O 79: Electronic Structure of Surfaces: Spectroscopy, Surface States I

Time: Wednesday 15:00–18:15 Location: WIL C307

Invited Talk O 79.1 Wed 15:00 WIL C307

Sensing the Quantum Limit in Scanning Tunneling Spectroscopy: From the Josephson Effect to Quantum Tunneling — •Christian R. Ast — Max-Planck-Institut für Festkörperforschung, Stuttgart

The tunneling current in scanning tunneling spectroscopy (STS) is typically and often implicitly modeled by a continuous and homogeneous charge flow. If the charging energy of a single-charge quantum sufficiently exceeds the thermal energy, however, the granularity of the current emerges. In this quantum limit, the capacitance of the tunnel junction mediates an interaction of the tunneling electrons with the surrounding electromagnetic environment and becomes a source of noise itself, which cannot be neglected in STS. Using a scanning tunneling microscope operating at 15 mK, we show that we operate in this quantum limit, which determines the ultimate energy resolution in STS. A theoretical description requires quantum electrodynamics to be included resulting in the $P(E)$-theory, which describes the probability for a tunneling electron to exchange energy with the environment. I will discuss this effect using a superconducting aluminium tip and a superconducting aluminium sample, where it is most pronounced. These considerations will be most important also at higher temperatures for extremely sharp spectral features, such as superconducting gaps, sharp Kondo peaks or Yu-Shiba-Rusinov states.

O 79.2 Wed 15:30 WIL C307

Photoemission tomography from extended 2D layers: the role of molecule/substrate interactions — •Peter Puschnig[1], Daniel Lüftner[1], Thomas Ules[1], Georg Koller[1], Xiaosheng Yang[2], Simon Weiss[2], Vitaliy Feyer[3], Stefan Tautz[2], Michael Ramsey[1], and Sergey Soubatch[2] — [1]Institute of Physics, University of Graz, Austria — [2]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, Germany — [3]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich, Germany

The valence band photoemission angular distribution (PAD) from highly oriented organic molecular layers has been shown to contain rich information on the spatial structure of orbitals and thereby also allows molecular orientations and conformations to be determined. In the past however, measured PADs have been often interpreted in terms of molecular orbitals computed for gas phase molecules.

In this contribution, we show how the photoemission tomography approach can be generalized to take into account two-dimensionally extended organic layers which are in contact with a substrate surface. To this end, we extend the initial state to a sum over Bloch states within the first Brillouin zone and further modify the plane wave final state such that the mean free path of the photoelectron is taken into account in an empirical manner. With the example of a monolayer of PTCDA on Cu(100) a detailed comparison of simulated and experimental momentum and band maps is then made which demonstrates show how the large substrate mediated intermolecular dispersion manifests itself.

O 79.3 Wed 15:45 WIL C307

Bulk and surface states on the Weyl-semimetal candidate Tellurium (Te) probed by spin integrated and spin resolved angle-resolved photoemission — •Florian Titze[1], Mattia Mulazzi[1], Maryam Nazarzadehmoafi[1], Christoph Janowitz[1], Taichi Okuda[2], Kazuki Sumida[3], and Andrei Varykhalov[4] — [1]Humboldt Universität zu Berlin — [2]Hiroshima Synchrotron Radiation Centre — [3]Hiroshima Graduate School of Science — [4]Helmholtz Zentrum Berlin

Te is a direct semiconductor with a band gap of 330 meV. At ambient conditions it crystallises in a hexagonal unit cell with 3 inequivalent atoms winding along its c-axis to form left & right helices making it non-centrosymmetric and chiral.

Lacking a symmetry centre together with a strong spin-orbit coupling induces exotic properties: The nested bands near the top of the valence band (at the H point of the Brillouin zone) provide conducting channels for holes, making Te a good thermoelectric material. Furthermore, non-degenerate bands cross near H at a point called a Weyl node, which is a source of Berry curvature. Because of this, the electron spin near H is predicted to be locked parallel to the electron momentum.

With high resolution angle-resolved photoemission spectroscopy, we mapped the electronic structure in great detail, parallel & perpendicular to the surface plane. We compared our data with bulk band structure calculations in order to identify electronic states and surface states. Finally, spin-resolved ARPES near H has been carried out to examine the predicted exotic spin texture.

