O 73: Electronic Structure of Surfaces 1

Time: Thursday 15:00–17:45 Location: S053

O 73.1 Thu 15:00 S053

Rashba-split image-potential state at Re(0001) — •Fabian Schöttke, Sven Schemmelmann, Peter Krüger, and Markus Donath — Westfälische-Wilhelms-Universität Münster, Germany

Since image states are located mainly in the vacuum in front of the surface, the influence of spin-dependent interactions on these states is a topic of ongoing debate in the literature. In particular, calculations predict Rashba-type spin splittings for image states [1], but experimental results of small spin splittings are controversial [2,3]. In addition, these two-photon-photoemission results using circular dichroism provide only indirect information about the spin polarization of states.

We measured the unoccupied surface electronic structure of Re(0001) with spin- and angle-resolved inverse photoemission. This method allows to investigate the spin orientations directly. We identified the $n = 1$ image state at a binding energy of $E_V - E = 0.68 \pm 0.04$ eV and with an effective mass of $m^*/m_e = 1.2 \pm 0.1$. Careful spin-resolved measurements for several angles of electron incidence allowed us to detect Rashba-type spin-dependent energy splittings of this state with a Rashba parameter of $\alpha_R = 105 \pm 33$ meV Å [4].

[1] McLaughlan *et al.*, J. Phys.: Condens. Matter **16**, 6841 (2004).
[2] Tognolini *et al.*, Phys. Rev. Lett. **115**, 046801 (2015).
[3] Nakazawa *et al.*, Phys. Rev. B **94**, 115412 (2016).
[4] Schöttke *et al.*, Phys. Rev. B **105**, 155419 (2022).

O 73.2 Thu 15:15 S053

Rashba-split surface state and spin-dependent photon emission from Re(0001) at $\bar{\Gamma}$ — •Sven Schemmelmann[1], Fabian Schöttke[1], Peter Krüger[2], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, Münster — [2]Institut für Ferstkörpertheorie, Westfälische Wilhelms-Universität, Münster

The unoccupied electronic structure of the Re(0001) surface around the center of the surface Brillouin zone was investigated by spin- and angle-resolved inverse photoemission [1]. The detected states were studied with respect to intrinsic and extrinsic spin-polarization effects. A surface state with Rashba-type spin splitting is detected close to the Fermi level, that disperses downward below the Fermi energy. Furthermore, for normal electron incidence, we observed spin-dependent photon emission from unpolarized bulk and surface states. The sign of the observed spin asymmetry varies for different states and depends on experimental parameters such as electron spin-polarization direction and photon-detection angle. Maximum spin asymmetry is observed if the electron spin polarization and the plane of photon emission are perpendicular. The asymmetry is zero if both are parallel [2]. The effect is traced back to the spin-orbit-induced hybridization of the involved states.

[1] S. Schemmelmann *et al.*, Physical Review B **104**, 205425 (2021)
[2] E. Tamura and R. Feder, Solid State Commun. **79**, 989 (1991)

O 73.3 Thu 15:30 S053

Distinct Tamm and Shockley surface states on Re(0001) - mixed by spin-orbit interaction — •Marcel Holtmann[1], Peter Krüger[1], Koji Miyamoto[2], Taichi Okuda[2], Pascal J. Grenz[1], Shiv Kumar[2], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany — [2]Hiroshima Synchrotron Radiation Center, Hiroshima University, 2-313 Kagamiyama, Higashi-Hiroshima 739-0046, Japan

Tamm and Shockley states - two paradigmatic concepts are used to describe surface states not only in electronic systems but also in photonic and phononic crystals. The Re(0001) surface hosts both types of electronic surface states in neighboring but qualitatively different energy gaps. Interestingly, spin-orbit interaction generates a double "W"-shaped energy vs. $\mathbf{k}_\parallel$ dispersion by mixing both types of states and lifting their spin degeneracy. By combining spin- and angle-resolved photoemission, tight-binding model calculations as well as density functional theory including the photoemission process, we develop verifiable criteria to distinguish between the two types of surface states and arrive at a consistent picture of the role of spin-orbit interaction in such a scenario.

