O 54: Electronic structure II

Time: Wednesday 15:00–17:15 Location: H33

O 54.1 Wed 15:00 H33

Momentum resolved imaging of the surface electronic structure of Cu(111) in multi-photon photoemission — •Christian Tusche, Cheng-Tien Chiang, Ahmet Akin Ünal, Aimo Winkelmann, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

We use a Photoelectron Emission Microscope (PEEM), combined with an imaging energy filter, to map the distribution of photoelectrons in energy and momentum space. In this "momentum microscope", the angular distribution of electrons leaving the sample is transferred from the back focal plane of the objective lens into two hemispherical analyzers. [1] The projected images directly show the parallel momentum component of the photoelectrons at a constant energy, and maps of the band structure are obtained as a series of parallel cuts through the Brillouin zone.

Combined with multi-photon photoemission (mPPE), using ultra short laser pulses ($h\nu$=3.1 eV), unoccupied electronic states situated in between the vacuum level and the Fermi energy can also be mapped. For instance, for the adsorption system Cs/Cu(111), 2PPE takes place resonantly through an unoccupied Cs-induced state located $\approx$2 eV below the vacuum level. This resonant photoemission channel is absent in a 1PPE experiment, using 6 eV photon energy. Using 3PPE, our experiments can be extended to the unoccupied part of the Cu(111) Shockley surface state and the image potential states.

[1] Krömker, Escher, Funnemann, Hartung, Engelhard, Kirschner: Rev. Sci. Instrum. **79**, 053702 (2008)

O 54.2 Wed 15:15 H33

One-dimensional Electron System of Au/Ge(001) Revealed by Angle-resolved Photoemission — •Sebastian Meyer[1], Jörg Schäfer[1], Christian Blumenstein[1], Aaron Bostwick[2], Eli Rotenberg[2], and Ralph Claessen[1] — [1]Experimentelle Physik 4, Universität Würzburg, 97074 Würzburg, Germany — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley 94720, California, USA

Self-organized atomic nanowires of noble metals on semiconductor surfaces are characterized by strict spatial separation and a high degree of charge confinement [1]. The ultimate width of single-atom dimension seems to be reached with gold chains on Ge(001).Thus they might offer the possibility to observe exotic properties, like a charge density wave (CDW), or, alternatively, a Luttinger liquid phase. Insight is gained by angle-resolved photoelectron spectroscopy (ARPES). We find that two shallow electron pockets disperse along the wire direction within the surface Brillouin zone, while a dispersion perpendicular to the wires is absent. This is confirmed by mapping the full Fermi surface (FS) topology, where sheets are found to be perfectly 1D without any interchain coupling. This is indicative of the virtual absence of coupling to the second dimension. Interestingly, while various nesting conditions are offered from the FS topology, no band back-folding from a CDW superstructure or energy gap opening is found, which opens a pathway for non-Fermi liquid physics. Thus the system emerges as a prototypical 1D electron system.

[1] J. Schäfer *et al.*, Phys. Rev. Lett. **101**, 236802 (2008).

O 54.3 Wed 15:30 H33

Angle-resolved photoemission in the multi-keV regime: first experimental data and theory for W and GaAs — •C. Papp[1,2,3], A. Gray[2,3], S. Ueda[4,5], J. Minar[6], L. Plucinski[7], C. Sakai[5], H. Yoshikawa[4], Y. Yamashita[4], S.-L. He[4], B. Balke[2,3,8], K. Kobayashi[4,5], C. Schneider[7], J. Braun[6], H. Ebert[6], and C. S. Fadley[2,3] — [1]Physical Chemistry II, Uni Erlangen — [2]Materials Science Division, LBNL — [3]Physics, UC Davis — [4]SPring 8 — [5]National Institute for Materials Science — [6]Physical Chemistry, Uni Munich — [7]Solid State Physics, Juelich Research Center — [8]Inorganic and Analytical Chemistry, Uni Mainz

