O 4: Electronic Structure of Surfaces I

Time: Monday 10:30–13:15 Location: MA 041

O 4.1 Mon 10:30 MA 041

Phonon-Mediated Electron Transport through CaO Thin Films — •Niklas Nilius[1], Yi Cui[2], and Hans-Joachim Freund[2] — [1]Institut für Physik, Carl von Ossietzky Universität, D-26111 Oldenburg, Germany — [2]Fritz-Haber-Institut der MPG, Faradayweg 4-6, D-14195 Berlin, Germany

Scanning tunneling microscopy has developed into a powerful tool for the characterization of conductive surfaces, for which the overlap of tip and sample wavefunctions determines the image contrast. On insulating layers, as the CaO thin-film grown on Mo(001) investigated here, direct overlap between initial and final states is not possible anymore and electrons are transported via hopping through the conduction-band states of the oxide. In this case, carrier transport is accompanied by strong phonon excitations, imprinting an oscillatory behavior onto the differential conductance of the system. The phonons show a characteristic spatial dependence and become softer around lattice irregularities in the oxide film, such as dislocation lines.

O 4.2 Mon 10:45 MA 041

Orientational Tuning Of The Two-Dimensional Electron Gases At The Low-Index Surfaces of SrTiO3 — •Tobias C. Rödel[1,2], Cédric Bareille[1], Franck Fortuna[1], François Bertran[2], Patrick Le Fèvre[2], Thomas Maroutian[3], Philippe Lecoeur[3], Marc Gabay[4], Marcelo J. Rozenberg[4], and Andres F. Santander-Syro[1] — [1]CSNSM, Orsay, France — [2]Synchrotron SOLEIL, Gif-sur-Yvette, France — [3]IEF, Orsay, France — [4]LPS, Orsay, France

Two-dimensional electron gases (2DEGs) in SrTiO3 have been studied extensively in the last decade after its discovery at the LaAlO3/SrTiO3 interface by Ohtomo & Hwang. This heterostructure displays many fundamentally interesting properties, such as field-effect induced insulator-to-superconductor transitions and the coexistence of magnetism and superconductivity.

To clarify the microcopic electronic structure of the 2DEG, we conducted angle resolved-photoemission spectroscopy (ARPES) experiments of a closely related system: the 2DEG at the surface of SrTiO3. Our group studied the 2DEGs at various different surface orientations of SrTiO3 (as well as KTaO3) at different synchrotron facilities.

Recent results demonstrate that the electronic structure of the 2DEG at the surface of SrTiO3 (Fermi surfaces, subband masses and orbital ordering) can be tuned by confining the electrons at different surface orientations. This occurs due to the different crystallographic symmetries of the surface and subsurface planes as well as the different effective electron masses along the confinement direction.

O 4.3 Mon 11:00 MA 041

Angle-resolved ultraviolet photoemission spectroscopy of quasicrystalline $BaTiO_3$ films on Pt(111) — •Richard Kraska[1], Konrad Gillmeister[1], Stefan Förster[1], Eva Maria Zollner[1], Klaus Meinel[1], Cheng-Tien Chiang[2,1], and Wolf Widdra[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

Bulk $BaTiO_3$ is a widely investigated perovskite. As recently discovered, thin films of this material can form a long-range ordered, quasicrystalline structure on the hexagonal Pt(111) surface with 12-fold rotational symmetry. Although the two-dimensional structure has been investigated by STM, LEED and XPS [1], no information on the electronic valence band structure has been reported so far. Here we present angle-resolved photoelectron spectroscopy data along the $[1\bar{2}1]$ and $[1\bar{1}0]$ directions of the substrate for a well-ordered quasicrystalline $BaTiO_3$-derived film using a photon energy of 21.22 eV. Comparing the data from the quasicrystalline film and from the clean platinum substrate, we can identify a weakly dispersive feature at 6 eV below the Fermi level that is assigned to the aperiodic structure.

[1] S. Förster, K. Meinel, R. Hammer, M. Trautmann, and W. Widdra, *Nature* **502**, 215 (2013)

O 4.4 Mon 11:15 MA 041

Employing Infrared Reflection Absorption Spectroscopy to Probe Polarons in Photoactive Oxides: TiO_2 and ZnO — •Fabian Bebensee, Hikmet Sezen, Alexei Nefedov, and Christof Wöll — Karlsruhe Institute of Technology (KIT), Institute of Functional Interfaces (IFG), Herrmann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

TiO_2 and ZnO are wide-band gap metal oxides exhibiting various desirable physico-chemical properties, e.g. high photocatalytic activity. In the context of photoexcitations, primarily excitons have been studied including their very recently reported ultrafast formation dynamics.[1] It is important to note that charge carriers generated from dissociation of excitons may be trapped in polaronic states. Consequently, the polaron binding energy becomes crucial for the photocatalytic activity, as this energy is not available to drive the desired reaction. Yet, only very little work has been devoted to these trap states. Here, we report a novel approach to study polarons in metal oxide single crystals by populating these trap states via UV-light irradiation and probe them using infrared reflection absorption spectroscopy (IRRAS). We will present results for TiO_2 (cf. [2]) and ZnO, where a number of previously unobserved bands ascribed to polaronic states appear in the IR-spectra upon irradiation and compare them to theoretical work. Exploiting time-resolved IRRAS, we were able to deduce lifetimes and binding energies of these states experimentally for ZnO.

