O 36: Poster Session III: Electronic structure of surfaces: Spectroscopy, surface states I

Time: Tuesday 10:30–12:30 Location: P

O 36.1 Tue 10:30 P

Phonon mediated tunneling into a 2D electron gas on the Be(0001) surface — •Hermann Osterhage, Karoline Oetker, Roland Wiesendanger, and Stefan Krause — Department of Physics, University of Hamburg, Germany

Beryllium is a very unique element among the metals. Whereas the bulk behaves almost like a semiconductor, the (0001) surface is much more metallic, originating from electronic surface states. In our experiments, the clean Be(0001) surface was investigated using scanning tunneling spectroscopy at low temperatures [1]. A pronounced surface state is identified, additionally manifested by the observation of bias-dependent standing wave patterns. Fourier analysis reveals a parabolic dispersion, being characteristic for Friedel oscillations. In contrast to previous studies [2], no indications for the formation of a charge density wave were observed.

Our spectroscopy data reveal symmetric steps in the tunneling conductance around the Fermi level, which we assign to the opening of inelastic tunneling channels via coupling to phonon modes. The Be(0001) surface is found to represent an almost ideal model system to shed light on the details of fundamental electron-electron and electron-phonon interactions in low dimensions.

[1] H. Osterhage *et al.* (submitted).
[2] P. T. Sprunger *et al.*, Science **275**, 1764 (1997).

O 36.2 Tue 10:30 P

The polar $KTaO_3$ (001) surface: Electronic structure and CO adsorption — •Martin Setvin[1,2], Michele Reticcioli[3], Zhichang Wang[2,4], Zdenek Jakub[2], Michael Schmid[2], Cesare Franchini[3], and Ulrike Diebold[2] — [1]Cherles University, Prague, Czech Republic — [2]TU Wien, Vienna, Austria — [3]University of Vienna, Vienna, Austria — [4]Xiamen University, Xiamen, China

Polar surfaces offer intriguing physical and chemical properties applicable in electronics or catalysis. Cleaving the $KTaO_3$ perovskite along its polar (001) plane provides a well-defined, bulk-terminated surface with KO and TaO_2 terminations [1]. As-cleaved surfaces exhibit a high concentration of in-gap states; these electrons predominantly reside at the TaO_2-terminated parts of the surface. These electrons can affect surface chemistry, as is demonstrated for CO molecules. CO has two adsorption configurations on the TaO_2 termination, and the CO differs in how it couples to the excess electrons. DFT calculations indicate that CO preferentially couples to electron bipolarons.

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O 36.3 Tue 10:30 P

Lifetime-measurements of surface electrons enclosured in a circular CO-Quantum Corral on Cu(111) — •Marco Weiss, Jakob Fuchs, Fabian Stilp, and Franz Josef Giessibl — University of Regensburg, 93040 Regensburg, Germany

Adsorbates scatter surface state electrons exhibited by a Cu(111) surface [1]. Artificial manipulation of these microscopic scatterers opens the path to a variety of manmade surface-potential landscapes. In 1993 Crommie et al. [2] assembled 48 Fe adatoms in a ring form shape with a diameter of about 15 nm. This so called Quantum Corral confines the surface electrons within a circular symmetric potential well. These past investigations revealed discrete, Bessel-type eigenstates of the enclosured electrons by using scanning tunneling microscopy and tunneling spectroscopy. But these studies on the Fe-Quantum-Corral showed a disadvantageous movement of the Corral-walls during spectroscopic measurements. [2]

Our solution approach for this problem is to use CO-molecules for upgrading the Quantum Corral with more stable walls. This permits a more reliable access for the spectroscopic analysis of this artificially built atomic feature. This poster presents the results of our spectroscopic investigations on the CO-Corral. The main focus is on determining the lifetime of such enclosuered surface state electrons.

[1] Crommie et al. Nature 363, 524 (1993)
[2] Crommie et al. Science 262, 218 (1993)

O 36.4 Tue 10:30 P

Importance of surface oxygen vacancies for ultrafast hot carrier relaxation and transport in Cu_2O: Insight from hybrid DFT — •Chiara Ricca[1], Lisa Grad[2], Matthias Hengsberger[2], Jürg Osterwalder[2], and Ulrich Aschauer[1] — [1]Department of Chemistry and Biochemistry and National Centre for Computational Design and Discovery of Novel Materials MARVEL, University of Bern, CH-3012 Bern, Switzerland — [2]Department of Physics, University of Zurich, Winterthurerstrasse 190, CH-8057 Zurich, Switzerland

Efficient Cu_2O-based electrodes for photochemical water splitting can be engineered through a deeper understanding of the surface defects and of the mechanisms responsible for the capture of the excited carriers that limit the generated photovoltage in Cu2O heterostructures. Using hybrid DFT calculations, we confirmed that the $(\sqrt{3} \times \sqrt{3})$-R30 reconstruction at the Cu_2O-(111) surface is associated with a 1/3 monolayer of charged surface oxygen vacancies forming ordered structures due to mutual repulsion. Comparison with experimental data obtained by two-photon photoemission spectroscopy indicates that the defect states associated with these vacancies can strongly suppress electron transport, while bulk defect states cannot act as electron traps. In particular, the excited electronic state of the singly charged oxygen vacancy plays a crucial role in the non-radiative electron capture process, with capture coefficients of about 10-9 cm^3/s and lifetimes of 0.04 ps, allowing to explain the experimentally observed ultrafast carrier relaxation.

