O 51 Hauptvortrag Kampen

Zeit: Mittwoch 09:45–10:30 Raum: TU EB301

Hauptvortrag O 51.1 Mi 09:45 TU EB301

Electronic structure of organic interfaces — •Thorsten Ulrich Kampen — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany

The energy level alignment at organic interfaces determines the efficiency of charge injection into organic films. Quite often the vacuum level alignment rule has been used to determine the energy level alignment at organic interfaces. Here, barrier heights can simply be calculated using the ionisation potentials or electron affinities of semiconductors materials and work functions of metals. For organic interfaces a conclusion has been reached that in general the vacuum levels do not align. This difference in vacuum levels is attributed to interface dipoles. Another important issue is the occurrence of a band-bending like electrostatic energy shift in organic layers, which has been observed in many metal/organic systems. In most cases this shift is confined to a regime of only a few nanometers, which cannot be accounted for using the conventional band bending theory of inorganic semiconductors. Shifts occurring in such small thickness ranges can be due to a change in the intermolecular interaction, namely, due to a change in the molecular orientation as a function of the film thickness. At intimate, abrupt, and defect free interfaces of organic semiconductors which show a band like dispersion in the highest occupied energy levels interface induced gap states govern the energy level alignment.

O 52 Elektronische Struktur IV

Zeit: Mittwoch 10:45–13:00 Raum: TU EB301

O 52.1 Mi 10:45 TU EB301

A photoelectron spectro-microscopy investigation of singleMoS$_2$ nanotubes — •A. Gloskovskii[1], M. Chincetti[1], S. A. Nepijko[1], G. Schönhense[1], H. A. Therese[2], G. H. Fecher[2], H. C. Kandpal[2], C. Felser[2], W. Tremel[2], and M. Klimiankou[3] — [1]Institut für Physik, Johannes Gutenberg -Universität, 55099 Mainz — [2]Institut für Anorganische und Analytische Chemie,Johannes Gutenberg - Universität, 55099 Mainz — [3]Institut für Materialforschung I, Forschungszentrum Karlsruhe GmbH, 76021 Karlsruhe

Nanostructured MoS_2 was prepared by thermal decomposition of $(NH_4)_2Mo_3S_{13}$ x H_2O in sealed tubes and nanotubes of MoS_2 were prepared by coating technique using SiO_2 rods as template. The samples were characterized by XRD, HRTEM, EELS, and XANES techniques. The electronic structure of MoS_2 was investigated by means of two photon photoemission spectroscopy (2-PPE) performed with a time-of-flight photoemission electron microscope (TOF-PEEM). The spatially resolved 2-PPE spectra show distinguished features arising in emission from the nanotubes. These features are explained by emission from the valence band via resonant excitation of an intermediate state in the conduction band. The size of the gap in semiconducting nanotubes will be discussed on hand of the 2-PPE spectra in comparison to electronic structure calculations. The electronic structure was calculated self-consistently by means of LMTO and FLAPW techniques. Comparing experimental and theoretical findings, we conclude that full potential methods are necessary to calculate electronic properties in particular for sulfide and oxide based nanotubes. (Funded by DFG in SFB 625 TP9.)

O 52.2 Mi 11:00 TU EB301

Quasi-one-dimensional surface states on Pt(110) — •Mariana Minca, Enrico Dona, Zhenrong Zhang, Alexander Menzel, and Erminald Bertel — Phys. Chemie, Univ. Innsbruck, A-6020 Innsbruck

Experimental investigation of the electron correlation responsible for the rich and technologically highly interesting phase diagram [1] of low-dimensional or even quasi-one-dimensional (Q1D) materials is difficult on account of the complex structure, surface reconstructions, and sensitivity to radiation damage of most model systems. Here we show that the clean missing-row reconstructed (1x2) Pt(110) surface can be used as a Q1D model system. The electron dispersion as measured by ARUPS at different photon energies reveals a Tamm-type Q1D surface resonance [2], which is derived from the very high bulk-DOS between the L and W point in the volume band structure [3]. Upon increasing the temperature, the corresponding quasiparticle peak at the Fermi Energy decays rapidly, as is seen in other weakly coupled Q1D systems. We discuss the unusual temperature dependence in terms of a coherent-incoherent transition.

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[2] S.D. Kevan (Ed.), *Angle-Resolved Photoemission* (Elsevier, Amsterdam 1992), p.99
[3] O.K. Andersen, Phys. Rev. B **2**, 883 (1970).

O 52.3 Mi 11:15 TU EB301

Fermi contours of a quasi-periodic 1-D film structure — •P. Moras[1], L. Ferrari[1], S. Gardonio[1], C. Carbone[1], J. Fuji[2], W. Theis[3], and K. Horn[4] — [1]Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, Trieste, Italy — [2]Laboratorio TASC, I.N.F.M, Trieste, Italy — [3]Freie Universitaet, Berlin, Germany — [4]Fritz-Haber-Institut, MPG, Berlin, Germany

Ag(111) films grown on GaAs(110) present in high-resolution STM images a quasi-periodic distribution of stripes running along the GaAs[1-10]-direction with two characteristic separations of 17 Å and 12 Å. The resulting one-dimensional superstructure can be described by a golden-mean Fibonacci sequence with a coherence length of about 125 Å. Angle-resolved photoemission has been used to examine the spectral functions of the sp-derived Ag electronic states as a function of the photoelectron momentum. While the dispersion of the Ag sp-quantum well states along the stripe direction is close to a free-electron-like parabola, it displays flatter bands and a complex branching structure perpendicularly to them. A close correspondence is found between the incommensurate wave vectors derived from the LEED pattern and those characterizing the Fermi contours of the Ag films in the two-dimensional reciprocal space.

O 52.4 Mi 11:30 TU EB301

Electron dynamics in vacancy islands — •J. Kröger[1], H. Jensen[1], R. Berndt[1], and S. Crampin[2] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel, Germany — [2]Department of Physics, University of Bath, Bath BA2 7AY, United Kingdom

The dynamics of Ag(111) surface state electrons confined to nanoscale hexagonal and triangular vacancy islands are investigated using scanning tunneling spectroscopy. The lifetimes of quantised states with significant amplitude near the centers of the vacancies are weakly affected by the geometry of the confining cavity. A model that includes the dependence of the lifetime on electron energy, vacancy size, step reflectivity and the phase coherence length describes the results well. For vacancy islands with areas in the range ≈ 40–$220\,\mathrm{nm}^2$ lossy scattering is the dominant lifetime-limiting process. This result and a corrected analysis of published experimental data improve the consistency of experimental and calculated surface state lifetimes.

O 52.5 Mi 11:45 TU EB301

Disorder induced local density of states oscillations on narrow Ag(111) terraces — •Karina Morgenstern[1], Karl-Heinz Rieder[1], and Gregory A. Fiete[2] — [1]Institut fuer Experimentalphysik, FB Physik, Freie Universitaet Berlin, Arnimallee 14, D-14195 Berlin, Germany — [2]Kavli Institute for Theoretical Physics and Department of Physics, University of California, Santa Barbara,CA 93106, USA

The local density of states of Ag(111) has been probed on disordered terraces of varying width by dI/dV-mapping with a scanning tunneling microscope at low temperatures. Shifts of the bottom of the surface state band edge lead to varying differential conductance for terraces of different widths. In contrast to perfect terraces, standing wave patterns are observed parallel to the step edges, i.e. in the non-confined direction. Scattering calculations for disordered terraces reproduce these spatial oscillations and all the qualitative features of the standing wave patterns