O 59: Electronic Structure of Surfaces I

Time: Wednesday 15:00–17:45 Location: REC C 213

Topical Talk O 59.1 Wed 15:00 REC C 213

Interplay of Inversion Symmetry Breaking and Spin-Orbit Coupling — •Maximilian Ünzelmann — Experimentelle Physik 7, Universität Würzburg and Würzburg-Dresden Cluster of Excellence ct.qmat

Inversion symmetry breaking (ISB) in crystalline solids provides an essential way of modifying electronic structures. For example, in combination with spin-orbit coupling (SOC), ISB allows for a lifting of spin degeneracy without the need for magnetism. Moreover, it is a source of Berry curvature, which is of fundamental importance in topological quantum matter. In this talk, two scenarios will be discussed, in which the interplay of ISB with SOC plays an important role: (i) At surfaces or interfaces, where inversion symmetry is inherently broken and the Rashba effect [1] enforces a locking of the electrons spin perpendicular to its momentum and (ii) in Weyl semimetals whose three-dimensional crystal structure has no inversion center, leading to the formation of Berry curvature monopoles, i.e., quantized topological charges [2].

As will be highlighted in this presentation, we find that ISB-induced unquenching of the so-called (atomic) orbital angular momentum (OAM) in the Bloch wave functions constitutes a key mechanism underlying the physics of both the Rashba effect and Weyl semimetals. Angle-resolved photoemission with variable light polarization provides detailed experimental access to the respective momentum-space orbital textures.

[1] M. Ünzelmann et al., Phys. Rev. Lett. **124**, 176401 (2020)
[2] M. Ünzelmann et al., Nat. Commun. **12**, 3650 (2021)

O 59.2 Wed 15:30 REC C 213

Unoccupied surface electronic structure of Re(0001) — •Fabian Schöttke, Sven Schemmelmann, Peter Krüger, and Markus Donath — Westfälische-Wilhelms-Universität Münster, Germany

The influence of spin-orbit interaction on the unoccupied electronic structure of the Re(0001) surface is investigated by spin- and angle-resolved inverse photoemission and density-functional theory calculations. In the two high-symmetry azimuths $\overline{\Gamma}\,\overline{\mathrm{K}}$ and $\overline{\Gamma}\,\overline{\mathrm{M}}$, we identify transitions into d-derived bulk states as well as different types of surface states. The Rashba-type spin-split hole pocket around $\overline{\Gamma}$ finds continuation in empty spin-split surface states for higher $\mathbf{k}_\parallel$, thereby forming W-shaped states whose lower parts are partially occupied.

Schöttke *et al.*, Phys. Rev. B **105**, 155419 (2022).

O 59.3 Wed 15:45 REC C 213

Establishing fundamentals of ARPES spin textures with the model material $PtTe_2$ — •Mohammed Qahosh[1], Gustav Bihlmayer[2], Jakub Schusser[3], Muthu Masilamani[3], Friedrich Reinert[3], Claus M. Schneider[1], and Lukasz Plucinski[1] — [1]PGI-6 Forschungszentrum-Jülich — [2]PGI-1/IAS-1 Forschungszentrum-Jülich — [3]Experimentelle Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg

A novel quantum material $PtTe_2$ is used to establish the connection between spin textures of angle-resolved photoemission spectroscopy (ARPES) and initial state spin textures. The crystal structure of 1T-$PtTe_2$ is trigonal, belongs to the space group 164 ($P\bar{3}m1$), that contains 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, a non-zero 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 the spin-polarization on the symmetries of the ARPES setup. This is performed in two geometries, with the reaction plane parallel to $\bar{K}$-$\bar{\Gamma}$-$\bar{K}$ and $\bar{M}$-$\bar{\Gamma}$-$\bar{M}$ 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 $\bar{K}$-$\bar{\Gamma}$-$\bar{K}$. However, we see asymmetries in the spin texture when the reaction plane is parallel to $\bar{M}$-$\bar{\Gamma}$-$\bar{M}$. For surface states, the asymmetries are due to the geometry-induced spin filtering in ARPES [1]. For bulk states, the effect might be additionally related to the asymmetric initial state dispersions. [1] T. Heider et al., arXiv:2210.10870 (2022)

O 59.4 Wed 16:00 REC C 213

Surface electronic structure of Re(0001): A spin-resolved photoemission study — •Marcel Holtmann[1], Peter Krüger[2], Koji Miyamoto[3], Taichi Okuda[3], Shiv Kumar[3], Kenya Shimada[3], and Markus Donath[1] — [1]Physikalisches Institut, WWU Münster, Germany — [2]Institut für Festkörpertheorie, WWU Münster, Germany — [3]HiSOR, Hiroshima University, Japan

