

O 77: Electronic structure I

Time: Thursday 16:00–17:30

Location: MA 043

O 77.1 Thu 16:00 MA 043

Electron-phonon coupling investigated by laser-photoemission spectroscopy in Pb/Si(111) — ●MATHIAS SANDHOFER, DIMITRIOS PAPOUTZIS, LAURENZ RETTIG, SIMON FREUTEL, LTAIEF BEN LTAIEF, ISABELLA AVIGO, MANUEL LIGGES, and UWE BOVENSIEPEN — Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg

We investigate different contributions to electron scattering rates in epitaxial Pb/Si(111) thin films by a linewidth analysis in photoemission spectroscopy, using frequency-quadrupled Ti:Sa laser pulses (6 eV). We consider contributions from electron-electron (e-e), electron-phonon (e-ph) and electron defect (e-df) scattering. For the investigated electronic quantum well states at five and seven monolayer film thickness the e-e contribution is 4 meV[1]. This simplifies the observation of the e-ph coupling through a temperature dependent linewidth analysis which is expected to yield a contribution one or two orders of magnitude higher[2]. A linear temperature-dependence of the linewidth is found for 40 K < T < 120 K, indicating the increase of e-ph scattering rate due to an increase of the number of phonons. The obtained e-ph coupling constant is $\lambda = 0.7 \pm 0.1$. For higher temperatures (T > 120 K) the linewidth remains constant. Supported by a lower linewidth for T = 40 K after heating to 180 K, we explain this by a decrease in e-df scattering through a reduction of defects.

[1] Kirchmann et al., Nature Physics 6, 782 (2010)

[2] Hong I-Po et al., Phys Rev B 80, 081409 (2009)

O 77.2 Thu 16:15 MA 043

Investigation of the hybridization between the unoccupied Shockley surface state and bulk electronic states on Cu(111) — ●AIMO WINKELMANN, A. AKIN ÜNAL, CHRISTIAN TUSCHE, CHENG-TIEN CHIANG, SAFIA OUAZI, SEBASTIAN WEDEKIND, MASAKI TAKADA, DIRK SANDER, JÜRGEN HENK, and JÜRGEN KIRSCHNER — Max-Planck-Institut für Mikrostrukturphysik, Halle

Shockley surface states and image-potential states in the bulk L -gap of the (111) surfaces of Cu, Ag, and Au are well-known models for the study of quasi-two-dimensional electron systems. We have applied k -resolved multiphoton photoemission using a *momentum microscope*, scanning tunneling spectroscopy using Fourier-transformation and Bessel-function fitting, together with first-principles electronic structure calculations to determine the dispersion of the occupied and unoccupied Shockley surface state of Cu(111). We verify that the dispersion of this state deviates significantly from the paradigmatic parabolic behavior of quasi-free electrons with increasing energy above the Fermi level [1]. Based on our calculations, we ascribe this deviation to the shift of the spectral weight of the surface state into the bulk, and of bulk states toward the surface, which leads to an enhanced hybridization between the states with increasing energy.

[1] A.A. Ünal, C. Tusche, S. Ouazi, S. Wedekind, C.-T. Chiang, A. Winkelman, D. Sander, J. Henk, J. Kirschner Phys. Rev. B 84, 073107 (2011)

O 77.3 Thu 16:30 MA 043

Spectral and spatial redistribution at the LaAlO₃/SrTiO₃ interface — ●TIM GÜNTHER¹, ANDREA RUBANO^{1,2}, THOMAS FINK¹, DOMENICO PAPARO³, LORENZO MARRUCCI³, FABIO MILETTO GRANOZIO³, UMBERTO SCOTTI DI UCCIO³, JOCHEN MANNHART⁴, and MANFRED FIEBIG^{1,5} — ¹HISKP, University Bonn, Germany — ²Fritz-Haber-Institut, Berlin, Germany — ³Dip. di Scienze Fisiche, University Naples, Italy — ⁴MPI for Solid State Research, Stuttgart, Germany — ⁵Materials Departement, ETH Zürich, Switzerland

A conductive two-dimensional electron liquid (2DEL) appears at the LaAlO₃/SrTiO₃ (LAO/STO) interface for a LAO thickness of $n \geq 4$ unit cells. Despite the tremendous research interest, many questions regarding the origin and characteristics of the 2DEL have to be addressed yet. In particular, this includes the electronic structure of the 'buried interface'. Optical second harmonic generation (SHG) is an ideal tool for studying interfaces, since it is sensitive to the interfacial symmetry breaking along the stacking direction. Using SHG with frequency-tunable amplified femtosecond laser pulses we obtain information about the structural reorganization of the interfacial STO conduction band for SHG photon energies up to 6.2 eV. A massive spectral weight redistribution is present for $n \geq 3$, indicating a global

reorganization of the conduction band structure. At low temperatures the spectral resolution is enhanced which alleviates the distinction of interfacial electronic transitions. Our data are supported by a theoretical framework based on symmetry selection rules that allows a specific assignment of interfacial O(2p)-Ti(3d) transitions to the SHG spectrum.