O 79.4 Wed 16:00 WIL C307

Spin-dependence in photoemission from strongly spin-orbit coupled systems — •Henriette Maass[1], Hendrik Bentmann[1], Eugene E. Krasovskii[2,3,4], Thiago R. F. Peixoto[1], Christoph Seibel[1], and Friedrich Reinert[1] — [1]Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg — [2]Departamento de Física de Materiales, Universidad del Pais Vasco UPV/EHU, 20080 San Sebastían/Donostia, Spain — [3]Donostia International Physics Center (DIPC), 20018 San Sebastían/Donostia, Spain — [4]IKERBASQUE, Basque Foundation for Science, 48013 Bilbao, Spain

Strong spin-orbit coupling governs the emergence of electronic states with an intrinsic spin polarization. Prominent examples are topological surface states which form for example on the surface of Bi_2Te_3, or Rashba-type spin-splittings in noble metals and surface alloys. Using spin- and angle resolved photoelectron spectroscopy we have investigated the spin- and orbital texture of the topological insulators Bi_2Te_3 and Bi_2Te_2Se as well as the surface alloy $BiAg_2$. Interestingly, whereas at first sight the measured photoelectron spin polarization strongly resembles the one expected for the ground state, strong modulations occur in both, the topological surface states as well as Rashba-type surface states, when the light polarization or photon energy is changed. These modulations reflect a strong influence of the symmetry of initial and final state as well as the experimental alignment on the measured photoelectron spin polarization. Our data yields insight into the relation between the result of a spin-sensitive photoemission experiment and the intrinsic spin-structure of material.

O 79.5 Wed 16:15 WIL C307

Electronic structure of a single crystal BiVO4 photocatalyst measured by angle-resolved photoemission spectroscopy — Mansour Mohammed[1,2], Matthias May[2], Christoph Janowitz[1], Michael Kanis[3], Reinhardt Uecker[4], Mario Brützmann[4], Roel van de Krol[3], and •Mattia Mulazzi[1,4] — [1]1Humboldt University in Berlin, Institute of Physics, 12489 Berlin, Germany — [2]2Assiut University, Department of Physics, Faculty of Science, 71515 Assiut Egypt — [3]3Helmoltz Zentrum Berlin für Materialien und Energie, Institute of Solar Fuels, 14109 Berlin, Germany — [4]4Leibniz Institute for Crystal Growth, 12489 Berlin, Germany

We measured by angle-resolved photoemission at low energy the valence band dispersion of BiVO4. The material, a wide-band gap n-type oxide, is a promising photoanode material for water splitting applications. A solar-to-hydrogen efficiency of ~5% was reached wiht a BiVO4 / double juntion a-Si tandem cell device. The bands measured in ARPES experiments are flat, with only a sizeable dispersion measured in the in-plane directions perpendicular to the (010) axis. We found a weak non-dispersive peak in the forbidden gap indicating localised states, which we attribute to point defects. To determine thee origin of the defects, we compared (for different photon energies) the in-gap peak and top-of-valence-band photoemission intensity ratio to the theoretical Mo and oxygen cross-sections. We found that the theory is in quantitative agreement with the experiment and attributed the in-gap peak to the Mo dopant. We discuss the consequences of the Mo states, which change the size and character of the band gap.

O 79.6 Wed 16:30 WIL C307

Effects of spin-orbit coupling on the optical responses of a material — •Tae Yun Kim[1], Andrea Ferretti[2], and Cheol-Hwan Park[1] — [1]Department of Physics and Astronomy, Seoul National University, Seoul 08826, Korea — [2]Centro S3, CNR-Instituto Nanoscienze, 41125 Modena, Italy

The electronic structure of a material involving heavy elements are significantly affected by spin-orbit coupling (SOC). Especially, since SOC allows the manipulation of the spin degree of freedom in a material by using light [1-4], understanding the SOC effects on the optical response is a matter of importance. In this contribution, we calculate and investigate the effects of SOC on the optical responses of a material based

on a fully-relativistic pseudopotential method [5-6].

[1] C.-H. Park and S. G. Louie, Phys. Rev. Lett. 109, 097601 (2012)

[2] C. Jozwiak, C.-H. Park, K. Gotlieb, C. Hwang, D.-H. Lee, S. G. Louie, J. D. Denlinger, C. R. Rotundu, R. J. Birgeneau, Z. Hussain and A. Lanzara, Nature Physics 9, (2013)

[3] J. H. Ryoo and C.-H. Park, Phys. Rev. B 93, 085419 (2016)

[4] Z.-H. Zhu, C. N. Veenstra, S. Zhdanovich, M. P. Schneider, T. Okuda, K. Miyamoto, S.-Y. Zhu, H. Namatame, M. Taniguchi, M. W. Haverkort, I. S. Elfimov, and A. Damascelli, Phys. Rev. Lett. 112, 076802 (2014)

