O 67: Focus Session: Unoccupied States by Inverse Photoemission II

The Other Half of the Picture: 50 Years of Direct Access to Unoccupied States by Inverse Photoemission

In 1981, J. Pendry evaluated the experimental access to electron states in solids: "Currently only half of the picture can be seen with photoemission. Inverse photoemission provides the other half." A complete picture of electron states needs both occupied and unoccupied states in order to describe, understand, and finally tailor macroscopic material properties. In 1976, V. Dose had submitted a first paper on Bremsstrahlung Isochromat Spectroscopy in the VUV range: "The physics involved may be most simply described as an inverse photoelectric effect." The first experiments provided surface-sensitive information on the density of unoccupied states. Later, momentum and spin resolution were added to investigate the spin-dependent E(k) dispersion of unoccupied electron states. During five decades, the technique was further developed by several groups worldwide to enhance the intensity and improve the resolution in energy, momentum, and spin. A wealth of information was gained about metals, semiconductors, ultrathin films as well as adsorbate systems. The experimental studies were accompanied by several theoretical approaches, which are able to accurately describe the unoccupied electronic structure and model the inverse photoemission process. In 2012, H. Yoshida extended the energy range to the near-UV range (low-energy inverse photoemission), which is especially suited to study organic samples due to a lower damage risk caused by the exciting electron beam.

Current research fields for inverse photoemission are, e.g., spin textures of exchange- and/or spin-orbit-induced influenced systems and topological insulators, gap structures in transition metal dichalcogenides, LUMO levels in semiconductors for photovoltaic applications, electronic structure of atomic-layer and quantum materials. This focus session will highlight recent advances obtained by inverse photoemission in different fields and material systems. Also, it will bring together researchers from different areas for addressing current trends and future applications of inverse photoemission from experimental as well as theoretical perspective.

Organized by Markus Donath, Fabian Schöttke and Peter Krüger (U Münster).

Time: Wednesday 15:00–18:00 Location: WILL/A317

Invited Talk O 67.1 Wed 15:00 WILL/A317

New frontiers of one step model of photoemission for quantum materials — •Jan Minar — New Technologies Research Center, University of West Bohemia in Pilsen, Pilsen, Czechia

Quantum materials feature intertwined electronic correlations, topology, and magnetism, requiring realistic treatments of spin-orbit coupling, interactions, and spin fluctuations. Spin- and time-resolved ARPES (STARPES) is a key probe of their electronic and spin structures, but its quantitative interpretation demands advanced theory. I will present a fully relativistic multiple-scattering Green function (KKR) [1] framework for spin-dependent photoemission that incorporates correlations via DMFT, spin fluctuations via the alloy-analogy model, and light-induced electronic excitations [2,3]. Applications include a one-step photoemission description of altermagnets such as RuO* and MnTe, where spin-ARPES reveals lifted Kramers degeneracy relevant for spintronics, and kagome magnets such as FeSn thin films, where persistent flat-band splitting and selective band renormalization expose strong correlation and topological effects. This framework provides a unified route to unravel spin dynamics in complex quantum materials [4,5,6].

References: [1] H. Ebert et al., Rep. Prog. Phys. 74, 096501 (2011) [2] J. Minár et al., Phys. Rev. B 102, 035107 (2020). [3] J. Braun et al., Physics Reports 749, 1 (2018). [4] J. Krempaský et al., Nature 626, 517 (2024). [5] A.D. Din et al., arXiv:2511.01690 (2025) [6] Z. Ren et al., Nature Communications 15, 9376 (2024).

O 67.2 Wed 15:30 WILL/A317

Surface-orientation-dependent unoccupied electronic states of Fe_3O_4 — •Jan Bieling and Markus Donath — Universität Münster, Germany

Experimental studies of the occupied electronic states of magnetite (Fe_3O_4) have revealed that the observed properties, such as band dispersions, are strongly surface-orientation-dependent [1,2]. However, comparable systematic studies of the unoccupied electronic states of different Fe_3O_4 surfaces are still lacking.

We report on the unoccupied electronic states of a well-characterized $Fe_3O_4(111)$ surface using angle-resolved inverse photoemission and compare the results with our previous study of $Fe_3O_4(100)$ [3]. This direct comparison allows for (re)interpreting the spectral features observed for both surfaces.

