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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[1] M. Imada, A. Fujimori, and Y. Tokura, Rev. Mod. Phys. **70**, 1039 (1998).
[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 and, thus, reveal the underlying reason for these obwervations.

O 52.6 Mi 12:00 TU EB301

Electrons in the competing potentials of a Moiré-type — •Christian R. Ast[1], Daniela Pacilé[1], Marco Papagno[1], Gero Wittich[2], Klaus Kern[1,2], and Marco Grioni[1] — [1]Ecole Polytechnique Fédérale de Lausanne, Lausanne — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

The effects of weak changes in the periodic potential on the electronic structure can be nicely studied in overlayer structures showing a Moiré-type superlattice. Angular resolved photoemission spectroscopy is used to study the valence bands of Pb on Ag(111), which produces a hexagonal Moiré superlattice at monolayer coverage having a lattice constant incommensurate with the surface. The measured electronic structure of the Pb monolayer is hardly influenced by the substrate due to the mismatch in lattice constants. However, within the monolayer the electrons feel the presence of two competing periodicities: The hexagonal primitive cell in the plane of the monolayer as well as the characteristic modulation of the Moiré structure normal to the monolayer plane with a much larger unit cell. A scenario will be proposed in which the superimposed modulation is not strong enough to change the Brillouin zone but does influence the overlap of orbitals normal to the monolayer plane.

O 52.7 Mi 12:15 TU EB301

Quantum Well States in thin films of In on Si(100) — •Jan Hugo Dil, Jeong-Won Kim, Thorsten Ulrich Kampen, and Karsten Horn — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Abteilung Molekülphysik, Faradayweg 4-6, 14195 Berlin

Experiments with ultrathin metal layers on metal or semiconductor substrates have recently resulted in a wide variety of discoveries; anomalous behaviour of the hall effect, self organisation into magic or preferred layers, and strong electron correlation effects are just a few of them. Moreover the quantum well states (QWS) formed in these structures allow for detailed studies of electron-phonon coupling. Here, we present a study of atomically flat layers of indium grown on a Si(100) substrate. QWS are

readily observed for a wide range of coverages. These can be discriminated into QWS lying above and below a bandgap. This bandgap corresponds to the one observed in the valenceband of bulk indium. In the direction parallel to the interface the QWS show a free electron like behaviour as expected from DFT calculations. In the energy region where the QWS cross the Fermi energy with free electron like behaviour electron-phonon coupling may be observed.

O 52.8 Mi 12:30 TU EB301

Characterization of nearly free electron bands in thin Al-Mg alloy films on Si(111) — •Massimo Tallarida[1], Lucia Aballe[2], Ashwani Kumar[1], Sudipto Roy Barman[3], and Karsten Horn[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]ELETTRA SpA, Trieste, Italy — [3]UGC-DAE Consortium, Indore, Indien

Thin films of Al-Mg alloys have been grown on Si(111) by MBE over a wide range of compositions, and were characterized by angle-resolved photoemission. For Al-rich alloys, electron confinement leads to the occurrence of quantum well states, and a surface state similar to that in the Al/Si(111) film is found. For Mg-rich compositions, only a broad surface state is observed. The occurrence of quantum well states and the surface state, and their binding energy dependence on alloy composition is explained in terms of the virtual crystal approximation, with an average electron density in the alloy system. The dispersion of the quantum well states in a direction parallel to the film shows a nearly free electron behaviour similar to that found in Al/Si(111). The variation of electron density in these alloy films open the way for a study of more complex metallic systems, e.g. an investigation of the influence of electron density of the electromagnetic response.

O 52.9 Mi 12:45 TU EB301

Molecular orbital shift of PTCDA on Au(111) and Au(788) — •Henning Jensen[1], Jörg Kröger[1], Riccardo Rurali[2], Nicolás Lorente[2], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität Kiel, D-24098 Kiel, Germany — [2]Laboratoire Collisions - Agrégats - Réactivité, Université de Toulouse, F-31062 Toulouse, France

Scanning tunnelling microscopy of 3,4,9,10-perylenetetracarboxylic-dianhydride adsorbed on Au(111) and Au(788) reveals two coexisting superstructures with different coordination numbers. Using single-molecule tunnelling spectroscopy we find that the energy of the second-to-lowest unoccupied molecular orbital varies significantly with coordination geometry. Theoretical modelling attributes this variation to a dipole moment induced by deformation of the molecular plane.