[5] L. Kleinman, Phys. Rev. B 21, 2630 (1980)

[6] Giovanni B. Bachelet and M. Schlüter, Phys. Rev. B 25, 2103 (1982)

O 79.7 Wed 16:45 WIL C307

Contribution of magnetic dopants to the electronic structure of the Topological Insulator Sb_2Te_3. — •Sonja Schatz[1], Thiago R. F. Peixoto[1], Hendrik Bentmann[1], Oleg E. Tereshchenko[2], Konstantin A. Kokh[2], and Friedrich Reinert[1] — [1]Experimentelle Physik VII, Universität Würzburg, D-97074 Würzburg — [2]Saint Petersburg State University, 198504 Saint Petersburg, Russia

Doped Topological Insulators with magnetic impurities have been shown to exhibit novel and exotic quantum phenomena. As has been reported recently, V-doped $(BiSb)_2Te_3$ features an insulating ground state below $T_C \sim 30$ K, and it forms a quantum anomalous Hall state below $T \sim 100$ mK [1]. For thin films of this system we already reported, that the existence of a $3d$ impurity band near the Fermi energy is expected to lead to the occurrence of a ferromagnetic superexchance interaction [2]. In this talk we will present studies of the Topological Insulator Sb_2Te_3 doped with different $3d$ transition metals and compare our results to first-principles calculations [3]. To investigate the electronic structure of these systems, angle-resolved photoemission and absorption experiments were performed in the soft X-ray regime at temperatures around $T \lesssim 30$ K. In particular the valence band was observed resonantly at the $2p$ absorption edge providing element specificity.

[1] C. Z. Chang *et al., Nature Materials* **14**, 473 (2015).

[2] T. Peixoto *et al., Physical Review B* **94**, 195140 (2016).

[3] J.-M. Zhang *et al., Physical Review B* **88**, 235131 (2013).

O 79.8 Wed 17:00 WIL C307

Investigation of the Mahan cones spin polarization of noble metal surfaces — •Benito Arnoldi, Johannes Stöckl, Mirko Cinchetti, Benjamin Stadtmüller, and Martin Aeschlimann — Department of Physics, TU Kaiserslautern, Erwin-Schroedinger-Strasse 46, 67663 Kaiserslautern, Germany

The angle resolved photoemission (ARPES) yield of noble metals such as Au, Ag or Cu recorded at low photon energies is dominated by direct optical transitions between free electron like sp-bands of the bulk band structure, the so called Mahan cones [1]. During the optical transition, the momentum conservation leads to an exchange of momentum between the photoelectron and the crystal lattice by adsorption of a reciprocal lattice vector.

Here, we employ spin and angle resolved laser ARPES with linear polarized light to gain insight into the spin polarization of these direct optical transitions for different noble metal surfaces. For $h\nu \approx 6$ eV and $h\nu \approx 3$ eV in the 1 photon photoemission emission (1PPE) and 2 photon photoemission (2PPE) process for the Au(111) surface, we observe clear spin-polarization of the Mahan cones along all high symmetry directions. Similar results will be presented for the Au(110) as well as for Cu(111) surface. A comparison of our results will allow us to reveal the influence of the spin-orbit coupling on the spin-polarization of the Mahan cones of noble metal surfaces. [1]New J. Phys. 14 (2012) 083027

O 79.9 Wed 17:15 WIL C307

Retrieving the initial-state spin polarization from spin-resolved photoemission: W(110) as a case study — •Jürgen Henk[1], Koji Miyamoto[2], Henry Wortelen[2], and Markus Donath[2] — [1]Martin-Luther-Universität Halle-Wittenberg, Halle — [2]Westfälische Wilhelms-Universität, Münster

Spin- and angle-resolved photoelectron spectroscopy (SARPES) aims at measuring the spin polarization of the initial states. In systems with sizable spin-orbit coupling, however, the photoemission process itself results in an additional spin polarization of the photoelectrons. This falsification can be considerable, even for surface states with spin-momentum locking.

We show that the initial-state spin polarization can be largely retrieved by combining SARPES data for selected setups. The idea is presented for optical orientation from the Dirac-type surface state of W(110). Theoretical spectra compare well with their experimental pendants; limitations of the approach are discussed.

