O 13: Electronic structure II

Time: Monday 15:00–16:45 Location: SCH A216

O 13.1 Mon 15:00 SCH A216

Self-assembled arrays of molecular quantum resonators — •Florian Klappenberger[1], Dirk Kühne[1], Wolfgang Krenner[1], Iñaki Silanes[2], Andres Arnau[2], Javier García de Abajo[3], Svetlana Klyatskaya[4], Mario Ruben[4], and Johannes Barth[1] — [1]Physik Department E20, TU München, Germany — [2]Departamento de Fisica de Materiales and Unidad de Fisica de Materiales, E-20018 San Sebastian, Spain — [3]Instituto de Óptica CSIC, Serrano 121, 28006 Madrid, Spain — [4]Institute of Nanotechnology, Forschungszentrum Karlsruhe, Karlsruhe, Germany

Confinement of Ag(111) surface state electrons by self-assembled, periodic, two-dimensional, nanoporous networks is studied by means of low-temperature scanning tunneling microscopy/spectroscopy and electronic structure calculation. We compare the case of a purely organic, hydrogen bonded Kagomé network constructed from dicarbonitrile-sexiphenylene molecules with the case of a Co-directed assembly of a metal-organic honeycomb network of the same molecule featuring a pore size of 24 nm^2. Both network types induce resonance states within the cavities with varying lateral electronic density distribution. The spectroscopic features of the resonances together with our analysis employing a boundary element method based on Greens functions indicate finite reflection at the boundaries of the cavities, thus transmission through the pore boundaries allows interaction of electrons in neighboring resonators. By the choice of the network we can steer the pore shape and size and hence engineer the electronic properties of the functionalized surface.

O 13.2 Mon 15:15 SCH A216

Temperature dependent quasiparticle renormalization in nickel metal — •Ruslan Ovsyannikov, Jaime Sánchez-Barriga, Jörg Fink, and Hermann A. Dürr — Helmholtz Zentrum Berlin, BESSY II, Albert-Einstein-Strasse 15, D-12489 Berlin, Germany

One of the fundamental consequences of electron correlation effects is that the bare particles in solids become 'dressed', i.e. they acquire an increased effective mass and a lifetime. We studied the spin dependent quasiparticle band structure of Ni (111) with high resolution angle resolved photoemission spectroscopy. At low temperatures (50 K) a renormalization of quasiparticle energy and lifetime indicative of electron-phonon coupling is observed in agreement with literature [1]. With increasing temperature we observe a decreasing quasiparticle lifetime at the Fermi level for all probed minority spin bands as expected from electron phonon coupling. Surprisingly the majority spin states behave differently. We actually observe a slightly increased lifetime at room temperature. The corresponding increase in Fermi velocity points to a temperature dependent reduction of the majority spin quasiparticle renormalization.

[1] M. Higashiguchi *et al.*, Phys. Rev. B 72, 214438 (2005)

O 13.3 Mon 15:30 SCH A216

Modulated spin polarization in nanostructures — •Sebastian Wedekind, Hirofumi Oka, Guillemin Rodary, Dirk Sander, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle(Saale)

Deposition of 0.7 ML Co onto the clean Cu(111) surface at room temperature leads to the formation of triangular two atomic layers high Co islands. We study the electronic properties of these nano islands by scanning tunneling microscopy (STM) and spectroscopy (STS) at 7 K. We observe pronounced spatial modulation patterns in the local density of states (LDOS) within the islands due to electron confinement. We explore the magnetic properties of the very same islands by spin-polarized STM and STS in a magnetic field of up to 4 T. Our spin-polarized measurements in field clearly identify the parallel and anti-parallel spin orientation states of tip and sample [1]. This enables us to measure the spatial distribution of the spin polarization within single Co islands. We find that the spin polarization is spatially modulated. Our results are discussed in view of recent theoretical predictions [2].

