O 16: Electronic Structure and Spin-Orbit Interaction II

Time: Monday 16:00–19:00 Location: GER 38

O 16.1 Mon 16:00 GER 38

Anisotropic two-dimensional electron gas at $SrTiO_3$(110) protected by its native overlayer — •Zhiming Wang[1], Zhicheng Zhong[2], Xianfeng Hao[1], Stefan Gerhold[1], Bernhard Stöger[1], Michael Schmid[1], Jaime Sánchez-Barriga[3], Andrei Varykhalov[3], Cesare Franchini[4], Karsten Held[2], and Ulrike Diebold[1] — [1]Institute of Applied Physics, Vienna University of Technology, Vienna, Austria — [2]Institute of Solid State Physics, Vienna University of Technology, Vienna, Austria — [3]BESSY, Albert-Einstein-Str. 15, D-12489 Berlin, Germany — [4]Faculty of Physics and Center for Computational Material Science, University of Vienna, Vienna, Austria

Two dimensional electron gases (2DEGs) at oxide heterostructures are attracting considerable attention, as these might substitute conventional semiconductors for novel electronic devices. Here we present a minimal set-up for such a 2DEG – the $SrTiO_3$(110)-(4×1) surface, natively terminated with one monolayer of chemically-inert titania. Oxygen vacancies induced by synchrotron radiation migrate underneath this overlayer; this leads to a confining potential and electron doping such that a 2DEG develops. Our angular resolved photoemission spectroscopy (ARPES) and theoretical results show that confinement along (110) is strikingly different from a (001) crystal orientation. In particular the quantized subbands show a surprising "semi-heavy" band, in contrast to the analogue in the bulk, and a high electronic anisotropy. This anisotropy and even the effective mass of the (110) 2DEG is tunable by doping, offering a high flexibility to engineer properties of this system. This work is supported by ERC Advanced Grant and FWF.

O 16.2 Mon 16:15 GER 38

Electronic structure of α- and ϵ-Fe_2O_3 nanoparticles: spin state and satellite structures — Jörg Haeberle[1], •Matthias Richter[1], Petr Brazda[2], Massimo Tallarida[1], and Dieter Schmeisser[1] — [1]Brandenburg University of Technology Cottbus-Senftenberg, Applied Physics and Sensors, K.-Wachsmann-Allee 17, 03046 Cottbus, Germany — [2]Department of Inorganic Chemistry, Faculty of Science, Charles University in Prague, Czech Republic

We report on spectroscopic investigation of α- and ϵ-Fe_2O_3 nanoparticles. α-Fe_2O_3 is commonly used as photocathode for water splitting for the hydrogen production. On the other hand ϵ-Fe_2O_3 is of interest because of its magnetic properties. For both well-defined nanoparticles we analyze the electronic structure and determine the partial density of states for the valence and conduction bands. From these data we can derive a band scheme and compare it with recent (band structure) calculations. The resPES data at the Fe2p absorption edge spectra are analyzed to give evidence about the involved spin states in both phases. We find that for the ϵ-Fe_2O_3 the majority is due to $Fe3d^5$ HS state. Contributions of the corresponding LS state are small and are found to be higher for the α-Fe_2O_3 phase. In α-Fe_2O_3 prepared by ALD we identify in addition a LS $3d^6\underline{L}$ state. In addition, a loss process can be identified upon resonant excitation at the Fe2p edge. It appears predominantly in the ϵ-Fe_2O_3 phase. We give a model to describe that loss process. It is used to also explain the appearance of the Fe2p core level satellites that are different for α- and ϵ-Fe_2O_3 phases.