Finally, we discuss our findings in the context of recent theoretical studies [4,5]. We report a very good agreement between our inverse photoemission spectra of $Fe_3O_4(100)$ and the theoretical results obtained from DFT+U+V for this surface.

[1] Y. Dedkov *et al.*, Phys. Rev. B **70**, 073405 (2004)
[2] W. Wang *et al.*, Phys. Rev. B **87**, 085118 (2013)
[3] J. Bieling and M. Donath, Phys. Rev. B **111**, 075117 (2025)
[4] N. Naveas *et al.*, J. Chem. Theory Comput. **19**, 8610-8623 (2023)
[5] N. Naveas *et al.*, Results Phys. **70**, 108158 (2025)

O 67.3 Wed 15:45 WILL/A317

Beyond the surface: Probing electronic structure with IPES in Valparaíso-Chile — Patricia Martínez[1], Rolando. Esparza[1], Jonathan Correa-Puerta[1], Valeria del Campo[1], Ricardo Henríquez[1], •Patricio Häberle[1], Sanber Viscaya[1], Eric Suárez-Morell[1], Patricio Vargas[1], Jean F. Veyan[2], Marcos Flores[3], and Samuel Hevia[4] — [1]Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso, Chile — [2]Department of Materials Science and Engineering, The University of Texas at Dallas, Richardson, Texas 75080, USA — [3]Physics Department, Facultad de Ciencias Físicas y Matemáticas, Universidad de Chile, Santiago, Chile — [4]Instituto de Física and CIEN-UC, Pontificia Universidad Católica de Chile, Av. Vicuña Mackenna 1860, Macul, Chile

Over the past few years, we have employed angle-resolved inverse photoemission spectroscopy (IPES) at the Valparaíso facility, utilizing both the isochromat mode and photon energy-resolving capabilities. This technique has enabled us to investigate systems exhibiting electronic structures modified by various forms of quantum confinement. We have characterized metallic thin films, carbon nanotubes, self-assembled monolayers (SAMs), and two-dimensional semiconductors. Whenever feasible, we have mapped unoccupied energy bands; however, in many instances, we have relied on simulations and inventive averaging to extract meaningful information from these low-symmetry nanoscale systems. A comprehensive overview of our experimental findings and future directions will be presented.

O 67.4 Wed 16:00 WILL/A317

Inverse photoemission studies of unoccupied electronic states of various Si(111)-based surfaces and interfaces — Younal Ksari, Hela Mrezguia, and •Jean-Marc Themlin — CNRS, Aix-Marseille Univ. University of Toulon, Marseille, France

We operate in Marseille an angle-resolved inverse photoemission (ARIPES) setup working in the isochromat mode. To illustrate the potential of this highly surface-sensitive technique, we give a comparative overview of the unoccupied part of the electronic structure of several Si(111)-based interfaces as revealed by ARIPES, from the hydrogenated H:Si(111) to 2D silicene monolayers grown on passivated Si(111) substrates.

The H-saturated (1x1) termination of Si(111) solely reveals bulk conduction band states. Upon segregation (B) or adsorption (H, As, Au) of foreign atoms on Si(111), specific surface states appear, leading to insulating (H, As, B) or metallic (Au) interfaces.

According to LEED, the adsorption of 1 ML of Si on the $\sqrt{3} \times \sqrt{3})R30°$ reconstructed Au- and B- substrates leads to the formation of a non-covalently bound Si bilayer, alias silicene, which adopts the symmetry of the passivated substrates. Specific unoccupied electronic states appear on each substrate, with dispersions profiles which do not exhibit a $\sqrt{3}\times\sqrt{3})R30°$ symmetry, small overall bandwidths and large bandgaps (resp. $>$ 2 eV and $>$ 1 eV), suggesting important correlation effects.

