O 41 Elektronische Struktur III

Zeit: Dienstag 10:45–13:00 Raum: TU EB107

O 41.1 Di 10:45 TU EB107

Systematic ARPES study of the influence of different adsorbates on surface states — •Frank Forster, Azzedine Bendounan, Johannes Ziroff, Felix Schmitt, and Friedrich Reinert — Experimentelle Physik II, Universität Würzburg, Germany

On the example of the (111) surfaces of Cu, Ag and Au we demonstrate that high and angle resolved photoemission spectroscopy (ARPES)($\Delta E = 3$ meV, $\Delta\Theta = 0.3°$) is a powerful tool for the study of the influence of differnt absorption processes on the electronic structure of these systems.

We discuss that only one monolayer of weak-interacting rare gases is reponsible for a characteristic shift of the Shockley-states towards and even above the Fermi level whereas bulk states of the substrates remain – except for band back-folding – almost unimpressed. Furthermore, the Au(111) surface state experiences an increase in the spin-orbit splitting up to 30%.

In contrast to the physisorption process of rare gases, a coverage of alkali metals on the nobel metal surfaces leads to a opposite effect on the Shockley-states, i.e., a decrease of the still detectable spin-orbit splitting and an increase in binding energy, until they reach the bottom of the L-gap and vanish in the bulk states.

These experimental results are supported by theoretical considerations which allow a deeper understanding of the electronic processes on adsorbate-substrate interfaces.

O 41.2 Di 11:00 TU EB107

Electronic structure of misfit layer chalcogenides — •Matthias Kalläne[1], Hans Starnberg[2], Kai Rossnagel[1], Sven Stoltz[2], and Lutz Kipp[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098, Germany — [2]Department of Physics, Göteborg University and Chalmers University of Technology, SE-412 96 Göteborg, Sweden

Misfit layer chalcogenides $(MX)_{1+x}(TX_2)_m$ (M=Sn, Pb, Sb, Bi; T=Ti, V, Cr, Nb, Ta; X=S, Se; $0.08 < x < 0.28$; m=1,2,3) result from an alternate stacking of MX and TX_2 slabs where the cubic MX layers are incommensurate with the hexagonal TX_2 layers in one of the two crystallographic directions parallel to the layers. To reach a better understanding of the electronic structure of these compounds we have performed angle-resolved photoelectron spectroscopy and photoelectron spectromicroscopy experiments. Our results reveal details about charge transfer from the MX to the TX_2 layers, interlayer bonding, possible effects of the incommensurability, and the domain structure of the cleavage planes. The photoemission experiments were carried out at HASYLAB (Germany), MAXLAB (Sweden), and the ALS (USA). Work at the University of Kiel is supported by DFG Forschergruppe FOR 353.

O 41.3 Di 11:15 TU EB107

Unoccupied electronic states on oxidized SiC(0001)-surfaces determined by inverse photoemission — •Kathrin Wulff, Ralf Ostendorf, Carsten Benesch, and Helmut Zacharias — Physikalisches Institut, Universität Münster, Wilhelm-Klemm Strasse 10, 48149 Münster

Starting from the silicon rich (3×3) reconstruction of SiC(0001) we prepared oxidized surfaces by hydrogen etching as well as molecular oxygen exposure ranging from 5000 L to 30000 L. LEED pictures show a (1×1)-reconstructed surface with a faint $(\sqrt{3} \times \sqrt{3})$R30° structure after oxidation, indicating a mainly disordered surface with only few patches of long range order. A distinct change in the shape of the Si_{LVV} AES peak which is similar to spectra taken on pure SiO_2 refers to the existence of Si-O bonds on the surface.

By applying inverse photoemission spectroscopy we find four electronic resonances above the Fermi level. Decreasing intensities with time caused by residual gas phase contaminants identify these structures as possible surface states. Finally, wave-vector resolved measurements show a flat dispersion for each resonance throughout the whole surface Brillouin zone.

