O 93: Electronic structure of surfaces: Spectroscopy, surface states III

Time: Friday 9:30–12:00 Location: HSZ/0201

O 93.1 Fri 9:30 HSZ/0201

Identifying Electronic Doorway States in Secondary Electron Emission — •Anna Niggas[1], Maosheng Hao[2], Peter Richter[3], Felix Blödorn[1], Florian Simperl[1], Alessandra Belissimo[4], Joachim Burgdörfer[2], Thomas Seyller[3], Wolfgang Werner[1], Florian Libisch[2], and Richard A Wilhelm[1] — [1]Institute of Applied Physics, TU Wien, Vienna, Austria — [2]Institute for Theoretical Physics, TU Wien, Vienna, Austria — [3]Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany — [4]Institute of Photonics, TU Wien, Vienna, Austria

Secondary electron emission following low-energy (<200 eV) electron impact is fundamental to particle-solid interactions but remains incompletely understood. While high-energy electrons are described by reflected primaries undergoing inelastic losses, the low-energy (<20 eV) region is often considered featureless. Coincidence spectroscopy has revealed hidden structures, notably the 3.3 eV X peak in graphite arising from plasmon excitation and interlayer-state hybridisation. Following that, we have measured low-energy secondary electrons from graphite and quasi-freestanding single- and bilayer graphene, enabling a controlled transition from bulk to two-dimensional systems. We observe layer-dependent features and, supported by density functional theory, attribute them to Feshbach-type resonances of quasi-bound above-vacuum states coupling to the continuum. The strong 3.3 eV resonance appears only in systems with five or more layers [1].

[1] A. Niggas et al., Phys. Rev. Lett. 135, 166401 (2025)

O 93.2 Fri 9:45 HSZ/0201

A novel approach to depth-resolved magnetic spectoscopy: grazing-incidence XMCD — •Umut Parlak[1], Katharina Wehrstein[1], Pia Maria Düring[1], Oliver Rehm[1], Endrit Kusari[1], David Capalbo[1], Andrei Gloskovskii[2], Christoph Schlueter[2], Lutz Baumgarten[3], and Martina Müller[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — [2]Deutsches Elektronen-Synchrotron, 22607 Hamburg, Germany — [3]Peter Grünberg Institut, PGI-6, Research Centre Jülich, 52425, Jülich, Germany

Magnetic depth profiling plays a key role in understanding inter- and intra-layer magnetic coupling mechanisms in multilayer thin films. We employ a synchrotron-based photoelectron spectroscopy approach (P22 beamline, DESY) to measure x-ray magnetic circular dichroism with depth-resolution taking EuO thin films grown on heavy metal (HM) underlayers as prototype sample. The presence of HM underlayer enables the near-total reflection x-ray excitation, where the incident and reflected x-rays interfere at the grazing angles forming high-intensity nodal points. The depth-resolution is achieved by probing at angles between 0.2 and 1°, i.e., tuning the position of the nodal points. Simulations of the x-ray intensity profile at these low angles allow us to optimize the MBE-grown MgO/EuO/HM trilayer structure for accessing both the upper and lower interfaces. Our results reveal the distribution of Eu^{2+} and Eu^{3+} ions throughout the EuO layer, which form ferromagnetic and paramagnetic oxides, respectively. The valency profile of the Eu ions directly aligns with the magnetic asymmetry profile.

O 93.3 Fri 10:00 HSZ/0201

Experimental Verification of the d-band Center Model in Au/Pt Systems: A Low-Energy XPS Study — •Justyna Piwowar[1,2,3] and Adam Lewera[3] — [1]Center for Quantum Nanoscience (QNS), Institute for Basic Science (IBS), Seoul 03760, Republic of Korea — [2]Ewha Womans University, Seoul 03760, Republic of Korea — [3]Faculty of Chemistry, University of Warsaw Pasteura 1 02-093 Warszawa

This work presents an experimental verification of the relationship between electronic structure and electrocatalytic properties in Pt-based materials, specifically critically evaluating the d-band center theory. Using Au-modified Pt as a model system, surface electronic properties were probed via X-ray Photoelectron Spectroscopy (XPS). We demonstrate that employing low-energy X-ray sources (Zr Mγ, 151 eV) provides superior surface sensitivity compared to standard sources (~1500 eV), allowing for the detection of subtle surface electronic shifts otherwise masked by bulk signals.

We observed a nonlinear evolution of electronic properties in Au/Pt thin films, specifically in core-level binding energies, which correlates with synergistic catalytic activity in formic acid oxidation. Detailed analysis of the valence band spectra reveals that significant modifications in the Density of States (DOS) near the Fermi level can occur even when the calculated shift in d-band center is negligible, due to spectral redistribution on both sides of the centroid. These findings indicate that the d-band center parameter alone may be insufficient to describe complex electronic structure modifications.