O 73.4 Thu 15:45 S053

Electronic structure of a square Te adlayer on Au(100) surface — •Begmuhammet Geldiyev[1], Tilman Kisslinger[2], Philipp Eck[3], Maximilian Ünzelmann[1], Tim Figgemeier[1], Jakub Schusser[1], Nikolai Tezak[1], Lutz Hammer[2], M. Alexander Schneider[2], Domenico Di Sante[3], Giorgio Sangiovanni[3], Hendrik Bentmann[1], and Friedrich Reinert[1] — [1]Experimentelle Physik 7 and Cluster of Excellence ct.qmat, Universität Würzburg — [2]Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg — [3]Institut für Theoretische Physik und Astrophysik and Cluster of Excellence ct.qmat, Universität Würzburg

In light of several theoretical predictions regarding the so-called square tellurene [1, 2], the growth and the electronic structure of Te deposited on a Au(100) surface is reported. At a coverage of 1/4 monolayer, Te forms a $p(2\times2)$ square lattice of adatoms on Au(100) as determined by a thorough LEED-IV characterization ($R_P = 0.085$) and STM. Utilizing angle-resolved photoemission spectroscopy and density functional theory an interface-like state with mixed Te $p_{x,y}$ and Au d orbital character is identified in addition to a complex multitude of backfolded bands of the substrate. Vastly differing Rashba parameters along the $\overline{\mathrm{XG}}$ and $\overline{\mathrm{XM}}$ lines cannot be explained within an (anisotropic) Rashba picture. The spin splitting rather depends on the momentum space texture of the atomic orbitals. Our work may stimulate further experimental explorations of symmetry and topology effects in 2D square-lattice systems. [1] Xian et al., 2D Mater. **4**, 041003, (2017)
[2] Zhang et al., Phys. Rev. B **98**, 115411, (2018)

O 73.5 Thu 16:00 S053

Interplay of exchange and spin-orbit interaction in ultrathin Ni films on W(110) — •Pascal Jona Grenz[1], Peter Krüger[2], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany — [2]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

Ferromagnetic adsorbates on high-Z substrates are prototypical systems for studying the combined influence of spin-orbit and exchange interaction on electronic states [1,2]. The unoccupied electronic states of ultrathin Ni films on W(110) were investigated with spin- and angle-resolved inverse photoemission. Measurements were performed along $\overline{\Gamma}\,\overline{\mathrm{N}}$ ($\overline{\Gamma}\,\overline{\mathrm{M}}$ with respect to the Ni(111) surface Brillouin zone), where the quantization axis of the Rashba-spin component is collinear to the easy magnetization axis. Remarkably, the observed unoccupied Ni-derived exchange-split states change their energy-momentum dispersion upon magnetization reversal. Density functional theory calculations show that this phenomenon is a consequence of substrate-induced spin-orbit coupling within the Ni adlayers.

[1] P. Moras *et al.*, Phys. Rev. B **91**, 195410 (2015)
[2] P.J. Grenz *et al.*, J. Phys.: Condens. Matter **33**, 285504 (2021)

O 73.6 Thu 16:15 S053

ARPES studies of Hf(0001) monocrystal: experiment and theory — •Saleem Ayaz Khan[1], Laurent Nicolai[1], Jean Zaraket[2,3], Maria Christine Richter[2,3], Olivier Heckmann[2,3], Laxman Nagi Reddy[2,3], Waly Ndiaye[2,3], Mauro Fanciulli[2,3], Karol Hricovini[2,3], and Jan Minar[1] — [1]NTC, Univiversity of West Bohemia, Plzeň, Czech Republic — [2]LPMS, CY Cergy Paris University, France — [3]DRF, IRAMIS, LIDYL, CEA Saclay, France