O 79.10 Wed 17:30 WIL C307

Surface states of transition-metal delafossite oxides — •Veronika Sunko[1,2], Helge Rosner[2], Pallavi Kushwaha[2], Lewis Bawden[1], Oliver J. Clark[1], Jonathon M. Riley[2,3], Deepa Kasinathan[2], Maurits W. Haverkort[2], Andrew P. Mackenzie[1,2], and Philip D.C. King[2] — [1]SUPA, School of Physics and Astronomy, University of St. Andrews, St. Andrews KY16 9SS, UK — [2]MPI-CPfS, Nöthnitzer Straße 40, 01217 Dresden, Germany — [3]Diamond Light Source, Harwell Campus, Didcot, OX11 0DE, UK

Delafossite oxides have recently attracted considerable attention because of their fascinating transport properties[1]. PdCoO2 and PtCoO2 are the most conductive oxides known at room temperature, with resistivities comparable to those of silver, copper and gold[2, 3]. This high conductivity is attributed to a single broad band crossing the Fermi level[3]. However, due to the polarity of the structure the electronic properties at the surfaces can be very different to those of the bulk[4]. We use angle resolved photoemission (ARPES) to show that the CoO2 terminated surfaces of (Pd,Pt)CoO2 do host a set of states which do not appear in the bulk, with much higher masses and stronger interactions. Comparing ARPES with density functional theory and model tight-binding calculations, we investigate the origin of these states, paying special attention to the role of the spin-orbit coupling.

[1] Moll et al., Science 351 (2016) 6277, Kikugawa et al., Nature Commun. 7 (2016) 10903 [2] Hicks et al., PRL 109 (2012) 116401 [3] Kushwaha et al., Science Adv. 1 (2015) e1500692 [4] Kim et al., PRB 80 (2009) 035116, Noh et al., PRL 102 (2009) 256404

O 79.11 Wed 17:45 WIL C307

Non-symmorphic band degeneracy at the Fermi level in ZrSiTe — •Andreas Topp[1], Judith M. Lippmann[1,2], Andrei Varykhalov[3], Viola Duppel[1], Shweta Sheoran[1], Bettina V. Lotsch[1,2,4], Christian R. Ast[1], and Leslie M. Schoop[1] — [1]Max Planck Institute for Solid State Research, D-70569 Stuttgart — [2]Department of Chemistry, Ludwig-Maximilians-Universität, D-81377 München — [3]Helmholtz-Zentrum Berlin für Materialien und Energie, Bessy II, D-12489 Berlin — [4]Nanosystems Initiative Munich (NIM) & Center for Nanoscience, D-80799 München

Three-dimensional Dirac semimetals, which accommodate massless Dirac or Weyl fermions, show exotic physical properties, e.g. an extremely high mobility and giant magnetoresistance. Compounds that contain non-symmorphic symmetries are especially interesting, because they exibit band crossings that are not affected by SOC. ZrSiS, hosting a square lattice of Si atoms, exhibits normal, as well as, non-symmorphically protected 3D Dirac crossings below and above the Fermi level [1]. Pinning these non-symmorphic crossings to the Fermi level can be difficult, since it requires a material with a half-filled band, that is usually not stable. Upon replacing S with Te, the resulting chemical uniaxial strain shifts the position of the non-symmorphic crossing. Here, we present ARPES data and DFT calculations confirming that the non-symmorphic crossing is located at the Fermi level in ZrSiTe, making this compound a strong candidate to investigate the effect of forced band degeneracies on transport properties.

[1] L. M. Schoop *et al.*, Nat. Comm. 7, 11696 (2016).

O 79.12 Wed 18:00 WIL C307

AiiDA Workflows with FLEUR for X-ray photoemission Spectroscopy — •Jens Bröder[1,2], Gregor Michalicek[1], Daniel Wortmann[1], Rudi Koslowski[2], Christian Linsmeier[2], and Stefan Blügel[1] — [1]Peter Grünberg Institute (PGI-1) and Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich GmbH, 52425 Jülich, Germany — [2]Institut für Energie- und Klimaforschung - Plasmaphysik, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

We present the plugin of the all-electron DFT code FLEUR[1] to AiiDA[2] (Automated interactive Infrastructure and database for material science) and our first established workflows to calculate electron binding energies and core level shifts (CLS) of X-ray photoemission (XPS) spectra of pure materials for surface science.

One workflow calculates CLS in the initial state approximation of

bulk and slab geometries. An other workflow uses super cell core-hole calculations to extract binding energies. Their first application will be the simulation of materials relevant for research on plasma wall interaction (PWI) in fusion. First results of different methods are compared to recent experimental data.

We acknowledge financial support in part from MAX (Materials design at the eXascale) Horizon 2020 EINFRA-5.

[1] www.flapw.de [2] G. Pizzi, et al. Comp. Mat. Sci. 111, 218-230 (2016)