[1] G. Rodary, S. Wedekind, D. Sander, and J. Kirschner, JJAP (in press)

[2] L. Niebergall, V. S. Stepanyuk, J. Berakdar, and P. Bruno, PRL **96**, 127204 (2006)

O 13.4 Mon 15:45 SCH A216

Surface reconstruction and energy gap of superconducting $V_3Si(001)$ — •Nadine Hauptmann, Michael Becker, Jörg Kröger, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Scanning tunneling microscopy of the superconductor $V_3Si(001)$ reveals a yet unknown surface reconstruction which is most likely induced by carbon. We suggest a structural model for the reconstructed surface, which is consistent with experimental data obtained by scanning tunneling microscopy and Auger electron spectroscopy. Superconductivity of the reconstructed sample persists as monitored by scanning tunneling spectroscopy of the superconducting energy gap. Financial support by the DFG is gratefully acknowledged.

O 13.5 Mon 16:00 SCH A216

Engeneering the band line up of Si(111) and organic semiconductors by -CH3, -H and -GaSe termination — •Thomas Mayer[1], Ralf Hunger[2], Andreas Klein[1], and Wolfram Jaegermann[1] — [1]TU-Darmstadt Fachbereich Materialwissenschaften — [2]now Solibro GmbH Thalheim

We report on the variation of the Si(111) ionization energy induced by surface dipoles of -CH3, -H, and -GaSe terminations. Photoelectron spectroscopy is used to determine the experimental dipoles which are compared to model calculations applying simple geometric and electronegativity arguments. The position of the vacuum level within bulk Si is derived to be 5.12 eV above the valence band maximum. In addition the variation of the band line up of Si(111) towards PTCDA and ZnPc is measured. While for -CH3 and -H terminations the Anderson model applies, for GaSe termination an additional interface dipole is induced. We relate this dipole to a varied molecule orientation.

O 13.6 Mon 16:15 SCH A216

Symmetry Analysis of Tunnel Current Eigenchannels — •Martyna Polok[1], Dmitry Fedorov[1], Steven Walczak[1,2], Peter Zahn[1], and Ingrid Mertig[1,2] — [1]Martin-Luther-Universität Halle, Institut für Physik, D-06099 Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Thanks to advances in Scanning Tunneling Microscopy (STM) it is now possible to probe both the electronic and magnetic properties of surfaces. We present an ab initio study of a tip approaching a Cu(001) surface decorated with a single Cu or Co adatom.

Electronic transport is calculated using the Kubo linear response theory in the Baranger and Stone formalism. This description is equivalent to the Landauer language, where conductance is understood as a sum over all transmission eigenchannels.

For a magnetic system additional channels created by the *3d* electrons can cause an increase in the tunnel current. The transmission amplitude of the eigenchannels depends on the overlap between those valence orbitals available at the Fermi energy ε_F. A detailed study of the local density of states shows that in the case of magnetic adatoms this is a spin dependent effect. For the investigated systems the majority spin current is dominated by electrons with spherically symmetric orbitals in the plane perpendicular to the transport direction (z), these are the s, p_z, and d_{z^2} orbitals. For the minority spin channel electrons with asymmetric orbitals, p_x, p_y, d_{xz}, and d_{yz}, dominate at the Fermi energy and therefore determine the current distribution.

O 13.7 Mon 16:30 SCH A216

Electron and Phonon Density of States of HOPG by Scanning Tunnelling Spectroscopy — •Norbert Maurer, Carsten Tröppner, and M. Alexander Schneider — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Motivated by the current interest in few-layer graphene and the widespread use of graphite as substrate we investigated the electronic structure of highly ordered pyrolytic graphite (HOPG) by low-temperature Scanning Tunnelling Spectroscopy in liquid Helium at 4.2K.

We find that the main features of the differential conductance (dI/dV) signal can perfectly be explained by a total density of states calculation as e.g. obtained from a TB-fit to the graphite band structure [1]. However, some of these features induce a structure in the sec-

ond derivative (d^2I/dV^2) signal. Hence both, first and second derivative signals have to be evaluated carefully to extract signatures of inelastic excitations [2]. We discuss the spatial dependence of electronic and inelastic contributions to the tunnelling conductance at step edges and within the HOPG unit cell.

[1] A. Grüneis, et al., arXiv:0808.1467v2 [cond-mat.mtrl-sci] [2] L. Vitali, et al., Phys. Rev. B **69**, 121414 (2004)