The surface electronic structure of Re(0001) has been investigated in a combined experimental and theoretical study. (Spin- and) angle-resolved photoemission was employed to unravel the spin-dependent $E(\mathbf{k}_\parallel)$ dispersion along the $\overline{\Gamma}\,\overline{\mathrm{M}}$ and $\overline{\Gamma}\,\overline{\mathrm{K}}$ directions. The results are compared with band structures from density-functional theory. Moreover, transitions into final states have been considered by inclusion of the corresponding matrix elements. A spin-orbit-induced mixing of Shockley- and Tamm-type surface states around $\overline{\Gamma}$ and close to E_F was reported recently [1]. Here, we extend the analysis to a wider $E(\mathbf{k}_\parallel)$ range showcasing a multitude of electronic states along the $\overline{\Gamma}\,\overline{\mathrm{M}}$ and $\overline{\Gamma}\,\overline{\mathrm{K}}$ directions. In particular, Rashba-type spin splittings are observed around the high-symmetry $\overline{\Gamma}$ and $\overline{\mathrm{M}}$ points. At variance with theoretical predictions [2], which describe a perfect hcp(0001) surface, we do not find any out-of-plane spin polarization. This is caused by monoatomic steps of a real Re(0001) surface with alternating terminations, which lead on average to an effective sixfold surface symmetry and vanishing net out-of-plane spin polarization.

[1] M. Holtmann *et al.*, Phys. Rev. B **105**, L241412 (2022)
[2] A. Urru and A. Dal Corso, Surf. Sci. **686**, 22 (2019)

O 59.5 Wed 16:15 REC C 213

Spectroscopic evidence for a new type of surface resonance at noble-metal surfaces — •Tobias Eul[1], Jürgen Braun[2], Benjamin Stadtmüller[1,3], Hubert Ebert[2], and Martin Aeschlimann[1] — [1]Technische Universität Kaiserslautern and Research Center OPTIMAS, 67663 Kaiserslautern, Germany — [2]Department Chemie, Ludwig-Maximilians-Universität München, 81377 München, Germany — [3]Institute of Physics, Johannes Gutenberg University Mainz, 55128 Mainz, Germany

We investigated the surface and bulk properties of the pristine (110) surface of silver using threshold photoemission by excitation with light of 5.9 eV. Using a momentum microscope, we identified two distinct transitions along the $\overline{\Gamma Y}$-direction of the crystal. The first one is a so far unknown surface resonance of the (110) noble-metal surface, exhibiting an exceptionally large bulk character that has so far been elusive in surface sensitive experiments. The second one stems from the well-known bulklike Mahan cone oriented along the ΓL-direction inside the crystal but projected onto the (110)-surface cut. The existence of the new state is confirmed by photocurrent calculations, and its character is analyzed.

O 59.6 Wed 16:30 REC C 213

One monolayer of Tl on Ag(111): Hybridization of image-potential states with Tl states — •Sven Schemmelmann[1], Patrick Härtl[2], Peter Krüger[3], Matthias Bode[2], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, Münster — [2]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg — [3]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, Münster

For one atomic layer of Tl on Ag(111) a moiré superstructure is observed. The unoccupied electronic structure of this superstructure is investigated by spin- and angle-resolved inverse photoemission. The experimental results are interpreted on the basis of DFT calculations. We observe several Tl-induced surface states and an image-potential state mainly located several Å in front of the surface. Surprisingly, we find a hybridization of this image state with a downward dispersing Tl band. This leads to spin-dependent spectral intensities that vary rapidly close to the hybridization point. The calculations show an expeditious change of the charge density from a resonant image-potential state towards a Tl-induced surface state in dependence of $\mathbf{k}_\parallel$.

O 59.7 Wed 16:45 REC C 213

Bulk and surface electronic structure of tunnel barrier Nb_3Br_8 in the field-free Josephson diode — •Mihir Date[1,2], Jonas.A. Krieger[1], Emily.C. McFarlane[1], Vicky Hasse[3], Claudia Felser[3], Stuart.S.P Parkin[1], Matthew Watson[2], and Niels.B.M Schröter[1] — [1]MPI-Halle, Weinberg 2, 06120 Halle (Saale), Germany — [2]Diamond Light Source Ltd. Didcot, OX11 0DE,

United Kingdom — [3]MPI-CPfS, Nöthnitzer Straße 40, 01187 Dresden, Germany

In this work, we report the bulk and surface electronic structure of Nb_3Br_8 probed using angle resolved photoemission spectroscopy (ARPES). Nb_3Br_8 is predicted to host trivial metallic surface states (obstructed surface states (OSS)) when cleaved between specific layers [1]. Although our in-plane electronic structure is consistent with the calculated orbital resolved bandstructure, we do not observe any signatures of the OSS. Nevertheless, the doubling of periodicity of the ARPES signal along the out-of-plane momentum direction, as compared to the Brillouin zone dimension, hints towards dimerization between alternate layers through the OSS. We discuss our results in connection with the recent discovery of the field-free Josephson diode effect in the $NbSe_2/Nb_3Br_8/NbSe_2$ heterostructures [2].

[1] Xu, Y. et al. arXiv:2106.10276 (2021).
[2]. Wu, H. et al. Nature 604 (2022).