We present first ARPES studies of the electronic structure of the Hf(0001) surface. High-Z materials have attracted much interest, because the strong spin-orbit coupling in combination with the broken inversion symmetry and an important effective electric field at the surface results in a spin-momentum locking. Spin-polarized electrons at the surface are of interest in physics and novel applications in electronics and data processing. Extra sharp peaks observed in experiment are identified thanks to *ab-initio* calculations performed within the SPR-KKR package. These extra states come from oxygen contamination of the highly reactive surface of Hf(0001). Further comparison is done on the ARPES level, thanks to the one-step model which include all matrix elements effect, resulting in an excellent agreement.

O 73.7 Thu 16:30 S053

Establishing fundamentals of ARPES spin textures with model material $PtTe_2$ — •Mohammed Qahosh, Honey Boban,

Xiao Hou, Claus-Michael Schneider, and Lukasz Plucinski — Electronic Properties-Peter Grünberg Institute (PGI-6).

A novel quantum material $PtTe_2$ is used to establish the connection between ARPES spin textures and initial state spin textures. $PtTe_2$ is predicted to host Dirac type-II fermions and a number of application-relevant properties. The crystal structure of the most stable 1T-$PtTe_2$ polytype is trigonal, belongs to the space group 164 ($P\bar{3}m1$), and exhibits 3-fold mirror planes and inversion symmetry. Since bulk 1T-$PtTe_2$ is both inversion-symmetric and non-magnetic, no bulk spin-polarized bands are allowed due to the Kramers degeneracy. At the surface, spin polarization is expected due to the broken inversion symmetry, however, it must obey the mirror and time-reversal symmetries.

We measured the dependence of spin-polarization on the symmetries of the ARPES experiment. This is performed in two geometries, with the reaction plane parallel to K-Γ-K and M-Γ-M reciprocal directions, i.e. either along or orthogonal to the crystal mirror plane. The measured spin texture is symmetric when the reaction plane is parallel to K-Γ-K. However, we could see asymmetries in the spin texture when the reaction plane is parallel to M-Γ-M. Such asymmetries are not allowed in the initial state and illustrate the mechanism of geometry-induced spin filtering in ARPES.

O 73.8 Thu 16:45 S053

Surface doping of the $MnBi_2Te_4$ family by rubidium deposition — •Klara Volckaert[1], Paulina Majchrzak[1], Raphaël Dubourg[1], Zhihao Jiang[1], Xing-Chen Pan[2], Yong Chen[1], and Søren Ulstrup[1] — [1]Department of Physics and Astronomy, Aarhus University, Denmark — [2]Advanced Institute for Materials Research, Tohoku University, Japan

Intrinsic magnetic topological insulators, in the form of $MnBi_2Te_4$, have recently been realised as a remarkable platform to study quantised magnetoelectric phenomena. Here we look into the surface electronic structure during rubidium deposition in a combined angle-resolved photoemission and core level study. We find that for $MnBi_2Te_4$, the initial electron doping effect from the adsorbed rubidium atoms is small. However, deposition on the higher stoicheometry compound $MnBi_4Te_7$ leads to a dramatic modification of the electronic structure, which is different for the surface terminated by a Bi_2Te_3 quintuple layer compared to a $MnBi_2Te_4$ septuple layer. Additionally, high rubidium deposition rates lead to a change of the electronic structure including a shift of the valence bands towards the Fermi level for both compounds, presumably due to Rb-Te-Bi alloying. A distinct quantization of the valence states is simultaneously observed. These results are the first to explore the tunability of electronic states the surface terminations of $MnBi_4Te_7$ with in situ alkali doping and substitution, which could modify the surface magnetic ordering.

