O 34: Methods: Atomic and Electronic Structure I

Time: Tuesday 15:45–17:45 Location: H42

O 34.1 Tue 15:45 H42

Calculations for isolated slabs: MgO/Ag(001), Callen effective charge of O in MgO layers, Ag(001) in external electric field — •Ferenc Tasnadi — IFW, Dresden, Germany

The main purpose of the talk is to prove the applicability of our newly developed local scheme for isolated slabs. In this model one can treat systems, like asymmetrically terminated slabs when the two surfaces have different work functions or slabs with polarization along the normal direction, without any additional artificial field and image interaction. The first application gives the complete electronic and geometric analysis of the MgO/Ag(001) insulator metal interface. In the second example the dynamical Callen effective charge of oxygen is calculated for several MgO layers by the finite-difference method. In the third application homogeneous external electric field is applied to calculate the location of the electrostatic mirror plane of several Ag(001) slabs. The results show that our local scheme together with the newly derived two dimensional Ewald method provide an effective method for isolated slabs.

O 34.2 Tue 16:00 H42

The Evaluation of I(V) Curves in Scanning Tunnelling Spectroscopy of Organic Nanolayers Revisited — •Christian Wagner, Robert Franke, and Torsten Fritz — Institut für Angewandte Photophysik; TU- Dresden George-Bähr-Straße 1; 01069 Dresden

In our contribution we want to verify whether the use of *scanning tunneling spectroscopy* (STS) evaluation methods developed for inorganic samples can be justified also for the case of organic nanolayers, or whether modifications are necessary. Here one have to keep in mind that the traditional approaches are derived for the case of bulk samples and low voltages. Since an organic adsorbate on a substrate presents a sample with a more complex structure and is further characterized by a large gap in the eV range, the answer to this question is not *a priori* clear. After discussing relevant quantities, i.e., the sample *density of states* (DOS) and *local density of states* (LDOS), we demonstrate the use of the simple and well known model of a 1D tunnel junction in WKB approximation in order to calculate the sample DOS for several STS results from literature dealing with ultra thin organic layers. In a subsequent discussion we conclude that the model is applicable to the orbital mediated tunneling process 'through' organic molecules and that it can be used to evaluate such STS measurements. By several examples we illustrate a weakness of the normalized differential conductivity as a method of STS I(V) curve evaluation and propose a new normalization algorithm as a solution to the problem.

O 34.3 Tue 16:15 H42

Scanning Tunneling Spectrocsopy of image potential states on NaCl/Ag(100) — •Hans-Christoph Ploigt, François Patthey, and Wolf-Dieter Schneider — Ecole Polytechnique Fédérale de Lausanne, Institut de physique des nanostructures, CH-1015 Lausanne, Switzerland

Image potential states are important two-dimensional electronic states at surfaces the binding energy of which reflects the nature of the substrate, especially the presence of adsorbates. These states are probed by Scanning Tunneling Spectroscopy. We prepared Ag(100) samples which are partially covered by NaCl islands of different thickness and measured dI/dV spectra with closed feedback loop at 50 K and 5 K with different tips (W, PtIr, Ni). The spectra on clean Ag(100) are reproduced with a simple one-dimensional model which includes the electric field of the tunnel junction. In this way, the work function and the radius of curvature of the tip have been determined and introduced as fixed parameters in a 1D model which includes a dielectric layer to calculate the spectra on NaCl/Ag(100). The resulting good agreement between simulation and experiment allows us to extract from the shift of the image potential/field emission states between clean Ag(100) and NaCl covered Ag(100) the work function change of the sample.

O 34.4 Tue 16:30 H42

Enhanced Rashba spin-orbit splitting in Bi/Ag(111) and Pb/Ag(111) surface alloys — •Gustav Bihlmayer[1], Stefan Blügel[1], and Eugene Chulkov[2] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, D–52425 Jülich, Germany — [2]Donostia International Physics Center, 20018 San Sebastian/Donostia, Basque Country, Spain

We present first-principles calculations of a $(\sqrt{3}\times\sqrt{3})R30°$ Bi/Ag(111) surface alloy. This alloy has recently been investigated experimentally using angle-resolved photoemission spectroscopy [1]. We find that the surface state in the L projected bulk-bandgap shows a Rashba-type spin-orbit splitting which 3 times larger than what has been observed on a clean Bi(111) surface. We explain this large enhancement, which was also found in experiments, by the strong distortion of the surface state wavefunction which is caused by the substantial outward relaxation of the Bi atom. For comparison we report on a similar surface alloy, Pb/Ag(111), where the strong Rashba-type splitting is found in the calculations. Experimentally, the situation seems to be a bit more complicated due to a second, close-by surface state which was also observed. We discuss the dependence of the two-dimensional bandstructure on the surface corrugation and compare to the experimental findings [2].