O 93.4 Fri 10:15 HSZ/0201

Spin Polarization of Photoelectrons Excited by Deep-UV Pulses with Orbital Angular Momentum — •Paul Valerian Möllers, Ruwen Quenter, and Helmut Zacharias — Center for Soft Nanoscience, Universität Münster

It is well known that circularly polarized light can excite longitudinally spin-polarized photoelectrons from centrosymmetric crystal surfaces [1]. The light carries an angular momentum of $\pm\hbar$, and the selection rules dictate that the photoexcitation occurs into final states with a specific total angular momentum. In the presence of spin–orbit interaction, states with different total angular momenta are energetically separated, and the excited electrons can exhibit a net spin imbalance. Light with helical wave fronts carries orbital angular momentum as a degree of freedom that is independent of its polarization and not limited to $\pm\hbar$ [2]. As the light always acts on the orbital electron angular momentum during photoexcitation, it appears plausible to assume that the optical orbital angular momentum could translate into a nonzero photoelectron spin polarization. This hypothesis has yet to be tested experimentally. We present preliminary results of spin-resolved photoemission measurements on Cu(111) and Au(111) surfaces that address this issue. [1] G. Borstel, M. Wöhlecke, Phys. Rev. B 26, 1148-1155 (1982) [2] S. S. R. Oemrawsingh et al., Appl. Opt. 43, 688-694 (2004)

O 93.5 Fri 10:30 HSZ/0201

Imaging stripe dynamics in superconducting nickelate — •Uladzislau Mikhailau[1], Luke C. Rhodes[1], Matthias Hepting[2], Masahiko Isobe[2], Pascal Puphal[2], and Peter Wahl[1,3] — [1]University of St Andrews, St Andrews, United Kingdom — [2]Max-Planck-Institute for Solid State Research, Stuttgart, Germany — [3]Physikalisches Institut, Universitat Bonn, Germany

In the Hubbard model, there is a competition between charge localization due to Coulomb repulsion and delocalization due to the energy reduction from electrons hopping between sites. When both tendencies are equally strong, a unique correlated stripe order can be stabilized [1]. Such a state is known to be realized in lightly doped high temperature superconducting cuprates and in nickelates.

Our STM investigation shows that commensurate stripe order forms in the metallic state of the recently discovered high-temperature superconductor $La_4Ni_3O_{10}$. Quasi-1D channels of delocalized charge appear as solitonic domain walls in charge density probed by STM. Interestingly, electrons tunnelling from the tip can induce local stripe fluctuations, pointing at the weak pinning of the order to the lattice.

Observation of stripe orders in normal states of high temperature cuprates and nickelates suggests shared correlated physics as a precursor to high-temperature superconductivity in both systems. Such experimental evidence is a valuable foundation for investigations into the mechanism of high-temperature superconductivity in both systems.

[1] J. Zaanen and O. Gunnarsson. Phys. Rev. B, 40(10):7391-7394 (1989).

O 93.6 Fri 10:45 HSZ/0201

Surface Rashba effect influence on bulk states: test case on Au(111) — •Laurent Nicolaï[1], Ján Minár[1], Christine Richter[2,3], Olivier Heckmann[2,3], Laxman Nagi Redi[2,3], Sourour Ayari[1], Aki Pulkkinen[1], Mauro Fanciulli[2,3], and Karol Hricovini[2,3] — [1]University of West-Bohemia in Pilsen, Czeck Republic — [2]CY Cergy Paris Université, France — [3]Université Paris-Saclay, CEA, France

Au(111) crystals are commonly used in the Photo-emission Spectroscopy field to calibrate instruments. When coming to spin-resolved ARPES, one uses the well-known surface states, spin-split due to the Rashba effect [1,2], as a reference. Au(111) being a centro-symmetric material, it is commonly assumed that bulk sates are spin degenerate.

However, we here present measurements attesting a spin polarisation of bulk states within the valence band. The measurements are complemented with ab-initio calculations confirming the existence of bulk states' spin polarisation on a fundamental level.

[1] Yu A. Bychkov and E. I. Rashba, J. of Phys. C: Sol. St. Phys., 17:6039-6045, 1984 [2] S LaShell et al. , Phys. Rev. Lett. 77 3419, 1996

O 93.7 Fri 11:00 HSZ/0201

calcQPI - a tool to simulate quasiparticle interference — •Peter Wahl[1,2], Luke Rhodes[1], and Carolina de Almeida Marques[1] — [1]SUPA, School of Physics and Astronomy, University of St Andrews, United Kingdom — [2]Physikalisches Institute, Universität Bonn

Quasiparticle interference imaging (QPI) is a powerful tool to study the low energy electronic structure of quantum materials and one of a few methods that can provide phase-sensitive information about the superconducting order parameter of unconventional superconductors, but the interpretation of QPI often requires complex modelling. This talk introduces calcQPI[1,2] as a new tool for the realistic simulation of QPI measurements. CalcQPI allows for the calculation of QPI from tight-binding models for a wide range of quantum materials, including magnetic materials, topological insulators and unconventional superconductors. I will give an overview of its capabilities and a few examples of how it can be applied to real materials.

