O 19 Electronic structure II

Time: Tuesday 11:15–13:00 Room: WIL A317

O 19.1 Tue 11:15 WIL A317

Surface state lifetimes from scanning tunnelling spectroscopy: A theoretical analysis — •Michael Becker[1], Simon Crampin[2], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Department of Physics, University of Bath, Bath BA2 7AY, United Kingdom

Recently the discrepancy between image state lifetimes measured by means of the scanning tunneling microscope (STM) and two-photon-photoemission spectroscopy was lifted [1]. The electric field applied in STM was shown to cause an increase in both the efficiency of the image state decay channels as well as their number. In the light of this work, we theoretically investigate the impact of the STM induced electric field on the inelastic electron-electron damping rate of the electron- and hole-like excitations in the Shockley surface state band at Ag(111). Our calculations within the GW approximation of many-body theory are based upon the approach developed by Chulkov and coworkers [2]. The results indicate that under typical tunnelling conditions the STM does not significantly alter the surface state wavefunction and so previous STM derived Shockley state lifetimes need not be corrected.

[1] S. Crampin, Phys. Rev. Lett. **95**, 046801 (2005)
[2] E. V. Chulkov, I. Sarria, V. M. Silkin, J. M. Pitarke, and P. M. Echenique, Phys. Rev. Lett. **80**, 4947 (1998)

O 19.2 Tue 11:30 WIL A317

Image-Potential States of Reconstructed Au(100) — •M. Alexander Schneider, Gero Wittich, Lucia Vitali, and Klaus Kern — Max-Planck-Institute for Solid State Research, 70569 Stuttgart, Germany

Electrons in image-potential states form an exemplary two-dimensional electron gas at the surface of many metals. As the major weight of the electron wavefunctions is found in the vacuum region they are attractive for studying the mechanisms limiting electron lifetimes which are larger than that of other electronic states in metal systems.
However, despite the low overlap with the surface region of a crystal, defects at surfaces modify the electronic states considerably. This is demonstrated in a low-temperature Scanning Tunneling Spectroscopy (STS) study of the image-potential states of reconstructed Au(100) (5x27). The interaction with the reconstruction introduces band-gaps in the dispersion of the image-potential states and causes a spatial anisotropy of the image potential states. STS allows to study the behavior of the electrons at defects like dislocations or step edges. We will discuss to what extent the (scattering) surface potential can be reconstructed from STS measurements.

O 19.3 Tue 11:45 WIL A317

Structure of the Adatom Electron Band of the Si(111)-7×7 Surface — •Josef Mysliveček[1], Anna Stróżecka[1], Jan Šteffl[2], Pavel Sobotík[2], Ivan Ošťádal[2], and Bert Voigtländer[1] — [1]Institut für Schichten und Grenzflächen (ISG 3) and cni – Center of Nanoelectronic Systems for Information Technology, Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Charles University, Faculty of Mathematics and Physics, Department of Electronics and Vacuum Physics, V Holešovičkách 2, 180 00 Praha 8, Czech Republic

Using a low temperature scanning tunelling spectroscopy we map the wave functions of the electrons in the adatom band of the Si(111)-7×7 surface in real space. We observe the splitting of the adatom electron states to "ring" (corner adatom) and "dimer" (center adatom) structures in agreement with recent theory and determine the relative energies of these structures. A high resolution of our measurement is a tradeoff for the loss of absolute energy scale due to transport limitations in tunelling spectroscopy of semiconductors at low temperatures.

O 19.4 Tue 12:00 WIL A317

Unoccupied surface state on Pt(111) revealed by scanning tunneling spectroscopy — •Jens Wiebe[1], Focko Meier[1], Katsushi Hashimoto[1], Gustav Bihlmayer[2], Stefan Blügel[2], Paolo Ferriani[1], Stefan Heinze[1], and Roland Wiesendanger[1] — [1]Institute of Applied Physics, Hamburg University, D-20355 Hamburg, Germany — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany

Surface states are known to play a crucial role in chemistry, magnetism and for the growth properties of surfaces of noble metals and late fcc transition-metals (Ni, Pd, Pt). For noble-metal (111) surfaces it is well known that a partly occupied surface state resides far inside the projected bulk *sp*-band gap. The situation is more complex for the transition-metals. Ni(111) has a partly occupied surface state, while the corresponding surface state on Pd(111) is unoccupied and far above the Fermi energy E_F. For Pt(111) the situation was controversial so far.

