O 95: Electronic Structure of Surfaces II: Spectroscopy, Surface States

Time: Thursday 15:00–17:30 Location: MA 144

O 95.1 Thu 15:00 MA 144

Towards Robust Dichroism in Angle-Resolved Photoemission Spectroscopy — •Jakub Schusser[1], Hibiki Orio[1], Maximilian Ünzelmann[1], Johannes Hessdörfer[1], Muthu P.T. Masilamani[1], Florian Diekmann[2,3], Kai Rossnagel[2,3], and Friedrich Reinert[1] — [1]Experimentelle Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, D-97074 Würzburg, Germany — [2]Ruprecht Haensel Laboratory, Deutsches Elektronen-Synchrotron DESY, D-22607 Hamburg, Germany — [3]Institute of Experimental and Applied Physics, Kiel University, D-24098, Germany

Dichroic techniques in angle-resolved photoemission spectroscopy are highly relevant in the field of topological materials, layered systems, etc. Dichroism is per se a matrix-element effect that depends on the initial and final states as well as the light-matter interaction. However, accessing the information about the initial state of the solid directly has so far not been possible. By comparing both experimental and theoretical SPR-KKR soft X-ray data in bulk WSe_2 we show the robustness of the newly introduced dichroic technique against variation of photon energy, light polarization and angle of incidence. Such robustness of the matrix-element effect hints at a leap towards accessing the initial state properties directly and encourages further investigation.

O 95.2 Thu 15:15 MA 144

Dichroic Photoemission Tomography of Orbital Vortex Lines in a Topological Semimetal — •Maximilian Ünzelmann[1], Tim Figgemeier[1], Philipp Eck[2], Begmuhammet Geldiyev[1], Philipp Kagerer[1], Jakub Schusser[1], Domenico Di Sante[3], Giorgio Sangiovanni[2], Friedrich Reinert[1], and Hendrik Bentmann[4] — [1]Experimentelle Physik 7 and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg — [2]ITPA Würzburg and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg — [3]Department of Physics and Astronomy, Univerity of Bologna — [4]Center for Quantum Spintronics, Department of Physics, NTNU, Norway

In this talk, we report on the discovery of orbital vortex lines (OVL) in the three-dimensional (3D) band structure of a topological semimetal. Using dichroic photoemission tomography, i.e., linear and circular dichroism applied at bulk-sensitive soft x-ray photon energies [1], we directly observe vortices of atomic orbital angular momentum (OAM) and trace their trajectories in full 3D momentum space. In the core of the OAM vortex we resolve a two-fold spin-degenerate Weyl nodal line [2]. The experimental data is supported by density functional theory as well as photoemission intensity calculations. Taken together, our experiments achieve the first imaging of non-trivial quantum-phase winding at line nodes.

[1] M. Ünzelmann et al., Nat. Commun., 12, 3650 (2021)
[2] M. Hirschmann et al. Phys. Rev. Mat., 5, 054202 (2021)

O 95.3 Thu 15:30 MA 144

Circular dichroism by core-level angle-resolved photoemission: Application of multiple and single-site scattering theory — •Trung-Phuc Vo[1], Olena Tkach[2,3], Sylvain Tricot[4], Didier Sébilleau[4], Olena Fedchenko[2], Hans-Joachim Elmers[2], Gerd Schönhense[2], and Ján Minár[1] — [1]New Technologies - Research Center, Univ West Bohemia, 30100 Pilsen, Czech Republic — [2]Johannes Gutenberg-Universität, Institut für Physik, 55128 Mainz, Germany — [3]Sumy State Univ, 40007 Sumy, Ukraine — [4]Univ Rennes, CNRS, IPR (Institut de Physique de Rennes), F-35000, Rennes, France

Photoelectron diffraction (PED) is a powerful and driving experimental technique for resolving surface structures with sub-ångstrom resolution, namely bonding geometries of atoms and the local environment of impurity or dopant atoms inside surfaces. In high energy regime, PED effects are found in ARPES measurements beside other obstacles (low cross-sections, large photon momentum transfer, non-negligible phonon scattering). Here, to disentangle these diffraction influences and pronounced Kikuchi patterns, we present a PED implement for SPRKKR package which makes use of multiple scattering theory and one-step model in photemission process. In contrast to the other real space implementations of the multiple scattering PED formalism, we propose to use k-space implementation based on the layer KKR method. The main advantage is that we can without convergence problems (wrt. the angular momentum and cluster size) address very broad kinetic energy range (20-8000eV). A so-called alloy analogy model can be utilized to simulate XPD at finite temperatures.