O 67.5 Wed 16:15 WILL/A317

Layer-Dependent Electronic Signatures of Tl on Ag(111) Revealed by Inverse Photoemission — •Sarah Laufer[1], Sven Schemmelmann[1], Yuichiro Toichi[2], Kazuyuki Sakamoto[2], and Markus Donath[1] — [1]Physikalisches Institut, Universität Münster — [2]Department of Applied Physics, The University of Osaka

The Tl/Ag(111) system is characterised by pronounced changes in its spatial and electronic structure when transitioning from sub-monolayer coverage to the monolayer [1,2] and further to the bilayer [3], making an accurate determination of the layer thickness essential. While low-energy electron diffraction and Auger electron spectroscopy provide valuable information on domain orientations and Tl coverage trends, neither technique allows an unambiguous identification of the bilayer. In contrast, inverse photoemission (IPE) gives direct access to unoccupied electronic states, which are highly sensitive to the Tl film thickness. We show that Tl/Ag(111) exhibits distinct layer-dependent unoccupied states whose characteristic intensity evolution with increasing Tl coverage enables a clear identification of the bilayer. These results highlight the particular strength of IPE as a layer-specific probe for ultrathin metallic films.

[1] P. Härtl *et al.*, Phys. Rev. B **107**, 205144 (2023)
[2] S. Schemmelmann *et al.*, Phys. Rev. B **109**, 165417 (2024)
[3] T. Kobayashi *et al.*, Nano Lett. **23**, 7675-7682 (2023)

O 67.6 Wed 16:30 WILL/A317

Modeling a transient Dirac-like surface state in Floquet-driven SnTe — •Aki Pulkkinen[1], Frédéric Chassot[2], Hugo Dil[3], Claude Monney[2], and Ján Minár[1] — [1]New Technologies-Research Centre, University of West Bohemia in Pilsen, Czechia — [2]Department of Physics and Fribourg Center for Nanomaterials, Université de Fribourg, Switzerland — [3]Institute of Physics, Ecole Polytechnique Fédérale de Lausanne, Switzerland

We present a theoretical analysis of the ultrafast transient cone-like dispersion observed in pump-probe photoemission experiments on SnTe[1]. A semi-infinite (111) surface Hamiltonian is constructed from a Wannier tight-binding model, and the surface Green's function is obtained using the recursive López-Sancho method[2] in extended Hilbert space. The effect of the pump pulse is introduced through a time-periodic Peierls substitution and a Jacobi-Anger expansion of the driven Hamiltonian into Floquet sectors. The Floquet-Green's-function calculations show that photoexcitation induces a transient hybridization between the Floquet replica of the valence band and the conduction band, producing a momentary band inversion at the surface. The inversion generates a short-lived Dirac-cone-like surface state, reproducing the main experimental feature. The results indicate that the transient cone originates from Floquet-induced reconstruction rather than structural or thermal effects, and demonstrate the role of strong periodic driving in reshaping surface electronic structure in SnTe. [1] F Chassot et al. 2025 arXiv:2502.11967 [2] M. P. Lopez Sancho et al. 1985 J. Phys. F: Met. Phys. 15 851

O 67.7 Wed 16:45 WILL/A317

Peak separation analysis for inverse photoelectron spectra: Comparing second derivative, curve fitting, and deconvolution — •ryotaro nakazawa[1,2], haruki sato[2], and hiroyuki yoshida[2] — [1]Institute for Molecular Science, Aichi, Japan — [2]Chiba University, Chiba, Japan

Inverse photoelectron spectroscopy (IPES) is a powerful technique for probing the unoccupied electronic states of materials. Recently developed low-energy inverse photoelectron spectroscopy (LEIPS) can significantly advance the study of unoccupied states, owing to minimal sample damage and suppressed dark counts compared to conventional IPES. However, the instrumental resolution remains at around 0.2 eV, which is one order of magnitude lower than that of photoelectron spectroscopy. Spectral broadening caused by the low instrumental resolution often results in overlapping peaks. Peak separation is therefore crucial in the analysis of LEIPS spectra. In this study, we compared three peak separation methods: second derivative, curve fitting, and deconvolution. These methods were applied to modeled and experimental LEIPS spectra of the lowest unoccupied molecular orbital-derived band of pentacene, which consists of two splitting peaks due to the two inequivalent molecules in the unit cell. We systematically and quantitatively evaluated the performance of each method in terms of analysis parameters and discussed its robustness to noise as well as its peak separation and detection capabilities. This work offers a practical framework for peak separation in LEIPS, with extensions to PES and a wide range of spectroscopies.

