from ∼tens of atoms (no significant overhead for smaller systems) and make large systems (hundreds of atoms and beyond) computationally feasible. Using a new all-electron NAO-based code,[1] we investigate the quantitative impact of basis orbital localization on three distinct physical classes of systems: Extended light-element biomolecules, compact transition metal clusters, and periodic bulk/surface systems. Strictly confined NAOs are achieved by imposing a cutoff potential with an onset radius r_c, and exploited by appropriately shaped integration domains. Conventional tight $r_c \leq 3$Å have no measurable accuracy impact in Alanine-based polypeptides, but introduce inaccuracies of 20-30 meV/atom in Cu_n clusters. We show how a rigorous exploitation of NAO localization is critical in dense periodic systems.

[1] V. Blum, R. Gehrke, P. Havu, V. Havu, X. Ren, M. Scheffler, *The FHI Ab Initio Molecular Simulations (aims) Project*, Fritz-Haber-Institut, Berlin (2006).

O 70.4 Fri 11:00 H42

Sampling of stable and metastable cluster structures by a first-principles Monte Carlo approach — •Ralf Gehrke, Volker Blum, Karsten Reuter, and Matthias Scheffler — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin

Size-selected nano-scale atomic clusters are now systematically becoming accessible in experiment, but characterizing their ground-state and metastable isomer ensemble averages from first principles requires a global and local exploration of vast configuration spaces. We here explore a first-principles Monte Carlo scheme to efficiently sample the minima of the corresponding total energy landscapes. The energetics is obtained at the density-functional theory level, using an all-electron local orbital based first principles code,[1] which allows to switch seamlessly from minimal size effective tight-binding like to meV-level chemically accurate basis sets within a single fundamental framework. The sampling strategies rely on basin hopping, using single and multiple atomic moves to create new trial structures. We demonstrate the reliability and performance of the approach for Cu and Si clusters, discussing in particular the suitability of minimal basis set runs for a coarse screening of the total energy landscapes.

[1] V. Blum, R. Gehrke, P. Havu, V. Havu, M. Scheffler, *The FHI Ab Initio Molecular Simulations (aims) Project*, Fritz-Haber-Institut, Berlin (2006).

O 70.5 Fri 11:15 H42

Efficient treatment of segregation phenomena at alloy surfaces: The UNCLE code — •Ole Wieckhorst and Stefan Müller — Universität Erlangen-Nürnberg, Lehrstuhl für Festkörperphysik, Staudtstr. 7, D-91058 Erlangen

The success of the Cluster Expansion (CE) method in alloy surface problems depends heavily on the number of Density Functional calculations (DFT) necessary to stabilize the CE Hamiltonian. That is, a "good choice" of input structures, as well as pair- and multibody figures, plays a crucial role for the efficiency of the method. In strongly ordering and symmetry-lowering systems, (surfaces, e.g.), it may even happen that other modern CE's fail to predict the system's properties. We show that our new UNCLE code efficiently selects and reduces the number of relevant layer-dependent pair and multibody interactions. Consequently, the necessary number of DFT calculations is greatly decreased. This is accomplished by use of a mixed-space representation for the bulk and a separate treatment of relaxation energies in the CE Hamiltonian. We will demonstrate that, even with these smaller input sets, the code quantitatively predicts segregation phenomena at alloy surfaces.

O 70.6 Fri 11:30 H42

Band structure mapping and calculations of $CuInS_2$(001) — •Carsten Lehmann[1], Christian Pettenkofer[1], and Volker Eyert[2] — [1]Hahn-Meitner-Institut, SE6, Glienicker Strasse 100, 14109 Berlin, Germany — [2]Universität Augsburg, Inst. f. Physik, Universitätsstrasse 1, 86135 Augsburg, Germany

The ternary compound semiconductor $CuInS_2$ is used as an absorber material for thin film solar cells. A better understanding of the detailed electronic structure might lead to an improvement of the junction properties with respect to the still limited photo voltage of the present devices. We report on band structure mapping via ARUPS on thin epitaxial layers of $CuInS_2$(001) prepared on sulfur passivated $GaAs$(100). To have a better control on the deposition process we introduced a MOMBE type deposition with an organic sulfur precursor. Samples were prepared and precharacterized in a dedicated UHV deposition and analysis system. ARUPS measurements were conducted at the beamline TGM7 at BESSY II. We will discuss the experimentally determined band structure in comparison to recent augmented spherical wave (ASW) calculations as based on density functional theory and the local density approximation (LDA). Beside earlier calcu-

lations presented by Zunger for some high symmetry directions along $k_{perpendicular}$ our calculations include for $k_{parallel}$ the experimental parameters of an ARUPS experiment thus allowing a direct comparison with our experimentally derived data rather than an idealistic run on the boundary of the brillouin-zone. Additionally we derive the effective mass from the valence band curvature.

O 70.7 Fri 11:45 H42

Geometric Analysis of Etch Pits for Intrinsic Defect Studies in Optical Crystals — •Christian Motzer and Michael Reichling — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück

Calcium fluoride is the material of choice in optical devices applying deep ultraviolet light. Intrinsic crystal defects, e.g. dislocations, may cause birefringence and reduce the laser damage threshold. Such defects, therefore, impose major limitations on optical lithography in the semiconductor industry. By etching the crystal surface such defects exhibit an enhanced reactivity and a characteristic etching figure remains that allows a characterisation of defects in the crystal. We have investigated the dimensions and geometry of etch pits created with hydrochloric and phosphoric acid on (111) CaF_2 cleavage plates by means of contact mode scanning force microscopy (SFM). By comparing geometric data, we can differentiate between two basic types. One etch pit type is related to dislocation defects terminating on the surface. Our measurements showed that the depth of those etch pits relates to the angle between the surface and the direction of dislocations. The other etch pit type is related to nm-sized local defects and has a typical geometric characteristic which differs from that of dislocation etch pits. High resolution SFM images reveal that there is a distinct transition when the core of these defects is dissolved. By comparing geometric data, we can differentiate between combinations of dislocations and these local defects.