O 73.9 Thu 17:00 S053

Theoretical and experimental HARPES study of Weyl-semimetal TaAs: The application of machine-learning — •Trung-Phuc Vo[1], Arian Arab[2], Sunil Wilfred D'Souza[1], Laurent Nicolaï[1], Tien-Lin Lee[3], Nitesh Kumar[4], Claudia Felser[4], Alexander Gray[2], and Ján Minár[1] — [1]New Technologies - Research Centre, University of West Bohemia, 301 00 Pilsen, Czech Republic — [2]Department of Physics, Temple University, Philadelphia, Pennsylvania 19122, USA — [3]Diamond Light Source Ltd., Didcot, Oxfordshire OX11 0DE, United Kingdom — [4]Max Planck Institute for Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany

The electronic structure properties of tantalum arsenide (TaAs), a Weyl semimetal, have been studied by soft and hard X-ray angle-resolved photoemission spectroscopy (ARPES) at energies of 440 eV and 2150 eV, respectively. For the first time, TaAs is experimentally investigated by the bulk sensitive photoemission in the hard X-ray regime. In order to interpret experimental data we performed one-step model of photoemission calculation which includes all matrix elements and final state effects. Due to the strong photon momentum effects and uncertainty in the tilt of experimental geometry we used a so-called machine learning algorithm combined with a free-electron final-state model to find best possible experimental parameters. Our findings re-emphasize the overwhelming accuracy of hard X-ray ARPES compared to the traditional ultraviolet and soft X-ray one in case of bulk electronic structure, motivating further material discoveries.

O 73.10 Thu 17:15 S053

Electron correlation in SrTiO3 studied by double photoemission spectroscopy with a MHz high-order harmonics laser source — •Robin Kamrla[1], Cheng-Tien Chiang[1,2], Frank Oliver Schumann[3], and Wolf Widdra[1] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany — [2]Academica Sinica, Institute of Atomic and Molecular Sciences, Taiwan — [3]Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

Photoelectron spectroscopy (PES) has provided deep insights into the electronic structure of solids. However, correlation effects can only be addressed indirectly. To observe such phenomena directly, double photoemission (DPE) spectroscopy is able to detect pairs of correlated photoelectrons that are emitted upon absorption of a single photon. Upon surface near doping, SrTiO3 (001) with a bandgap of 3.4 eV forms a two-dimensional electron gas (2DEG). In this contribution we present PES and DPE data for SrTiO3 (001) with and without 2DEG states at the surface, obtained by a high-order harmonic (HHG) light source at 25.2 and 30.0 eV. PES reveals a change in spectral weight of the O2p states and a surface band bending of 250 meV upon flipping SrTiO3 (001) into the 2DEG state and oxygen vacancy derived states emerging within the bandgap. In DPE, a band-bending induced shift of 500 meV, changes in the intensity of the O2p derived two hole states as well as emission from vacancy-valence pairs are identified via the two-electron sum energy spectrum. In addition, the role of Auger decays for the shallow Sr4p and O2s core level will be discussed.

O 73.11 Thu 17:30 S053

Doping of 1D topologically protected edge states on the (001) surface of the topological crystalline insulator (Pb,Sn)Se — •Florian Keller, Artem Odobesko, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Topological crystalline insulators (TCI) are a class of materials with topological protected surface states protected by crystalline symmetry. A particularly popular representative of this material class is (Pb,Sn)Se which exhibits four Dirac cones per Brillouin zone. It has been shown that surface step edges with a height equivalent to an odd number of atomic layers results in a topologically protected one-dimensional edge state which is characterized by a peak at the Dirac energy [1]. Theoretical analysis suggests that this state is caused by the broken translation-invariance at the step edge and originates from flat-dispersing bands which connect pairs of surface Dirac nodes [1]. Due to intrinsic doping, the energy of the edge modes of as-grown crystals is usually well separated from the Fermi level. Here we investigate the behavior of these one-dimensional edge modes during Fe surface doping. Since Fe donates charge to p-doped PbSnSe, it results in a downwards-bending of the surface band structure. We observe a peak splitting as the Dirac energy gets close to the Fermi level. We discuss the potential origins of this observation in terms of electron correlations.

[1] Sessi, Paolo, Science 354, 6317 (2016)