O 59.8 Wed 17:00 REC C 213

Termination dependent many-body interactions of the surface states of $PdCoO_2$ revealed by ARPES-based microscopy — •Gesa-Roxanne Siemann[1], Edgar Abarca Morales[1,2], Philip A. E. Murgatroyd[1], Tommaso Antonelli[1], Seunghyun Khim[2], Matthew Watson[3], Cephise Cacho[3], Andrew P. Mackenzie[1,2], and Phil D. C. King[1] — [1]University of St Andrews, UK — [2]MPI for Chemical Physics of Solids, Dresden, Germany — [3]Diamond Light Source, UK

The layered ABO_2 structure of the delafossite oxides yields markedly different electronic structures at their A- and BO_2-terminated surfaces which are either electron- (A-termination) or hole-doped (BO_2-termination) with respect to the bulk[1]. A prominent example is $PdCoO_2$ where a giant Rashba effect can be observed on the CoO_2 terminated surface[2], while the Pd terminated surface hosts ferromagnetic states which are absent in the bulk[3,4]. However, the study of these states has often been hampered by the size of domains of each distinct surface termination. Here we show how these problems can be circumvented using micro-ARPES performed in a spatially-resolved mode. Our measurements further reveal strong signatures of self-energy modulations on both surfaces due to coupling to bosonic modes, making them the ideal playground to study varying coupling mechanisms and their tunability in the same sample. [1]A. P. Mackenzie, Rep. Prog. Phys. 80, 032501 (2017), [2]V. Sunko et al., Nature 549, 492-496 (2017), [3]F. Mazzola et al., PNAS 115(51)12956-12960 (2018), [4]F. Mazzola et al., npj Quantum Materials 7, 20 (2022)

O 59.9 Wed 17:15 REC C 213

The Meservey-Tedrow-Fulde vortex in epitaxial aluminum near the monolayer limit — •Werner M.J. van Weerdenburg[1], Anand Kamlapure[1], Eirik Fyhn Holm[2], Niels P.E. van Mullekom[1], Xiaochun Huang[1], Manuel Steinbrecher[1], Peter Krogstrup[3], Jacob Linder[2], and Alexander A. Khajetoorians[1] — [1]Institute for Molecules and Materials, Radboud University Nijmegen, the Netherlands — [2]Center for Quantum Spintronics, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway — [3]NNF Quantum Computing Programme, Niels Bohr Institute, University of Copenhagen, Denmark

The critical magnetic field of 2D superconductors is greatly enhanced for fields parallel to the 2D plane. In the case of aluminum, this gives rise to a spin-splitting of the coherence peaks, referred to as the Meservey-Tedrow-Fulde (MTF) effect. In the MTF regime, it has been proposed that unconventional odd-frequency (ω_o) spin-triplet pairing is promoted [1], but their presence is experimentally hard to detect. Here, we study vortices in thin epitaxial Al films on Si(111) in the MTF regime by applying a vector magnetic field with a large in-plane component, and find experimental evidence of odd-frequency pairing [2]. Strikingly, we find that the shape of the vortex structure is strongly modified and exhibits a gapless region. Numerical simulations confirm a connection between this vortex shape and the presence of ω_o pairing, highlighted by a paramagnetic Meissner effect.

[1] J. Linder & J. Robinson, Scientific Reports **5**, 15483 (2015)
[2] W. van Weerdenburg et al., arXiv:2210.10645 (2022)

O 59.10 Wed 17:30 REC C 213

Exploring polaron stability and defect structures in $Li_4Ti_5O_{12}$ (LTO): A combined theoretical and experimental approach — •Yu-Te Chan[1], Matthias Kick[2], Cristina Grosu[2], Christoph Scheurer[1], and Harald Oberhofer[3] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Massachusetts Institute of Technology, Cambridge, USA — [3]University of Bayreuth, Bayreuth, Germany

Spinel $Li_4Ti_5O_{12}$ (LTO) is a promising anode material for next-generation all-solid-state Li-ion batteries (ASSB) due to its "zero strain" charge/discharge behavior. Pristine LTO suffers from poor ionic and electronic conductivity. Oxygen vacancies, produced by tailored sintering protocols, yield a performant, blue LTO material. Vacancy induced polarons have been proposed as one of the origins of increased electronic conductivity. However, detailed knowledge about polaron stability, distribution, and dynamics in LTO bulk and surface have been lacking. By performing *Hubbard corrected density functional theory* (DFT+U) calculations we are able to show that in fact polaron formation and a possible polaron hopping mechanism can not only play a significant role in enhancing electronic conductivity but boost Li^+ diffusion nearby, in line with the experimentally observed improved conductivities.[1,2] In combination with positron lifetime spectroscopy data and machine learning models, we arrive at a rather complete picture of the bulk vs. surface defect chemistry in LTO particles and the resulting mixed ionic electronic conductivity. [1] M. Kick et al., J. Phys. Chem. Lett. 11 (2020), 2535 [2] M. Kick et al., ACS Appl. Energy Mater 4 (2021), 8583