O 77.4 Thu 16:45 MA 043

Energy level alignment and ultrafast electron dynamics at pristine and pyridine-covered ZnO(10 $\bar{1}$ 0) — ●JAN-CHRISTOPH DEINERT, DANIEL WEGKAMP, JULIA STÄHLER, and MARTIN WOLF — Fritz-Haber-Institut der MPG, Abt. Physikalische Chemie, Faradayweg 4-6, 14195 Berlin

Organic adlayers on semiconductor surfaces are promising candidates for highly functional molecular electronics devices, e.g. organic LEDs. Such hybrid systems may exhibit electronic and excitonic properties that go beyond the linear combination of the two material classes' stand-alone properties. An example is the formation of new interface states through hybridization of molecular and semiconductor states. Efficient functionalization requires sound knowledge of both occupied and unoccupied electronic structure at the hybrid interface. In our experiment we can directly access these states and examine their ultrafast dynamics upon excitation using femtosecond time-resolved two-photon photoemission (2PPE). Characterization of the pristine ZnO(10 $\bar{1}$ 0) surface yields the valence and conduction band (CB) edge energies. Besides a time-dependent down shift of the sample work function by few 10 meV, our spectra show the hydrogen-induced downward shift of the CB minimum below E_F . Furthermore, we directly monitor the hot electron relaxation in the ZnO CB on femtosecond timescales and subsequent formation of a long-lived state. Adsorption of pyridine leads to a massive reduction of the work function of the sample up to $\Delta\Phi = -2.7$ eV, which makes this system a good candidate for further studies of energy level alignment.

O 77.5 Thu 17:00 MA 043

Character of the valence band states in the Kondo surface alloys CeAg_x/Ag(111) and CePt₅/Pt(111) — ●HOLGER SCHWAB^{1,2}, MATTIA MULAZZI^{1,2}, KENYA SHIMADA³, and FRIEDRICH REINERT^{1,2} — ¹Physikalisches Institut, Experimentelle Physik VII und Wilhelm Conrad Röntgen Research Center for Complex Material Systems (RCCM), Universität Würzburg, D-97074 Würzburg — ²Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, D-76021 Karlsruhe — ³Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima 739-0046, Japan

Recently we have shown the transition from the single impurity to the Kondo lattice regime in the surface alloy CePt₅. [1] Now we have prepared a new Ce based surface alloy: CeAg_x. The electronic and crystal structures of both materials have been investigated by means of low-energy electron diffraction and angle-resolved photoelectron spectroscopy (ARPES). With resonant PES near the 4d-4f absorption edge we were able to infer the weight of the 4f-electron spectral function with respect to single-particle density of states. While the typical Kondo features at the Fermi energy (Kondo resonance and spin orbit partner) in the CePt₅ surface alloy are observed, CeAg_x shows a different behaviour. By comparing our experiments to model calculations [2,3], we were able to estimate the Kondo temperature in the two systems and investigate parameters contributing to the hybridisation.

[1] M. Klein et al., Phys. Rev. Lett. 106, 186407 (2011).

[2] F. Patthey et al., Phys. Rev. B 42, 8864 (1990).

[3] S. Gardonio et al., Phys. Rev. Lett. 107, 026801 (2011).

O 77.6 Thu 17:15 MA 043

Spectroscopic Characterisation of Insulating and Superconducting Cement 12CaO-7Al₂O₃ (C12A7) — ●ANNA BULING¹, JOHN MCLEOD², MANFRED NEUMANN¹, ERNST KURMAEV³, HIDEO HOSONO⁴, and PETER SUSHKO⁵ — ¹D-Fachbereich Physik, Universität Osnabrück — ²CA-Department of Physics and Engineering Physics, University of Saskatchewan — ³RU-Institute of Metal Physics, Russian Academy of Sciences - Ural Division, Yekaterinburg — ⁴JP-Materials and Structures Laboratory, Tokyo Institute of Technology — ⁵UK-University College London

The nanoporous complex oxide C12A7, which is a wide bandgap in-

ulator, is produced as a main constituent of commercial alumina cement but has great potential for other applications in electronics and catalysis. By introducing oxygen deficiency, conductivity can be realized in the system up to superconductivity with a $T_C \approx 0.14 - 0.4$ K. Currently, there are two competing models explaining the existence of conductivity in this compound: One involves the electron hopping along framework lattice sites, the other the electron transfer via a cage conduction band.

Here we present the investigation of insulating and superconducting $C12A7$ by means of X-ray photoemission, X-ray absorption and X-ray emission spectroscopy measurements completed with DFT calculations to illuminate the relations in the conduction and the valence bands. Our measurements suggest that free electrons in oxygen-deficient $C12A7$ occupy a narrow band which exists between the main conduction band and the valence bands.