O 67.8 Wed 17:00 WILL/A317

The role of light polarization in inverse photoemission — •Marcel Holtmann, Pascal J. Grenz, and Markus Donath — Physikalisches Institut, Münster University, Germany

In inverse photoemission (IPE), electrons are directed onto a surface and the light emitted during radiative transitions into unoccupied states is detected. By detecting the emitted photons as a function of the kinetic energy of the electrons impinging at a defined angle of incidence, the dispersion of conduction-band states can be traced. We focus on the role of light polarization in IPE and how the simultaneous detection of photons with multiple detectors provides additional symmetry information.

In the spirit of "50 years of IPE", this talk aims to give an overview of this aspect of IPE analysis. Building on early work from the 1980s [1,2], we will present measurements of the AgTe/Ag(111) surface alloy. The polarization contrast allows us to identify the orbital character of spin-dependent unoccupied states. We will also discuss the recent improvement of our setup, in which a polarizing mirror was added to the photon detector [3], enabling us to select the detected light polarization.

[1] M. Donath *et al.,* Solid State Commun. **60**, 237 (1986)
[2] T. Fauster *et al.,* Phys. Rev. B **40**, 7981 (1989)
[3] P. J. Grenz *et al.,* Rev. Sci. Instrum. **96**, 033905 (2025)

O 67.9 Wed 17:15 WILL/A317

Sub-100 meV low-energy inverse photoelectron spectroscopy using an electrostatic monochromator — •Tomoko Onishi[1], Taichi Suruga[1], Daichi Honma[1], Masaya Kai[1], Issei Ishimori[1], François C. Bocquet[2], F. Stefan Tautz[2], Harald Ibach[2], and Hiroyuki Yoshida[1] — [1]Chiba University, Chiba, Japan — [2]Forschungszentrum Jülich, Jülich, Germany

Inverse photoelectron spectroscopy (IPES) is the optimal experimental method for probing unoccupied electronic states but its applicability has been limited by modest energy resolution. This resolution is determined by the convolution of the electron energy spread and photon-detector bandwidth. The best reported resolution to date is 165 meV, limited by the photon detector [1]. Low-energy IPES (LEIPS) [2], using an optical bandpass filter, achieves a photon-detection resolution of 38 meV. However, the total resolution remains limited to 250 meV due to electron-beam thermal broadening [3]. In this work, we report a LEIPS system with an electron source consisting of a LaB6 cathode, electrostatic monochromator, and deceleration lens system. This design is based on high resolution electron energy loss spectroscopy (HREELS). We modified it to deliver several hundred nA with a capability of energy scan for LEIPS [4]. An electron energy spread of 90 meV is obtained, resulting in a total LEIPS energy resolution of 98 meV. [1] M. Budke et al., Rev. Sci. Instrum. 78, 083903 (2007). [2] H. Yoshida, Chem. Phys. Lett. 539*540, 180 (2012). [3] H. Yoshida, J. Electron Spectrosc. Relat. Phenom. 204, 116 (2015). [4] H. Ibach et al., Rev. Sci. Instrum. 94, 043908 (2023).

O 67.10 Wed 17:30 WILL/A317

Towards high resolution IPES in the VUV range — Giacomo Merzoni[1], Samuele Comizzoli[1], Giacomo Panzera[1], Lucio Braicovich[1,2], and •Giacomo Ghiringhelli[1,3] — [1]Politecnico

di Milano, Italy — [2]ESRF, Grenoble, France — [3]CNR/SPIN, Politecnico di Milano, Italy

Since its concept was introduced and its feasibility was demonstrated, the conceptual interest of angle-resolved inverse photoemission (ARIPES) has not declined. Unfortunately, for decades technical challenges have kept ARIPES in a niche. At the same time direct photoemission, ARPES, has become a popular and unmissable technique for the determination of the electronic structure of solids. ARPES spectra are commonly measured with energy resolution better than 30 meV, a figure still unachieved in ARIPES. Which explains the different popularity of the two complementary techniques.

Is it possible to design today an ARIPES instrument that better exploits the technological progress undergone over the years by detectors and optical elements for VUV radiation, and by monocromatized electron-beam sources?

We present some ideas guiding the realization of an ARIPES apparatus working in the 20-100 eV energy range. Aiming at a combined instrumental bandwidth smaller than 50 meV, it is based on a high-luminosity grating spectrometer and a 2D position sensitive semiconductor detector.

O 67.11 Wed 17:45 WILL/A317

2D IPES intensity maps of MoS_2 — •Patricia Martínez-Rojas, