O 5 Electronic structure I

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

O 5.1 Mon 11:15 WIL A317

Probing of bulk band edges by STM: An ab initio analysis — •Alexey Dick and Jörg Neugebauer — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Scanning tunneling microscopy (STM) is an extensively used surface-sensitive tool that allows to address an ever extending range of surface phenomena. Recently it became possible to study electron dynamics by analyzing electron standing wave patterns created in the vicinity of surface imperfections. In the past these studies had been mainly restricted to surface states since bulk states have been assumed to decay too fast in the vacuum region accessed by STM.

To analyze whether STM can be extended to access bulk properties such as the dispersion of the projected bulk band edge (BBE), we have performed a theoretical STM study on various noble metal (110) surfaces. A repeated slab geometry and density functional theory based on a plane-wave pseudopotential approach have been employed to accurately describe surface properties.

A careful analysis of our results explains well recent experimental studies on silver (110) surfaces [1]. It shows that probing of the BBE is possible due to coupling of the bulk and surface states and an enhancement of the bulk state density at the edge of the projected bulk bands. Such an enhancement occurs due to the bulk band-folding in the direction perpendicular to a surface. Since the underlaying effect is general, our results can be used to understand the resolution of the BBE on other metallic surfaces.

[1] J.I. Pascual *et al.*, submitted to Phys. Rev. Lett.

O 5.2 Mon 11:30 WIL A317

Stark-Effect in STM induced Light Emission — •Germar Hoffmann[1], Peter Johansson[2], and Richard Berndt[3] — [1]Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Universität Hamburg, 20355 Hamburg,Germany — [2]Department of Natural Sciences, University ofÖrebro, Sweden — [3]IEAP, Christian-Albrechts-Universität zu Kiel,24098 Kiel

The tunnelling current in a scanning tunnelling microscope gives rise to the emission of photons. Owing to the small lateral dimension of the tunnelling current filament high lateral resolution can be achieved. The effect can be used for optical spectroscopy of nanoscale objects such as individual molecules. In STM induced light emission of Na layers on Cu(111) photon emission spectra reflect quantum well transitions. The energy of these transitions can be varied by the electric field of the tip, akin to a Stark effect. We will present experimental observations and numerical calculations for clean substrates, a number of Na coverages and various quantum well states. The results will be discussed in relation to recent observations of STM-induced molecular fluorescence.

O 5.3 Mon 11:45 WIL A317

Electronic structure of the 6H-SiC$(11\bar{2}0)$ non-polar surface — •Marco Bertelli[1], Jan Homoth[1], Martin Wenderoth[1], Rainer G. Ulbrich[1], Angela Rizzi[1], M. Clelia Righi[2], and Alessandra Catellani[3] — [1]IV. Physikalisches Institut, Georg-August Universität Göttingen, Germany — [2]CNR-INFM National Center on nanoStructures and bioSystems at Surfaces (S^3) and Dipartimento di Fisica, Università di Modena e Reggio Emilia, Modena, Italy — [3]CNR-IMEM, Parco Area delle Scienze, Parma, Italy and S^3

We studied the 6H-SiC$(11\bar{2}0)$ surface reconstruction by means of combined cross-section scanning tunneling microscopy and ab-initio simulations. The n-doped Si-terminated 6H-SiC(0001) substrates were cleaved in ultra high vacuum and measured in-situ by STM at room temperature. The experimental results show an unreconstructed surface. The surface unit cell resembles the stacking sequence of the 6H polytype. The most prominent feature in the occupied state images within the cell is a depression at the inversion point.

In agreement with the experimental observation, the theoretical calculations predict a relaxed surface, but no reconstruction. Correspondingly bond lengths and angles change along the stacking sequence only for the outermost layer, with Si atoms moving inwards of ca. 0.22 Å. C atoms positions are almost unchanged, but for a depression of 0.07 Å at inversion. In general, the up and down arrangement of C and Si atoms is responsible for the observed features in STM images: filled states appear to be concentrated on the carbon atoms and the empty states on the Si atoms.

O 5.4 Mon 12:00 WIL A317

Neutral phosphorus atoms in Si(111)-2×1 stabilize local buckling of π-bonded chains — •J. K. Garleff[1], M. Wenderoth[1], R. G. Ulbrich[1], C. Sürgers[2], H. v. Löhneysen[2,3], and M. Rohlfing[4] — [1]IV. Physikalisches Institut der Universität Göttingen, Friedrich-Hund-Platz. 1, 37077 Göttingen, Germany — [2]Physikalisches Institut and DFG Center for Functional Nanostructures (CFN), Universität Karlsruhe, 76128 Karlsruhe, Germany — [3]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — [4]School of Engineering and Science, International University Bremen, P. O. Box 750561, 28725 Bremen, Germany

Substitutional phosphorus (P) atoms in the Si(111)-2×1 surface have been studied with scanning tunneling microscopy at 8 Kelvin. The unexpected *neutral* charge state of embedded P atoms at low temperature has been established by experimental observation: (i) Peak positions in the differential conductance at the P atom and on the clean Si surface coincide. (ii) The P-induced contrast pattern is restricted to a single or double π-bonded chain. (iii) Atomic corrugation significantly changes around charged defects, but remains unaffected at P atoms. The absence of extra charge at substitutional P atoms in Si(111)-2×1 proves that its electronic properties are dominated by the surface states. The surface band gap of clean Si(111)-2×1 itself strongly decreases to higher temperature. This points on weaker buckling of the π-bonded chains at increased temperature. We explain the spectroscopic contrast of P atoms at room temperature [1] by a locally stabilized buckling of the π-chains.

[1] T. Trappmann *et al.*, Europhys. Lett. **38**, 177 (1997)

O 5.5 Mon 12:15 WIL A317

Visualization of the Molecular Jahn-Teller effect in an insulating K4C60 Monolayer — •Andre Wachowiak[1,2], R. Yamachika[2], K. H. Khoo[2], Y. Wang[2], M. Grobis[2], D.-H. Lee[2], Steven G. Louie[2], and M. F. Crommie[2] — [1]Institute of Applied Physics, University Hamburg, 20355 Hamburg, Germany — [2]Department of Physics, University of California at Berkeley, Berkeley, CA, USA

Unlike atoms in an elemental solid, the building blocks of a molecular solid are more susceptible to tuning. C60 based bulk solids can be tuned between metallic, insulating and superconducting states by changing the charge state and/or local environment of the constituent molecules. This flexibility arises through a sensible interplay between intramolecular Coulomb interaction, electron-phonon coupling, and local charging on an energy scale comparable to the narrow electronic bandwidth. By low temperature scanning tunneling microscopy we have examined how molecular electronic structure is strongly influenced due to charge doping and local electron-phonon interaction in extended monolayer films. In particular, the Jahn-Teller effect, a charge-induced mechanical deformation of molecular structure, is directly visualized at the single molecule level in an insulating K4C60 monolayer[1]. [1] A. Wachowiak et al. Science 310 (2005) 468

O 5.6 Mon 12:30 WIL A317

Scanning Tunneling Microscopy (STM) and Spectroscopy (STS) Investigation of Ultra-thin Epitaxial Nobel Metal Films on Sapphire — •Christof Dietrich, Berndt Koslowski, Gerd Kästle, Hans-Gerd Boyen, and Paul Ziemann — Abteilung Festkörperphysik, Universität Ulm, D-89069 Ulm

Ultra-thin epitaxial Au(111) and Ag(111) films have been prepared on (0001)-oriented sapphire with a niobium buffer layer. Despite their thickness of just 2nm, the nobel metal films are electrically conductive and, according to XRD, exhibit excellent epitaxial properties as well as outstanding smoothness over macroscopic scales [1,2]. Room temperature STM measurements revealed highly ordered smooth surfaces with large terraces and mono-atomic steps. STS measurements on these samples reproducibly showed prominent signatures which can be nicely explained by quantum well states due to the confinement of the electrons perpendicular to the film. Additionally, a thickness-dependent shift of the onset of the Shockley-like surface state was observed in the I(V) spectra possibly indicating a thickness dependent strain in the films.

[1] Growth of thin, smooth, epitaxial (111) oriented Gold films on c-cut Sapphire; G.Kästle, H.-G. Boyen, B. Koslowski, A. Plettl, F. Weigl and P. Ziemann, Surf. Sci. 498, 168 (2002). [2] Size-Effect of the resistivity of thin epitaxial Gold Films, G. Kästle, H.-G. Boyen, A. Schröder, P. Ziemann, Phys. Rev. B 70, 165414 (2004).