ARPES is the technique of choice for studying the electronic structure of solids and surfaces. However, the measurements are very surface sensitive, probing only about 1 nm into the material. In order to study bulk properties, the use of highenergy photons in the multi-keV regime is suggested. ARPES in the multi-keV regime is now possible via hard x-ray undulator beamlines, together with angle-resolving spectrometers. We will present first hard x-ray ARPES experiments on a tungsten (110)and a GaAs(001) crystal at energies of up to 6 keV. Data obtained at 30 K clearly show band structure effects for both materials, as well as photoelectron diffraction effects for corelevels and more localized valence-band states. The data will be compared with the results of both free-electron final-state theory and one-step theory including matrix element effects. Methods for correcting low-temperature data for residual phonon effects will be considered. Funded by the Humboldt foundation and the DOE (DEAC02-05CH11231).

O 54.4 Wed 15:45 H33

Stabilization of bulk-like α-Mn on W(110): LEED, PES, and DFT studies — •Elena Voloshina[1], Yuriy Dedkov[2], and Manuel Richter[3] — [1]Freie Universität Berlin, Germany — [2]Fritz-Haber Institut der Max-Planck Gesellschaft, Berlin, Germany — [3]IFW Dresden, Germany

Manganese can be considered as the most complex of all metallic elements from the crystallographic point of view. Assuming regular structural trends as in the series of the 4*d* and 5*d* transition metals, one would expect crystallization of Mn in a hcp structure. Being a member of the 3*d*-row where elements crystallize in bcc, fcc, or hcp structures, Mn behaves in a completely different way. Depending on temperature and pressure, it exists in five allotropic forms [1]. α-Mn, the stable phase below 1000K, has an exotic bcc crystal structure containing 58 atoms in the conventional cubic unit cell. Here we demonstrate a successful stabilization of bulk-like α-Mn films with (110) orientation on W(110). The (3 x 3) overstructure observed for the Mn film with respect to the original W(110) LEED pattern is consistent with the suggested structural model. Density functional total energy calculations confirm that this structure, a strained α-Mn phase, is close in energy to the ground state phase and thus can be prepared under carefully controlled conditions. It is metastable, though, and can be destroyed by annealing at 300°C. Angle-resolved PE spectra show weak but distinct dispersions of the electronic states in the valence band that confirm a high quality of the studied Mn films.

[1] J. Hafner *et al.* PRB **68**, 014407 (2003); PRB **68**, 014408 (2003).

O 54.5 Wed 16:00 H33

Electronic structures of thin NaCl (100) films grown on a Ag (111) surface — •Sarah-Charlotta Heidorn, André Sabellek Sabellek, and Karina Morgenstern — Institut für Festkörperphysik, Abteilung ATMOS, Hannover, Deutschland

In nanoelectronics, ultrathin epitaxical insulating films are needed to separate conducting material in electronic devices of the future. NaCl is a prototype wide bandgap insulator and its electronic interactions with metals are of great interest. We present a quantitative low-temperature scanning tunnelling spectroscopy study of the interface state of nanoscale NaCl(100)-islands on Ag(111) and of the surface state on Ag(111) close to NaCl(100)-islands. The interface state energy of NaCl(100) on Ag(111) depends on island-size and -geometry. Additionally, indications for size quantization on islands are observed. The surface state on the Ag(111) shifts close to the polar edges of NaCl(100)-islands. Details of the spatially resolved dI/dV-spectra will be discussed in the presentation.

O 54.6 Wed 16:15 H33

Field Emission Resonances on Au Atomic Chains: Periodic Energy Variations on a sub-nm Scale — •Stefan Polei, Ingo Barke, Kristian Sell, Viola von Oeynhausen, and Karl-Heinz Meiwes-Broer — Institut für Physik, Universität Rostock, Universitätsplatz 3, D-18051 Rostock

We present scanning tunneling spectroscopy (STS) data of field emission resonances (FER) on the quasi one-dimensional Si(111)5x2-Au structure. The image-state derived FER are investigated by dI/dV measurements in the energy range near the vacuum energy and above. A distinct splitting of the first peak in dI/dV curves is observed when varying the location perpendicular to the chains. The effect appears on a length-scale of less than one nanometer. We assign the splitting to variations of the local work function [1].

[1] H. C. Ploigt, C. Brun, M. Pivetta, F. Patthey, and W. D. Schneider, Phys. Rev. B 76, 195404 (2007).

O 54.7 Wed 16:30 H33

The Interplay of Conductance, Force, and Structure Change in Metallic Point Contacts — •Markus Ternes[1,2], César González Pascual[3], Chris P. Lutz[1], Franz J. Giessibl[4], Pavel Jelňek[5], and Andreas J. Heinrich[1] — [1]IBM Research Division, Almaden Research Center, San Jose, California — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [3]Instituto Ciencia de Materiales de Madrid, Spain — [4]Institute of Experimental and Applied Physics, University of Regensburg, Germany — [5]Institute of Physics, Academy of Sciences of the Czech Republic, Prague

A combined scanning tunneling and atomic force microscope was used to measure simultaneously the conductance and the short-range force between an atomically sharp tip and a single metal adsorbate on a metal surface. We found that in the tunneling regime the conductance as well as the attractive short-range force increased exponentially as the tip approached the adsorbate. In the transition regime between tunneling and point-contact a stronger than exponential increase in the conductance was found for a Cu atom on a Cu(111) surface probed with a Cu tip but not for a Pt atom on a Pt(111) surface. To explain the subtle details of the experimental findings, extensive density functional calculations where performed showing that both studied systems show a profound structural change when the transition between tunneling and point-contact occurs. The structural change strongly influences the conductance and forces between tip and sample. The experimental and numerical results are in excellent agreement and give new detailed inside into the transition and formation of metallic point-contacts.

O 54.8 Wed 16:45 H33

Electronic structure of carboxylate molecules on Cu(110) surface: An experimental and theoretical investigation — •Vasile Caciuc, Christina Lennartz, Nicolae Atodiresei, Silvia Karthäuser, Rainer Waser, and Stefan Blügel — Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany

In the present contribution we report on a combined experimental and theoretical study focused on the electronic structure of aromatic organic molecules like benzoic acid ($C_7H_6O_2$) and pyridine-2-carboxylic acid ($C_6H_5NO_2$) adsorbed on the Cu(110) surface. A special focus of our study is to investigate the role of the substitution of an CH functional group by an N atom or by the addition of a second carboxylic group on the electronic properties of the adsorbate-substrate system. In particular, the electronic structure of the molecule-Cu(110) surface was analyzed by recording the differential conductance dI/dV curves, whose shape show a significant dependence on the tip-molecule distance. A clear picture of the nature of the molecule-substrate states that lead to the observed shape of the dI/dV curves was achieved by comparing the experimental differential conductance with the calculated density of states for the carboxylate-surface systems under consideration.

O 54.9 Wed 17:00 H33

Nanoporous supramolecular networks: From quantum confinement to caged rotators — •Florian Klappenberger — Physik Department E20, TU München, Germany

Making use of molecular self-assembly of dicarbonitrile-sexiphenyl (NC2Ph6) molecules, we confine the surface state of the Ag(111) surface with various nanoporous networks and investigate their properties by means of low-temperature scanning tunneling microscopy/spectroscopy and electronic structure calculation. The case of a hydrogen-bonded chiral Kagome superstructure induces a complex dichotomous electronic tessellation. An analysis employing a boundary element method based on Greens functions indicates a uniform repulsive scattering potential for the molecular building blocks. In a Co-directed metal-organic honeycomb network employing the same molecules, Co atoms scatter clearly different from the organic linkers with slight attractive potential for electrons at the Fermi energy, thus with strongly altered character than isolated Co adatoms. Further evaporation of NC2Ph6, acting as guest molecules, leads to the self-assembly of three-winged supramolecular units within the honeycomb pores and to further confinement of the surface state electrons. Thermal activation induces rotation of the trimeric unit and thus produces a dynamic quantum confinement. A temperature-dependent study yields the rate of the motion of the self-assembled rotor and shows various modes of motion.