O 41.4 Di 11:30 TU EB107

Rechnungen zur energie- und winkelaufgelösten Photoemission an GaN(0001) Oberflächen — •Thomas Strasser und Wolfgang Schattke — Institut für Theoretische Physik und Astrophysik, Leibnizstr. 15, 24098 Kiel

Galliumnitrid hat in der Optoelektronik erheblich an Bedeutung gewonnen. Jedoch sind Fragen zur elektronischen und geometrischen Struktur seiner Oberfläche offen. Die Photoelektronenspektroskopie ist aufgrund ihrer Oberflächenempfindlichkeit ein geeignetes Mittel zu ihrer Klärung.

Ausgangspunkt der Untersuchung sind theoretische Oberflächenmodelle der 1x1 aus Gesamtenergierechnungen von Wang et. al. [1]. Für diese werden gerechnete Spektrenserien in nichtnormaler Emission entlang verschiedener hochsymmetrischer Richtungen gezeigt und mit Hilfe von Matrixelementen, Zustandsdichten und komplexen Endzustandsbändern analysiert.

Zum Vergleich stehen experimentelle Ergebnisse von Dhesi und Chao zur Verfügung [2,3]. Beide Experimente wurden an 1x1 GaN Oberflächen durchgeführt, zeigen aber dennoch charakteristische Unterschiede. Ziel ist es, diese mit Hilfe des Einstufenmodells auf mikroskopischer Ebene zu verstehen.

[1] Fu-He Wang et al.; Phys. Rev. B 64, 035305 (2001).
[2] S.S. Dhesi et al.; Phys. Rev. B 56, 10271 (1997).
[3] Y.-C. Chao et al.; Phys. Rev. B 59, R15586 (1999).

O 41.5 Di 11:45 TU EB107

Polarization-Dependent Domain Contrast on cesiated Si(100) in Photoemission Electron Microscopy — •D. Thien, M. Horn-von Hoegen, and F.-J. Meyer zu Heringdorf — Institut für Laser und Plasmaphysik, Universität Duisburg-Essen (Campus Essen), 45117 Essen

On the Si(100) surface, two types of terraces are present with either (2x1) or (1x2) reconstruction. In Low Energy Electron Microscopy (LEEM) dark-field contrast can be observed if a diffraction spot of only one of the two superstructures is used for imaging of the related domain. In Photoelectron Emission Microscopy (PEEM), however, such contrast has not yet been observed. Using a polarized light source such as a 532nm-laser (2.4eV) for illumination of a Cs covered Si(100) surface, however, we observe a polarization dependent photoemission signal of the two different terraces. Ultraviolet Photoemission Spectroscopy (UPS) and Medium Energy Ion Spectroscopy (MEIS) studies of Cs on Si(100) indicate the transfer of the Cs 6s electron to the previously unoccupied upper dangling bond state of the Si(100) surface [1], which acts as initial state for the photoemission process. This lowers the work function while leaving the geometry of the silicon substrate unchanged. The polarization dependence of this contrast is strong enough to be observed even with a green laser pointer.

[1] J.Günster et al., Surf.Sci.359(1996)155-162

O 41.6 Di 12:00 TU EB107

The electron-phonon coupling on Mg(0001) — •T. Kim[1], T.S. Sørensen[1], E. Wolfring[1], H. Li[2], E.V. Chulkov[3], and Ph. Hofmann[1] — [1]Institute for Storage Ring Facilities, University of Aarhus,8000 Aarhus C, Denmark — [2]Department of Physics, Zhejiang University,Hangzhou 310027, China — [3]Donostia International Physics Center (DIPC), 20018 San Sebastián/Donostia, Basque Country, Spain

The influence of many-body effects on surface state lifetimes, and in particular the role of the electron-phonon coupling, has recently attracted considerable attention. Work has mostly concentrated on surface states located in wide gaps of the projected band structure, such as the L-gap surface states of the (111) noble metal surfaces or the surface state on Be(0001). Here we report results from the deeply penetrating surface state which is located in a narrow gap at the Brillouin zone centre of Mg(0001). The temperature-dependent photoemission linewidth of this state is used to determine the electron-phonon mass enhancement parameter λ. λ, as well as the electron-electron contribution to the surface state linewidth at zero temperature, are compared to first-principles calculations and good agreement is found.