O 36.5 Tue 10:30 P

Fermi Surface Tomography of Palladium via Momentum Microscopy — •Xin Liang Tan[1], Kenta Hagiwara[1], Ying-Jiun Chen[1,2], Jakub Schusser[3], Iulia Cojocariu[1], Vitaliy Feyer[1], Jan Minar[3], Claus M. Schneider[1,2], and Christian Tusche[1,2] — [1]Forschungszentrum Jülich, Peter Grünberg Institut, Jülich — [2]Fakultät für Physik, Universität Duisburg-Essen, Duisburg — [3]New Technologies Research Centre, University of West Bohemia, Pilsen, Czech Republic

The Fermi surfaces, which describe all thermodynamical and transport quantities of solids, of transition metals are often failed to be modeled by one-electron mean-field theory due to strong correlations among the valence electrons. Moreover, relativistic spin-orbit coupling pronounced in heavier elements lifts the degeneracy of the energy bands and modifies the Fermi surface. Palladium, a 4d metal attributed to both significant spin-orbit coupling and electron correlations, is ideal for a systematic and fundamental study on the two fundamental physical phenomena and their interplay in electronic structure. We will explore the experimentally determined electronic structure of palladium in four-dimensional energy-momentum space ($E_{Binding}$,k_x,k_y,k_z) obtained via momentum microscopy. The complete 3D-Fermi surface of palladium and corresponding isoenergy surfaces at higher binding energies were tomographically mapped with an energy- and polarization-variable light source. Spin-orbit coupling and electron correlations in palladium will be presented in the context of energy-momentum relations across the Fermi surface and isoenergy surfaces.

O 36.6 Tue 10:30 P

Emergence of unusually high Na2IrO3 surface conductivity prepared in UHV — •Máté Stark[1], Thomas Dziuba[1], Ina Pietsch[2], Philip Gegenwart[2], and Martin Wenderoth[1] — [1]IV. Physikalisches Institut, Georg-August-Universität Göttingen, Germany — [2]Lehrstuhl für Experimentalphysik VI, Zentrum für elektronische Korrelationen und Magnetismus, Universität Augsburg, Germany

Na2IrO3 is a prototypical material in the honeycomb iridate family, where both a spin liquid ground state and topologically insulating behaviour are theoretically predicted [1]. In this work, we perform transport measurements of freshly cleaved Na2IrO3 crystals in ultra-high vacuum. Making use of the insulating nature of bulk Na2IrO3 allows us to separate surface-related conductivity of freshly cleaved crystals from bulk transport. We compare the electrical conductivity of the uncleaved and cleaved surface as well as of the surface after degradation in air as a function of temperature between 150 K and 300 K. We find a severe deviation from the usual variable-range-hopping transport [2] and complete domination of the surface conductivity for low temperatures. The freshly cleaved crystal showed a saturation of the sheet resistance at about 2,9 kΩ at low temperatures. After the degradation of the surface in air, the conductivity of the surface decreased, and we

measured a general change in the temperature dependence compared to the freshly cleaved surface. Work supported by DFG through SPP 1666 and TRR80. Ref.: [1] Phys. Rev. 108, 106401 (2012), [2] Phys. Rev. B82, 064412 (2010)

O 36.7 Tue 10:30 P

Photoexcitation of Bulk Polarons in Rutile TiO2 — •Alex Tanner[1,2], Bo Wen[3], Yu Zhang[1,2], Li-min Liu[4], Helen Fielding[1], Annabella Selloni[3], and Geoff Thornton[1,2] — [1]Department of Chemistry, University College London, 20 Gordon Street, London WC1H 0AJ, United Kingdom — [2]London Centre for Nanotechnology, University College London, 17-19 Gordon Street, London WC1H 0AH, United Kingdom — [3]Department of Chemistry, Princeton University, Princeton NJ 08540, United States — [4]School of Physics, Beihang University, Beijing, 100083, China

In recent years there has been considerable interest in the physics of polarons at reduced TiO2 surfaces. This includes two photon photoemission spectroscopy (2PPE) studies, which have proposed that polaron excitation may represent an alternative vector to band gap excitation in photocatalysis. These studies show that surface-localized polarons in rutile TiO2(110) couple with excited electronic states ca. 2.6 eV above the conduction band minimum. However, readily oxidised surface polarons likely have a minimal contribution in catalytic applications. In contrast, polarons in bulk TiO2 remain protected and therefore offer intriguing potential.

With 2PPE and hybrid density functional theory, we find bulk polarons are less bound by 0.2 eV compared with polarons at the surface. Because the excited state is also shifted to higher energy, bulk polarons have the same resonance energy as at the surface with a threshold at 3.1 eV. This is degenerate with the band gap, suggesting that bulk polarons could also provide an additional contribution to the photoyield.