O 95.4 Thu 15:45 MA 144

VUV Polarimeter for Inverse Photoemission — •Pascal Jona Grenz, Patrick Geers, Lennard Strompen, and Markus Donath — Physikalisches Institut, Universität Münster, Germany

In photoemission (PE) experiments, the use of polarized light for excitation provides access to orbital information of the electronic states under investigation. In inverse photoemission (IPE), the equivalent is the analysis of the polarization of the emitted light. So far, this light-polarization analysis was neglected due to the much lower cross-section in IPE compared with PE and the lack of suitable optics in the VUV (vacuum ultraviolet) spectral range.

In this contribution, we present a VUV polarimeter for IPE. A mirror with a polarizing coating of high reflectivity in Brewster angle geometry is used. With the high reflectivity and polarization power, this provides an easy-to-use attachment to the established photon detector [1]. We performed IPE measurements of the well-studied Cu(111) surface state by detecting *p*- and *s*-polarized light separately. The data show a strong dependence of the photon intensity on the polarization directions. Our results are in accordance with polarization-dependent PE measurements of the occupied part of the surface state [2].

[1] Thiede *et al.*, Meas. Sci. Technol. **29**, 065901 (2018)
[2] Mulazzi *et al.*, Phys. Rev. B **79**, 165421 (2009)

O 95.5 Thu 16:00 MA 144

Double Photoemission of C_{60} on $SrTiO_3$(001) with pulsed laser radiation — •Kathrin Plass[1], Robin Kamrla[1], Frank O. Schumann[2], and Wolf Widdra[1] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), Germany — [2]Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

Via photoelectron spectroscopy, important insights into the electronic structure of solids were obtained. However, correlation effects can only be addressed indirectly. With double photoemission spectroscopy (DPE), such phenomena can be observed directly by detecting pairs of correlated photoelectrons emitted upon absorption of a single photon [1]. C_{60} is classified as a strongly correlated material with a highly structured valence band. In this contribution we present DPE data for C_{60} thin films on $SrTiO_3$(001), obtained by a laboratory high-order harmonic (HHG) light source, operating at MHz repetition rates [2]. For different photon energies, we analyze the 2D energy maps of correlated electron pairs and compare the resulting sum energy spectra to simulations using a two-electron density of states [3,4]. This allows us to determine orbital-resolved two-electron binding energy shifts in C_{60} for the first time.

[1] J. Berakdar et al., Phys. Rev. Lett. **81**, 3535 (1998)
[2] A. Trützschler et al., Phys. Rev. Lett. **118**, 136401 (2017)
[3] M. Cini, Solid State Communications **24**, 681 (1977)
[4] G. A. Sawatzky, Phys. Rev. Lett. **39**, 504 (1977)

O 95.6 Thu 16:15 MA 144

On the unoccupied electronic structure of Fe_3O_4(100) — •Jan Bieling and Markus Donath — Universität Münster, Germany

The (100) surface of magnetite (Fe_3O_4) undergoes a $(\sqrt{2} \times \sqrt{2})R45°$ reconstruction. While its occupied states have been extensively investigated, studies addressing the empty ones are lacking.

We examined the unoccupied electronic structure of a pristine and well-characterized Fe_3O_4(100) surface by angle-resolved inverse photoemission. A threefold split, almost non-dispersive 3*d*-related spectral feature is observed. It is attributed to band groups originating from tetrahedrally and octahedrally coordinated iron atoms. The latter give rise to two spectral features since the t_{2g} and e_g orbitals are non-degenerate due to crystal-field splitting.

Based on our present study, we showcase the inherent limitations of using the second derivative to analyze electron spectroscopical data. Extracted peak positions can significantly deviate from the underlying ones, as demonstrated by synthetically generated spectra.

O 95.7 Thu 16:30 MA 144

Unusual Behavior of the Spin-Split L-Gap Surface Resonance at Pt(111) — •Fabian Schöttke, Peter Krüger, and Markus Donath — Universität Münster, Germany

We investigate the unoccupied electronic structure of Pt(111) with focus on the surface resonance (SR) at the bottom of the L gap. SR is discussed in the literature to be either typically free-electron like or hybridized with bulk states [1]. With different approaches within density-functional theory, we demonstrate that the lattice constant is crucial for the energetic position and dispersion behavior of SR. For experimentally obtained structural parameters as derived from low-energy electron diffraction studies [2], the hybridization-induced shape of SR results. In the case of hybridization, close to $\overline{\Gamma}$, a downward dispersing branch of SR splits off with predominantly one spin direction. This behavior is a distinct deviation of the usual parabolic upward dispersing L-gap surface states. By spin- and angle-resolved inverse photoemission, we measure the dispersion of SR in close vicinity to $\overline{\Gamma}$ and find a scenario of spin-split spectral features in agreement with the aforesaid theoretical results. Furthermore, we elucidate how the position of SR at the bottom of the L gap leads to hybridization with the d bands in comparison with L-gap surface states/resonances at other fcc(111) surfaces [3].