O 16.3 Mon 16:30 GER 38

Electronic structure of the Co oxide catalyst for OER — •Matthias Richter and Dieter Schmeisser — Brandenburg University of Technology Cottbus-Senftenberg, Applied Physics and Sensors, K.-Wachsmann-Allee 17, 03046 Cottbus, Germany

The electronic structure of the cobalt oxide based catalysts is analyzed using synchrotron radiation photoelectron spectroscopy. Cobalt oxide is used in photoelectrochemical cells for photocatalytic water splitting in order to produce solar fuels. We discuss our resonant data in terms of the partial density of states of the valence and conduction band. For the individual Co3d states, we determine their configuration, their spin, and their energy level relative to the Fermi energy. At resonant excitation we find the Co2p partial DOS to exhibit sharp features next to the VBM for increased cobalt oxidation state instead for a broad emission at around 6eV below E_F for a low oxidation state. The former are found in $LiCoO_2$ and other Co-oxide systems with a Co^{3+} ground state. We attribute such sharp features to the low spin (LS) configuration of Co^{3+} and deduce that in the Co oxide catalyst layers with increased thickness there is evidence for the corresponding LS contributions. In contrast, our data prove the Co^{2+} ground state for thin pristine cobalt oxide films and demonstrate that it is exclusively in the $Co3d^7$ high spin state. In addition, both cobalt oxide configurations Co^{2+} in a HS state and Co^{3+} in a LS state have characteristic oxygen to Co charge transfer states in the band gap. We attribute the trivalent charge transfer state to be the active state for the oxygen evolution reaction.

O 16.4 Mon 16:45 GER 38

The role of spin-orbit coupling in the electronic structure of bulk and thin film $CaIrO_3$ — •Kerstin Dörr, Yuriy Mokrousov, Stefan Blügel, and Marjana Lezaic — Peter Grünberg Institut, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Transition-metal oxides (TMO) feature a multitude of interesting properties, such as metal-insulator transitions or high-temperature superconductivity. Furthermore, Mott physics plays a major role, with an enhanced onsite Coulomb repulsion U driving the system into an insulating state. While this is true for well-studied $3d$ TMOs, in $5d$ TMOs the situation is different owing to larger extent of d-orbitals and reduced values of U. On the other hand the large atomic number of $5d$ elements promotes strong spin-orbit coupling (SOC). The interplay between strong SOC and small Coulomb repulsion can drive the $5d$ TMOs into a novel spin-orbital Mott state. Here, we investigate these effects in Iridium-based TMOs from first principles calculations using the full-potential linearized augmented plane-wave method [1]. In particular, we focus on the perovskite and postperovskite phases of $CaIrO_3$ and investigate the modifications of their bulk bandstructures in thin films.

[1] www.flapw.de

O 16.5 Mon 17:00 GER 38

A combined LEEM/PEEM study on ferroelectric domains in perovskite crystals — •Hatice Doğanay[1], Ingo Krug[1], Daniel Gottlob[1,2], Stefan Cramm[1], and Claus M. Schneider[1,2] — [1]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich — [2]Fakultät für Physik, Universität Duisburg Essen

We investigated the local electronic structure in domains of BaTiO3(001), which is considered a model perovskite-type ferroelectric oxide with potential for technological applications [1] due to its large dielectric permittivity, spontaneous polarization, piezoelectricity, and nonlinear optical responses. Polarized x-rays and variable photon energy enables photoelectron microscopy (PEEM)with element selective contrast and nanospectroscopy of the electronic structure differences between the ferroelectric domains. AES and LEED show that the surface is BaO terminated with a (2x2) reconstruction. For a clean surface the MEM-LEEM transition shift between different ferroelectric domains was 300 mV. Such a significant value is related to opposite polarizations perpendicular to the surface, pointing either outwards (P+) or inwards (P-). Equally important, in order to study the charge anisotropy with spatial resolution, XAS measurements have been performed. Accordingly, we were able to image the ferroelectric domains with the help of performed and calculated XLD Spectra, recorded at our UE56/1-SGM beamline (BESSY-II, Berlin) with an aberration-corrected LEEM/PEEM. [1] Shimizu et al. J. Phys.: Condens. Matter 25 (2013) 132001

O 16.6 Mon 17:15 GER 38

The origin of TiO_2 shallow gap states evidenced from resonant photoelectron spectroscopy (RPES) and AFM on anatase single crystal (101) surface, nanocrystalline anatase films and ALD titania ante and post annealing — •Philip Reckers[1], Mariel Dimamay[1], Sara Trost[2], Thomas Riedl[2], Thomas Mayer[1], and Wolfram Jaegermann[1] — [1]Technical University of Darmstadt, Surface Science, Germany — [2]Wuppertal University, Electronic Devices, Germany

Transparent, conductive and catalytic active TiO_2 with all its polymorphs is of high interest as it is used e.g. for water splitting, in DSSC and OSC. Gap states in TiO_2 play a crucial role as they influence e.g. charge transport and act as recombination centers. We investigated TiO_2 samples with respect to gap states by the use of res-

onant photoelectron spectroscopy. We detected two different band gap states. Deep gap states (DGS), that are attributed to oxygen defects are found around 1.3 eV and shallow gap states (SGS) are occupied from the Fermi level to about 0.35 eV binding energy. On a single crystal (SC) anatase (101) surface only SGS were detected. DGS and SGS states are observed on sintered nanocrystals (NC). Together with images from AFM we were able to ascribe the SGS to under coordinated Ti sites. The measured DOS fits well to the calculated DOS tailing into the energy gap inherent to NC as 1D line defects of under coordinated Ti sites form at (101) intersections[1]. Similar defects are located at edges of terraces on SC surfaces that form along the (101) direction. [1]F.Nunzi, F.De Angelis, E.Environ. Sci.,2013,6,4,1221-1229

O 16.7 Mon 17:30 GER 38

SPLEED at metallic and adsorbate-covered surfaces — •Stephan Borek[1], Dmytro Kutnyakhov[2], Christian Langenkämper[3], Christian Thiede[3], Jan Minár[1], Jürgen Braun[1], Gerd Schönhense[2], Hans Joachim Elmers[2], Markus Donath[3], and Hubert Ebert[1] — [1]Ludwig-Maximilians-Universiät München — [2]Johannes-Gutenberg-Universiät Mainz — [3]Westfälische-Wilhelms-Universität Münster

The development of SPLEED (Spin-Polarized Low-Energy Electron Diffraction) as a surface-sensitive method has been pushed dramatically in theory as well as in experiment during the last decades. In particular, it is a very important tool for the study of the geometry of crystal surfaces as well as the surface potential barrier. Within the development of a multichannel-vector-spin polarimeter at BESSY various sensor materials have been investigated. Starting from this we perform fully relativistic SPLEED calculations using the SPRKKR package to investigate the resulting spin-dependent reflectivity in dependence on the energy and the scattering angles (polar and azimuthal). We present SPLEED calculations for various materials (W(001), Fe(001), Fe(001) p(1x1) O) and show their characteristics in view of reflectivity, asymmetry and the figure of merit. A comparison between experiment and theory will be made. Funded by BMBF (05K13UM1, 05K13WMA).

O 16.8 Mon 17:45 GER 38

Efficient photoemission spectroscopy via a MHz high-harmonic light source — •Andreas Trützschler[1,2], Michael Huth[1], Cheng-Tien Chiang[1,2], Jürgen Kirschner[1,2], and Wolf Widdra[2,1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120, Halle(Saale), Germany — [2]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, D-06120, Halle(Saale), Germany

We demonstrate an efficient photoemission setup by combining time-of-flight (ToF) spectroscopy with a laboratory MHz pulsed light source with photon energies from 16 to 40 eV. The light is provided by high-order harmonic generation driven by a compact fiber laser system. The high flux of 10^9 photons per second (at 25 eV) at the sample position together with the efficient collection of photoelectrons using ToF spectroscopy allows rapid band mapping of the electronic band structure. As an example we demonstrate photoemission experiments on Ag(100), which reveal the valence band electronic structure within 10 seconds measurement time without remarkable space-charge effects.