[1] Deinert, et al., PRL 2014, 113, 057602.

[2] Sezen, et al., Sci Rep 2014, 4, 3808.

O 4.5 Mon 11:30 MA 041

High Resolution Electron Energy Loss Study of Pd and Pt Phthalocyanine on Ag(111) — •Jessica Sforzini, Francois Bocquet, and Stefan Tautz — Peter Gruenberg Institute 3, Forschungszentrum Juelich, 52428 Juelich, Germany

We have investigated the geometrical and the vibrational properties of Pd and Pt Phthalocyanine on Ag(111) by Low Energy Electron Diffraction (LEED) and by High Resolution Electron Energy Loss Spectroscopy (HREELS). The LEED patterns show that the molecules grow highly ordered on the surface. The HREELS spectrum is dominated by vibrational modes with symmetry A2u that produce an out-of-plane variation in the dipole moment. This indicates a flat adsorption geometry. The asymmetric vibrational losses, between 1000 and 1500 cm^{-1}, indicate the presence of an interfacial dynamical charge transfer that is more pronounced in the case of Pd molecules. We also studied both systems after exposure to molecular hydrogen, but observe no drastical changes in the behavior with the central metal type.

O 4.6 Mon 11:45 MA 041

One- and many-electron computational scheme for XES and NEXAFS spectra calculation within DFT and pseudopotential approach — •Roman Ovcharenko[1], Elena Voloshina[1], Alexander Shulakov[2], and Yuriy Dedkov[3] — [1]Institut für Chemie, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 2, 12489 Berlin, Germany — [2]V. A. Fock Institute of Physics, Saint-Petersburg State University, 198504 Saint-Petersburg, Russia — [3]SPECS Surface Nano Analysis GmbH, Voltasraße 5, 13555 Berlin, Germany

In this work we present the density functional method using the PAW pseudopotential and the plane wave basis set for X-ray emission and absorption spectra calculation of simple metals and graphene-like systems. As it is well known, smoothed pseudo wave functions differ from the standard all-electron crystal orbitals in the atomic core region which is particularly important for X-ray matrix elements calculation. Therefore, to calculate the probabilities of X-ray spectra, we have reconstructed all-electron orbitals in the core region leaving wave function outside core sphere unchanged.

Moreover, even after such reconstruction many materials demonstrate spectral features which cannot be described by one-electron treating. The problem is in originally many particle nature of the dynamical core-hole screening during X-ray transition, which partially can be overcome by adopting Mahan-Nozieres-De Dominicis theory. The results of numerical application of such one- and many-electron approaches to a number of simple metals as well as graphene-like systems is the topic of present talk.

O 4.7 Mon 12:00 MA 041

First principles exploration of noble metal lanthanide sur-

face alloys — •Matthieu Verstraete[1], Bin Xu[1], Lucia Vitali[2], Laura Fernandez[2], Frederik Michael Schiller[2], Maider Ormaza[2], and Enrique Ortega[2] — [1]University of Liège, Liège, Belgium — [2]Universidad del Pais Vasco, San Sebastian, Spain

The electronic and magnetic structure of X_2L alloys of noble metals (X = Ag Au Cu) with lanthanides (L = La Gd Ce...) is investigated by first principles calculations, to explain and complement a series of surface science techniques (ARPES, XRD, STM, STS, MOKE). The complex interplay of magnetic, strain, and chemical variables produces a variety of different electronic states for very similar geometric structures. STM profile inversions, relativistic and spin polarized band splittings, and a series of hole and electron like surface states all result from varying the noble metal or lanthanide. The common point in these systems is the existence of an experimental "sweet spot" in the synthesis, generating a homogeneous surface alloy showing a hexagonal motif and a long range moiré pattern. Density functional theory band and structure calculations shed light on the nature of the states and their magnetism.

Xu, B. et al. in preparation (2015)

Ormaza, M. et al. in preparation (2015)

Ormaza, M., et al. Phys. Rev. B 88, 125405 (2013)

Corso, M., et al. Phys Rev Lett 105, 016101 (2010)

O 4.8 Mon 12:15 MA 041

Interface electronic structure and charge transfer processes in layered ferecrystalline [(SnSe)1.15]5(TaSe2)5 compound: Photoemission study — •Pavel Shukrynau[1], Lars Smykalla[1], Matthias Falmbigl[2], David Johnson[2], and Michael Hietschold[1] — [1]Institute of Physics, Technische Universität Chemnitz, Reichenhainer Straße 70, D-09107 Chemnitz, Germany — [2]Materials Science Institute and Chemistry Department, University of Oregon, Eugene, Oregon 97403, USA

In situ synchrotron radiation photoelectron spectroscopy was used to characterize electronic structure at the cleaved interface of the layered ferecrystalline [(SnSe)1.15]5(TaSe2)5 material. Detailed analysis of the Sn 3d, Ta 5d and Se 4p core levels spectra obtained at various incident angles revealed significant differences in chemical bonding of atoms in surfaces with divers terminating layers. On the basis of energy positions and widths of the Sn-derived features of the valence band spectra, a weak coupling between SnSe and TaSe2 layers is suggested. However, the Ta 5d signal reveals different electronic structures depending on the terminating layer. The observed changes can be attributed to stronger interaction between TaSe2-TaSe2 layers and a large charge transfer between Se 4p and Ta 5d orbitals. Comparisons were made with classical misfit compounds.