[1] P. Wahl, L.C. Rhodes, C.A. Marques, calcQPI: A versatile tool to simulate quasiparticle interference, SciPost Phys. Codebases 61 (2025). [2] P. Wahl, L.C. Rhodes, C.A. Marques, Codebase release 1.0 for calcQPI, SciPost Phys. Codebases 61-r1.0 (2025).

O 93.8 Fri 11:15 HSZ/0201

Defect-driven polarity compensation on weakly polar $BaTiO_3$ (001) and $SrTiO_3$ (001) surfaces. — •Darin Joseph[1], Llorenç Albons[4], Florian Ellinger[2], Michele Reticcioli[2,3], Martin Setvin[4], and Cesare Franchini[1,2] — [1]University of Bologna, Italy — [2]University of Vienna, Austria — [3]CNR-SPIN, L' Aquila, Italy — [4]Charles University, Prague , Czech Republic

$BaTiO_3$ (001) and $SrTiO_3$ (001), commonly classified as Tasker Type I and nonpolar, exhibit surface instability, as evidenced by A-site (Ba/Sr) adatoms and vacancies on cleaved surfaces observed in experiments. Density Functional Theory (DFT) calculations revealed the work function variation between the TiO_2 and AO terminations and an electric field in the vacuum of asymmetric slabs, which are typically associated with polar surfaces. Our study reveals that both perovskites exhibit weak polar stacking along the crystallographic axis, leading to surface charges on the pristine terminations and creating an unfavorable electrostatic environment. Our analysis shows that the experimentally observed A-site defects act as compensation mechanisms by counterbalancing these charges to restore charge equilibrium. Charge compensation occurs at 12.5% Sr adatom and 12% vacancy coverage for $SrTiO_3$ and at approximately 12-13% defect concentration for $BaTiO_3$. These theoretical values are consistent with the experimental defect concentrations.

O 93.9 Fri 11:30 HSZ/0201

3D Mapping of Photoelectron Diffraction Patterns at Very Low Energies — •O. Tkach[1], T.-P. Vo[2], D. Biswas[3], J. Liu[3], O. Fedchenko[1,4], T.-L. Lee[3], J. Minár[2], H.-J. Elmers[1], and G. Schönhense[1] — [1]Univ., Mainz — [2]Univ. of West Bohemia, Czech Republic — [3]Diamond Light Source, UK — [4]Goethe Univ. Frankfurt

The full-field recording architecture of momentum microscopes (MMs) efficiently captures the (E,k) valence band structure along with the corresponding dichroism and spin texture [1]. Here, we apply the same approach to photoelectron diffraction (PED) in the low-energy range. Capturing PED in a solid angle up to 2π, including the corresponding core-level CDAD [2] reveals a wealth of structure far beyond that of standard PED measurements. The experiments are compared with calculated three-dimensional (E,k_x,k_y) patterns obtained via one-step photoemission calculations using the PED implementation [3] within the SPRKKR package. Calculated results over a wide range of kinetic energies ($106 - 1036$ eV) for the Ge 3d core level reveal striking patterns that change rapidly with photon energy. The high-energy end provides insight into bulk (Kikuchi-) diffraction, while the lower end with its high surface sensitivity yields structural information about the surface. This is indicative of the transition from a localized core level to an itinerant, time reversed LEED photoemission final state. In general, these results bridge the gap between PED analysis and electronic structure investigations.

[1] Medjanik et al. Nat. Mater 16, 615 (2017); [2] Tkach et al. Ultramic. 250, 113750(2023); [3]Vo et al. npj Comput. Mater.11, 159(2025)

O 93.10 Fri 11:45 HSZ/0201

Shaping Surface States: The Art of Designing Quantum Corrals — •Nadine Egger, Simon B. Hollweger, and Oliver T. Hofmann — Institute of Solid State Physics, TU Graz, Austria

Quantum corrals enable precise control over electron behavior on surfaces and can be designed to carry out tasks such as atomic-scale logic operations. However, determining the optimal corral shape and the precise placement of the individual building blocks is a nontrivial task. To address this, we introduce a simulation-based framework that automatically designs corral geometries to achieve specific functionalities. The approach combines surface-state electron simulations with an optimization algorithm that identifies not only the number of atomic building blocks required but also their optimal arrangement on the surface. As a first application, the framework is applied to design corrals capable of performing basic logic operations, such as AND or NOT gates. Beyond these examples, this method offers a versatile path toward creating atomically precise nanostructures with customized functional properties, paving the way for future developments in quantum device engineering.