We measured the dispersion of an unoccupied surface state on Pt(111) by imaging scattering states at point defects and step edges using scanning tunneling spectroscopy. By comparison to first-principles electronic structure calculations the state is assigned to an *sp*-derived surface band at the lower edge of the projected bulk band-gap. In $dI/dV(V)$-curves, the onset of the surface-state band appears as a rather broad feature. Its shape results from two spin-orbit split branches with nearly linear dispersion, one of them merging into bulk states at higher energies. We found no indications for a surface state below E_F.[1]

[1] J. Wiebe, *et al.*, Phys. Rev. B **72**, 193406 (2005)

O 19.5 Tue 12:15 WIL A317

STS study of Fe monomers and multimers on InAs(110) surfaces — •Tomohiro Matsui, Christian Meyer, Lilli Sacharow, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg

The local density of states on and around single Fe atoms (monomers) and Fe multimers (dimers, trimers and tetramers both perpendicular and parallel to the As rows of the substrate) on n-InAs(110) surfaces were studied by scanning tunneling spectroscopy at $T \sim 6$ K.

Different states are observed for a monomer as peaks in the tunneling spectrum: The most prominent peak is spatially localized mainly on the Fe atom, while the other states are spread to the As or In atoms next to the Fe. Their shapes are strongly anisotropic reflecting the asymmetry of the substrate lattice. The peak structure changes by manipulating the atom laterally suggesting different bonding configurations of the Fe to the substrate.

On multimers, the main peak related to the Fe is found at lower energies. The peak shifts in energy from one side to the other side of the multimer. However, this behavior is observed only for the perpendicular case presumably because of the asymmetry of the substrate lattice. For the parallel tetramers, on the other hand, three symmetric states are observed. The first is extended over the whole tetramer, while the others are localized on the end or the middle atoms of the tetramer.

O 19.6 Tue 12:30 WIL A317

Image states on ferromagnetic surfaces explored by tunneling spectroscopy — •Andre Kubetzka, Matthias Bode, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, 20355 Hamburg, Germany

Above metal surfaces a series of hydrogenlike states can exist in the potential well created by the attractive image potential and the surface projected bulk band gap, which hinders a decay into the crystal, with energies between the Fermi and the vacuum level. These so-called image or image-potential states have been investigated in the past by inverse photoemission (IPE) and tunneling spectroscopy [1].

In ferromagnets the band gap is spin dependent which results in a small spin-splitting of these states. The first experimental investigation with spin-resolved IPE determined a value of 18 meV for Ni(111) [2]. We will present first results for image states on Fe(110), employing low temperature spin-polarized scanning tunneling spectroscopy.

[1] G. Binnig *et al.*, Phys. Rev. Lett. **55**, 991 (1985)
[2] F. Passek and M. Donath, Phys. Rev. Lett. **69**, 1101 (1992)

O 19.7 Tue 12:45 WIL A317

Organic small bandgap semiconductors: Electronic properties of quaterrylene derivatives on Au(111) — •Robert Franke, Christian Wagner, Sebastian Franke, and Torsten Fritz — Institut für Angewandte Photophysik, George-Bähr-Straße 1, 01069 Dresden

The understanding of the electronic properties of organic thin films is of large interest for their application in novel devices. As the electronic properties of perylene derivatives [1] and other medium-sized pla-

nar aromatic molecules [2] have already been studied intensively, we have now investigated larger organic molecules, namely quaterrylene (QT) and quaterrylenebisdicarboximide (QTCDI) on Au(111) in UHV. This class of materials is especially interesting due to their long-wavelength absorption in the NIR.

Ultrathin films of QTCDI and QT were investigated by Tunnelling Spectroscopy. In case of QTCDI we found a HOMO-LUMO gap of about 2.2 eV. This result is in good agreement with our optical measurements of QTCDI on mica where the optical gap is found to be 1.8 eV, indicating an exciton binding energy of about 0.4 eV. For thin QT films we obtained an electronic bandgap of 2.5 eV, which fits nicely to the fact that the smaller QT-molecule is expected to have a larger gap than the larger QTCDI molecule.

[1] M. Toerker, T. Fritz, H. Proehl, R. Gutierrez, F. Großmann, and R. Schmidt PRB 65 (2002) 245422 [2] H. Proehl, M. Toerker, F. Sellam, T. Fritz, and K.Leo PRB 63 (2001) 205409