O 4.9 Mon 12:30 MA 041

Orbital signatures of Fano-Kondo lineshapes in STM adatom spectroscopy — •Sebastian Frank and David Jacob — MPI of Microstructure Physics, Halle, Germany

Scanning tunnel spectroscopy has become a routine tool for probing the Kondo effect of magnetic atoms deposited on conducting surfaces [1]. The Kondo effect manifests itself as so-called Fano line shape in the measured conductance spectrum. However, it is often unclear which of the d-orbitals causes the observed Kondo signature in the conductance. Here we fill this gap by finding the Kondo signatures of individual d-orbitals. To this end, we perform DFT calculations augmented by local dynamic correlations. We add correlations to specific d-orbitals only, instead of the entire d-shell, and compute the corresponding conductance curves. The Fano line shapes strongly depend on the type of the correlated orbital, the effective interaction parameter U and the d-level position. Furthermore, we laterally displace our model STM tip to find the spatial evolution of the Fano signature. Hence it is possible to identify the d-orbital responsible for the observed Fano line shape.

[1] Madhavan et al., Science 280, 567 (1998); Li et al., PRL 80, 2893 (1998); Knorr et al., PRL 88, 096804 (2002)

O 4.10 Mon 12:45 MA 041

A new setup for investigation of advanced materials by means of dynamic-XPS — •Sergey Babenkov[1], Olga Molodtsova[1], Victor Aristov[1,2,3], Frank Scholz[1], Joern Seltmann[1], Ivan Shevchuk[1], Leif Glaser[1], and Jens Viefhaus[1] — [1]DESY Hamburg, Germany — [2]Uni Hamburg, Germany — [3]ISSP RAS, Russia

Using dynamic-XPS method is a big step toward understanding of fast processes on the solid surfaces and subsurfaces of advanced materials, which are taking place during changing of different conditions. The experimental setup for such experiments, based on a hemispherical electron spectrometer Argus (Omicron NanoTechnology GmbH), has been built up, commissioned and currently is available for regular users of beamline P04 (PETRA III, DESY). Such combination allows to acquire both traditional scanning and extremely fast snapshot (down to 0.1 sec/spectrum) XPS spectra of several core levels (CL). It opens new possibilities to real time characterization of the fast processes both from quantitative and qualitative point of view by dynamical measuring of XPS. The concept was verified by real time XPS characterization of thermally induced process of graphene formation on model cubic-SiC(001)/Si(001) wafer. We were able to control time/temperature/rare-gas pressure parameters and follow the changes in C 1s CL spectra. Moreover, we present the dynamic-XPS study of controllable metal-organic interface formation (Indium/CuPcF4) at room temperature conditions. This work was supported by grants of RFBR No 13-02-00818, 14-02-00949, BMBF-Project No. 05K12GU2, PSP-Element No. U4606BMB1211.

O 4.11 Mon 13:00 MA 041

Elektronische Eigenschaften von Au(111) mittels Dichtefunktionaltheorierechnungen — •Ari Paavo Seitsonen — Institut für Chemie, Universität Zürich, Schweiz — Département de Chimie, École Normale Supérieure, Paris, Frankreich

Die Fischgräten-Rekonstruktion (engl. Herringbone) von der Au(111) Oberfläche hat Forscher besonders seit der Rastertunnelmikroskopieuntersuchung [1] inspiriert. Die elektronischen Eigenschaften sind unter anderem durch winkelabhängige Photoelektronenspektroskopie gemessen worden [2].

In den letzten Jahren sind zwei Dichtefunktionaltheorierechnungen zu der Geometrie und elektronische Reaktivität der rekonstruktuierten Au(111) erschienen [3,4]. Wir haben diese Untersuchungen weitergeführt, da wir die elektronische Struktur, darunter den Oberflächenzustand in der Näher von der Fermi-Energie, analysiert haben. Wir diskutieren sowohl die Bandstruktur wie die Spin-Bahnspaltung des Zustandes.

[1] Johannes V Barth, Harald Brune, Gerhard Ertl and Rolf Jürgen Behm, *Physical Review B* **42**, 9307 (2010)

[2] S. LaShell, B. A. McDougall and E. Jensen, *Physical Review Letters* **77**, 3419 (1996)

[3] Yun Wang, Noel S Hush and Jeffrey R Reimers, *Physical Review B* **75**, 233416 (2006)

[4] Felix Hanke and Jonas Björk, *Physical Review B* **87**, 235422 (2013)