[1] C. R. Ast et al. arXiv:cond-mat/0509509 (2005)
[2] D. Pacilé et al. Phys. Rev. B **73**, 245429 (2006)

O 34.5 Tue 16:45 H42

Giant spin-orbit splitting in the surface alloy Bi/Ag(111): A theoretical explanation — •Jürgen Henk, Arthur Ernst, and Patrick Bruno — Max-Planck-Institut für Mikrostrukturphysik, Halle (Saale)

The Rashba-Bychkov effect at (111) surfaces of noble metals, in particular Au, results in a spin-orbit splitting of the L-gap surface states, in analogy to a two-dimensional electron gas. Recent photoemission experiments for the surface alloy Bi/Ag(111) also found a spin-orbit splitting but the size of the splitting is unexpectedly large (Chr. Ast *et al*, cond-mat/0509509). Usual explanations of the effect by the atomic contribution to the spin-orbit coupling and by the gradient of the surface-barrier potential fail.

Relativistic first-principles calculations give strong support for a new mechanism. The interplay of the conventional Rashba-Bychkov contribution to the spin-orbit interaction and the in-plane gradient of the surface potential leads to the giant splitting of the Bi-derived surface states. In addition, the spin polarization of these states is considerably rotated out of the surface plane. The latter prediction suggests investigations by means of spin-resolved photoemission.

O 34.6 Tue 17:00 H42

Spin-orbit coupling in the band structures of the layered charge-density-wave compunds 1T-TaS_2 and 2H-$TaSe_2$ — •Kai Rossnagel[1] and Neville Smith[2] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel, Germany — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

Empirical tight-binding calculations on the layered charge-density-wave materials 1T-TaS_2 and 2H-$TaSe_2$ have been performed and are found to replicate the basic phenomenology of the electronic structure near the Fermi level as revealed by angle-resolved photoelectron spectroscopy (ARPES). In the case of 1T-TaS_2, the combination of spin-orbit coupling and the $\sqrt{13}\times\sqrt{13}$ reconstruction generates a distinct and very narrow band at the Fermi level [1]. For 2H-$TaSe_2$, the large spin-orbit splitting of the Ta 5d levels causes a significant change of Fermi surface topology and the combination of spin-orbit coupling and the 3×3 reconstruction gives rise to Fermi surface sheet-dependent energy gapping [2]. Our results highlight the importance of spin-orbit interaction in any understanding of the correlation effects and charge-density-wave transitions in these two materials.

[1] K. Rossnagel and Neville V. Smith, Phys. Rev. B **73**, 073106 (2006).
[2] K. Rossnagel and Neville V. Smith, to be published.

O 34.7 Tue 17:15 H42

$1T - TiSe_2$: Semimetal or Semiconductor? — •Julia Rasch, Torsten Stemmler, and Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin

Even though the semimetallic behavior of $1T-TiSe_2$ seemed to be well established by band structure calculations and previous photoemission results (see e.g. [1]), this conclusion has been challenged recently. Two

high-resolution photoemission investigations deduced semiconducting behavior, however with a very small band gap [2,3]. But such a conclusion is afflicted, on principle, by the problem of measuring an unoccupied conduction band by photoemission.

In the present contribution this problem is solved by the idea of H_2O adsorption onto the van der Waals-like surface, causing a distinct bending of the bands and resulting in an completely filled lowest conduction band. The detailed analysis yields undoubtedly semiconducting behavior for $1T - TiSe_2$ and interesting new properties of semiconductors with extremely small band gaps.

[1] O. Anderson, R. Manzke, M. Skibowski, Phys. Rev. Letters 55, 2188 (1985) [2] K. Rossnagel, L. Kipp, M. Skibowski, Phys. Rev. B 65, 235101 (2002) [3] T.E. Kidd, T. Miller, M.Y. Chou, T.-C. Yang, Phys. Rev. Letters 88, 226401 (2002)

O 34.8 Tue 17:30 H42

The origin of the Te 4d core level splitting in transition metal dichalcogenides with distorted CdI_2-structure — •Thorsten Zandt, Robert Heimburger, Christoph Janowitz, and Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin

Typically quasi-two-dimensional transition metal dichalcogenides exhibit the charge density wave phenomena. These show up e.g. as a superstructure in electron diffraction (e.g. LEED) or Fermi surface nesting in angular resolved photoemission. In addition, an observed attending splitting of certain core levels has also been interpreted to be caused by the charge density wave.

In this contribution we present a detailed temperature dependent soft x-ray photoemission study of Te 4d core levels of transition metal ditellurides. In some materials with distorted CdI_2-structure we found a splitting of the Te 4d core levels, *but no* superstructure in LEED. It will be argued the core level splitting, at least in the distorted ditellurides, is more likely due to the geometric zig-zag chains of the transition metals than a charge density wave effect.