O 19: Clean surfaces I

Time: Monday 17:30–19:00 Location: A 053

O 19.1 Mon 17:30 A 053

Electron coincidence studies from S-overlayers on Cu(100) and Ni(100) — •Changhui Li[1], Swapnil Patil[1], Zheng Wei[1], Lucie Behnke[1], Frank O. Schumann[1], Gianluca di Filippo[2], Giovanni Stefani[2], and Jürgen Kirschner[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120Halle — [2]Dipartimento di Fisica, Università Roma Tre,Rome, Italy

In a previous double photoemission study of a Cu(100) surface we proved that the Auger process proceeds via a single step rather than a two-step process. The evidence was the emergence of a diagonal line in the 2D-Energy spectrum in the coincidence experiment [1]. In related coincidence measurements on atomic targets diagonal lines in the 2D-Energy distributions are reported in the literature. In order to bridge the gap between solids and atomic targets we prepared S-layers on a solid surface. We exposed a Cu(100), a oxygen passivated Cu(100) and a Ni(100) surface to H_2S gas. This caused the formation of S overlayers with nominal coverages of 0.25, 0.48 and 0.5 ML. We excited these structures with circular polarized light. The photon energy was adjusted such that the S 2p photoelectron and related Auger electron were both in the energy window of our coincidence spectrometer. We do not find a continuous energy sharing between photoelectron and Auger electron. Furthermore, we did not observe a helicity dependence of the coincidence and singles spectra. This means that the Auger emission from S proceeds via a two-step process.

[1] G. van Riessen, Z. Wei, R. S Dhaka, C. Winkler, F.O. Schumann, and J. Kirschner, J. Phys.: Condens. Matter 22, 092201 (2010).

O 19.2 Mon 17:45 A 053

Electronic Surface Properties of Transparent Conducting Oxides from First Principles: In_2O_3, SnO_2, and ZnO — •Benjamin Höffling[1,2], Sebastian Küfner[1,2], and Friedhelm Bechstedt[1,2] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität,Max-Wien-Platz 1, 07743 Jena,Germany — [2]Eutropean Theoretical Spectroscopy Facility (ETSF)

Transparent Conducting Oxides (TCOs) are important for their usage as transparent electrodes in optoelectric and photovoltaic devices as well as transparent electronics. The surface properties of these materials are therefore of great interest for future technical applications. Electronic parameters like the ionization energy, the electron affinity and the work function can be used for electronic band alignment with other semiconducting materials. The possible existence of electronic surface states in the fundamental band gap and the influence of dangling bonds play a crucial role for the efficiency of charge carrier separation in photovoltaic applications. Yet all of these key parameters are still controversially discussed in literature. We employ Density Functional Theory and most modern Quasiparticle Theory to predict electron affinity, ionization potential, surface energy and surface band structures for different surface orientations and terminations of the TCOs In_2O_3, SnO_2 and ZnO. The results are compared with experimental observations and interpreted with regard to possible applications in optoelectric devices.

O 19.3 Mon 18:00 A 053

Bulk and Surface Characterization of In2O3(001) Single Crystals — •Daniel Hagleitner[1], Manfred Menhart[1], Peter Jacobson[1], Sara Blomberg[2], Karina Schulte[2], Edvin Lundgren[2], Frank Kubel[3], Christoph Puls[3], Andreas Limbeck[3], Herbert Hutter[3], Lynn Boatner[4], Michael Schmid[1], and Ulrike Diebold[1] — [1]Institute of Applied Physics, TU Wien, Austria — [2]Division of Synchrotron Radiation Research, Lund University, Sweden — [3]Institute of Chemical Technologies and Analytics, TU Wien, Austria — [4]Materials Science and Technology Division, Oak Ridge National Laboratory, USA

Indium oxide, In2O3, has drawn increased attention from researchers over recent years. When doped with SnO2, the material is commonly referred to as Indium Tin Oxide (ITO), which is the prototypical Transparent Conducting Oxide (TCO). ITO combines high optical transparency in the visible range with a conductivity approaching that of a metal. Despite the technological importance of ITO, surprisingly little is known about its surface properties or those of pure indium oxide. We will present STM, STS, PES, LEIS and XRD results of high-quality single crystals grown by the flux method. In particular, we will discuss atomically-resolved STM images of the In2O3(001) single crystal surface depending on the surface preparation (reduced/oxidized/hydrogenated) conditions. PES and STS data show a significant difference of the electronic structure (surface states, band bending) depending on the surface preparation.