O 41.7 Di 12:15 TU EB107

Influence of electron-phonon-coupling on the spectral function of nitrogen induced adsorbate states on Cu(100) — •Christian Bumiller, Thordis Michalke, Christian Kant, and René Matzdorf — Institut für Physik, Universität Kassel

We investigated the self organized surface of the adsorbate system nitrogen on copper (Cu(100)c(2×2)N) by means of angle resolved photoelectron spectroscopy (ARPES). Temperature dependent photoelectron spectra reveal a very strong electron-phonon-coupling of the nitrogen induced states on Cu(100). The strong coupling is very interesting for electronic states close to the Fermi level. One adsorbate state shows exceptional behaviour when approaching the Fermi energy. The spectral function changes drastically with the energy position. Here the real part of the self energy for the electron-phonon-coupling is visible. We show the influence of the self energy at different temperatures and binding energies. The characteristic features of the spectra are explained with the Eliashberg theory using the Einstein and Debye models for the phonon density of states.

O 41.8 Di 12:30 TU EB107

PES and LEED-IV measurements of Cu(100)c(2×2)N in comparison with theoretical studies — •Ch. Kant[1], Th. Michalke[1], Ch. Bumiller[1], J. Braun[2], A. Postnikov[3], and R. Matzdorf[1] — [1]Institut für Physik, Universität Kassel — [2]Universität Münster — [3]Universität Osnabrück

The atomic structure of the self organized nanopatterned adsorbate system Cu(100)c(2×2)N is still under discussion and the electronic bandstructure was not measured so far. Although it is known since 30 years, that nitrogen adsorbs at the fourfold hollow site, the positions of the outermost copper-atoms, which may undergo a strong reconstruction due to the incommensurate adsorption of nitrogen, is not clarified completely. We present the first angle resolved photoemission spectra of this system. The measurements are compared with detailed theoretical calculations based on the one-step model of photoemission. These calculated spectra are very sensitive to the positions of N- and Cu-atoms. The results from the calculations may help to understand the atomic structure of the adsorbate system. In addition we use LEED-IV analysis to evaluate the models of the surface structure.

O 41.9 Di 12:45 TU EB107

Energy and angle resolved measurement of the $(1\pi)^{-1}$ photoemission cross section of CO adsorbed on Pt(111) — •Grigorios Tsilimis, Sebastian Wegner, Jörg Kutzner, and Helmut Zacharias — Physikalisches Institut, Westfälische Wilhelms-Universität, Wilhelm-Klemm-Straße 10, D-48149 Münster

The c(4×2)-2CO-covered Pt(111) surface is investigated by energy and angle resolved photoelectron spectroscopy (ARUPS) using high-order harmonic radiation. Femtosecond pulses of a table–top, high–repetition rate (1 kHz) Ti:sapphire laser system are focussed into rare gases to generate high-harmonic radiation in the range of $h\nu = 20$ to 120 eV ($60 - 11$ nm). Both the coarse tunability in steps of 3.1 eV as well as a fine tuning within a single harmonic are utilized in the measurements.

The photoemission cross section of the CO-induced structures, in particular the pronounced $CO(1\pi)^{-1}$-emission at photon energies around $h\nu = 32$ eV is analyzed by means of partial wave decomposition. The influence of the surface on the electronic structure of the adsorbed CO leads to a different $(1\pi)^{-1}$-emission compared to oriented gas phase CO molecules.