[1] A. Dal Corso, Surface Science **637-638**, 106 (2015).
[2] L. Hammer, T. Kißlinger, A. Schneider, private communication.
[3] Braun & Donath, Europhys. Lett. **59**, 592 (2002).

O 95.8 Thu 16:45 MA 144

On the unoccupied electronic structure of Hf(0001) — •Lennard Strompen[1], Vincent Reinartz[1], Sven Schemmelmann[1], Karol Hricovini[2], Saleem Khan[3], Jan Mínar[3], and Markus Donath[1] — [1]Universität Münster, Muenster, Germany — [2]CY Cergy Paris University, Paris, France — [3]University of West Bohemia, Pilsen, Czech Republic

Spin-orbit-induced effects are of particular importance in the surface electronic structure of high-Z materials. In our study, we focus on the unoccupied electron states at the so far unexplored Hf(0001) surface. The first challenge was to prepare a well-ordered and clean Hf(0001) surface, which, according to the literature, is known to show considerable impurities, in particular oxygen. After having developed a successful preparation recipe, we used spin- and angle-resolved inverse photoemission to determine the energy vs wavevector dispersion of the unoccupied states along the high-symmetry directions $\overline{\Gamma\mathrm{M}}$ and $\overline{\Gamma\mathrm{K}}$. Besides bulk-related spectral features and an image-potential-induced surface state, we identify surface-related features, which are interpreted on the basis of calculations of the electronic structure.

O 95.9 Thu 17:00 MA 144

Electronic structure of the $(\sqrt{3}\times\sqrt{3})R30°$ $TlAg_2$ surface alloy on Ag(111) — •Sven Schemmelmann[1], Patrick Härtl[2], Peter Krüger[3], Matthias Bode[2], and Markus Donath[1] — [1]Physikalisches Institut, Universität Münster — [2]Physikalisches Institut, Experimentelle Physik II, Universität Würzburg — [3]Institut für Festkörpertheorie, Universität Münster

The $BiAg_2$ surface alloy on Ag(111) exhibits a giant Rashba splitting which is one order of magnitude larger than the splitting of the L-gap surface state on Au(111) [1]. We investigate the unoccupied electronic structure of the similar $(\sqrt{3}\times\sqrt{3})R30°$ $TlAg_2$ surface alloy by scanning tunneling spectroscopy (STS) and angle-resolved inverse photoemission (IPE) [2]. We observe two dominant empty-state electronic features, which are attributed to downward dispersing s, p_z-derived states and to states with p_z orbital symmetry, respectively. On the basis of bandstructure and charge distribution calculations, we discuss the variation of the binding energies of the respective electronic features observed by STS and IPE.

[1] Ast et al., Phys. Rev. Lett. 98, 186807 (2007)
[2] Härtl et al., Phys. Rev. B 107, 205144 (2023)

O 95.10 Thu 17:15 MA 144

Insights into the dominant confinement mechanism and a spatially inhomogeneous broadening effect in quantum corrals — •Marco Weiss, Michael Schelchshorn, Fabian Stilp, Alfred J. Weymouth, and Franz J. Giessibl — Institute of Experimental and Applied Physics, University of Regensburg, Universitätsstraße 31, 93053 Regensburg

Understanding the factors influencing the lifetime of electronic states in artificial quantum structures is of great significance for advancing quantum technologies. This study focuses on CO-based quantum corrals on a Cu(111) surface. Tunneling spectroscopy measurements revealed a strong correlation between the size of the quantum corral and spectral width, characterized by a predominant Gaussian line shape. We attribute this dominant Gaussian-shaped lifetime broadening to the interaction of surface state electrons with the corral boundary.

To further investigate this phenomenon, we constructed corrals of the same size but varying wall densities. Our findings indicate that the energetic behavior of resonant eigenstates in a quantum corral is predominantly dictated by elastic processes, such as tunneling, rather than lossy interactions with the wall, like bulk coupling or inelastic scattering.

Due to our characterization of the interaction between resonant electrons states and their confining boundary, the observations made in our work enhance the understanding of lifetime limiting factors in artificial quantum structures, paving the way for more predictive simulations and more controllable quantum systems.