O 19.4 Mon 18:15 A 053

***SnO_2*: Band Structure Measurements by ARPES and Determination of Resistivity and Carrier Concentration** — •Stephan Machulik[1], Valentina Scherer[1], Christoph Janowitz[1], Helmut Dwelk[1], Alicia Krapf[1], Klaus Irmscher[2], and Recardo Manzke[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, Berlin, Germany

So far the experimental band structure of SnO_2 has only been measured on thin films or the surface of crystals prepared by sputtering [1]. These methods however lead to oxygen deficient and reconstructed surfaces. For the cleaved surfaces of single crystals, investigated by us, a higher resolution for the band structure measurements was obtained, due to less surface imperfections. By comparing our results with HSE hybrid functional band structure calculations good agreement has been found [2]. Prior to the angular resolved photoemission (ARPES) measurements the resistivity (ρ) and the carrier concentration (n) was determined by van der Pauw measurements.

[1] M. Batzil and U. Diebold, Progress in Surface Sience 79 (2005) 47-154

[2] J. B. Varley, A. Janotti, and C. G. Van de Walle, Physical Review B 81, 245216 (2010)

O 19.5 Mon 18:30 A 053

Ab-initio study of tin dioxide surfaces: stability and electronic structure — •Sebastian Küfner[1], Andre Schleife[2,1], Benjamin Höffling[1], and Friedhelm Bechstedt[1] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, D-07743 Jena, Germany — [2]Department of Physics, University of California, Santa Barbara, California 93106-9530, USA

SnO_2 as an transparent conducting oxide is an interesting material for application in transparent circuits, photovoltaic or optoelectronic devices. However, the electronic structures as well as the relative stability of different orientations and terminations of SnO_2 surfaces are not well known.

We apply the density functional theory to calculate the total energies and the atomic geometries of the low-index surfaces (001), (100), (110), (111) of rutile SnO_2. From a comparison to the quasiparticle bulk band structure we conclude that the results of the approximate LDA-$\frac{1}{2}$ scheme are sufficiently accurate while they can be obtained at significantly lower computational cost. Therefore, the LDA-$\frac{1}{2}$ method is used to calculate the surface band structures.

Calculating the surface free energy depending on the oxygen chemical potential, we find the oxygen-terminated (100) and (110) surfaces to be most stable, in accordance with experiments and other ab-initio results. We show that the insulating character is conserved for the surfaces (except for the tin terminated (110) one) even though surface states appear in the fundamental band gap. Furthermore, we obtain the ionization energies and electron affinities.

O 19.6 Mon 18:45 A 053

k-space microscopy with synchrotron radiation on Ag and Bi_2Te_3 — •Marten Patt, Vitaliy Feyer, Lukasz Plucinski, Carsten Wiemann, and Claus Michael Schneider — PGI-6, Forschungszentrum Jülich GmbH, Jülich, Germany

Momentum resolved photoelectron detection combined with an imaging energy filter gives access to a robust bandstructure imaging of the full k-space with comparatively short acquisition times. With our *NanoESCA* installation at the *Nanospectroscopy Beamline* at the synchrotron *ELETTRA* (Italy)[1] we combine this method with a microspot refocused synchrotron beam, which provides a defined excitation region (ca. 10 μm). The complete angular distribution of the excited electrons at one kinetic energy is measured parallel in one acquisition with an angular resolution $< 0{,}09$ Å^{-1}.

We present results of the well-known Ag (001) single crystal Fermi surface as well as of Bi_2Te_3, which belongs to a new class of materials:

the topological insulators [2]. Clear Dirac cone features are visible. Furthermore, we discuss the possibility of future time-resolved measurements due to the efficiency of this method.

[1] http://www.elettra.trieste.it/beamlines/NASP

[2] J.E. Moore, Nature (London) 464, 194 (2010)