O 16.9 Mon 18:00 GER 38

Electron pair emission detected by time-of-flight spectrometers: new perspectives — •Michael Huth[1], Cheng-Tien Chiang[1,2], Andreas Trützschler[1,2], Wolf Widdra[2,1], Frank O. Schumann[1], and Jürgen Kirschner[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120, Halle(Saale), Germany — [2]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, D-06120, Halle(Saale), Germany

We present results for electron coincidence spectroscopy obtained by using two time-of-flight (ToF) spectrometers. Electron-pair emission from a Cu(111) surface detected in coincidence and excited by electron impact allows to resolve the dispersion of the Shockley surface state in the momentum distribution. By combining the two ToF spectrometers with a high-order harmonic generation light source opens up new perspectives to enable (γ,2e) spectroscopy in the laboratory that required synchrotron radiation in the past. Utilizing this setup we report results for (γ,2e) on NiO(001) on Ag(001) excited with light at 30 eV photon energy.

O 16.10 Mon 18:15 GER 38

Energy relations in positron-electron pair emission — •Frank O. Schumann[1], Iuri S. Brandt[1], Zheng Wei[1], and Jürgen Kirschner[1,2] — [1]Max-Planck Institut für Mikrostrukturphysik, Halle, Germany — [2]Martin-Luther Universität, Halle, Germany

The impact of a primary positron onto a surface leads to the emission of a correlated positron-electron pair. By means of a lab-based positron beam we studied this pair emission from a Ag(100) surface. We analyzed the energy spectra in a symmetric emission geometry. We found that the available energy is shared in an unequal manner among the partners. On average the positron carries a larger fraction of the available energy. The unequal energy sharing is a consequence of positron and electron being distinguishable particles. We provide a model which explains the experimental findings.

O 16.11 Mon 18:30 GER 38

Spin-orbit-induced spin polarization on W(110) — •Henry Wortelen[1], Jürgen Henk[2], Anke B. Schmidt[1], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

Despite W(110) being nonmagnetic, its electronic structure exhibits spin-polarized states due to spin-orbit interaction, e.g., a spin-polarized Dirac-cone-like surface state below the Fermi level [1,2]. We report on the unoccupied electronic structure of W(110) investigated with spin-resolved inverse photoemission experiments and calculations. We compare results for $\bar{\Gamma}$-$\bar{N}$ and $\bar{\Gamma}$-$\bar{H}$, which are inequivalent due to the two-fold symmetry. A complex spin structure is observed for the surface states, which even depends on the photon detection angle. This shows that the measured spin polarization does not necessarily resemble the spin structure of the respective electronic state.

[1] K. Miyamoto et al., Phys. Rev. Lett. **108**, 066808 (2012)
[2] H. Mirhosseini et al., New J. Phys. **15**, 033019 (2013)

O 16.12 Mon 18:45 GER 38

Spin-split surface state above the Fermi level on Ta(110) — •Bernd Engelkamp[1], Henry Wortelen[1], Jürgen Henk[2], Anke B. Schmidt[1], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

Recent experimental and theoretical photoemission studies on W(110) have been focused on a spin-polarized Dirac-cone-like surface state within a spin-orbit-induced symmetry gap [1, 2]. Browsing the periodic table for another heavy element with bcc structure yields only tantalum. On Ta(110), with one valence electron less compared to W(110), the spin-orbit-induced symmetry gap is expected above the Fermi level.

Using spin- and angle-resolved inverse photoemission we identified a spin-split surface state along the $\bar{\Gamma}$-$\bar{H}$ direction. We present our experimental results in combination with spectral density calculations in both high-symmetry directions $\bar{\Gamma}$-$\bar{H}$ and $\bar{\Gamma}$-$\bar{N}$.

[1] K Miyamoto *et al.* Phys. Rev. Lett. **108**, 066808 (2012)
[2] H Mirhosseini *et al.* New J. Phys. **15**, 033019 (2013)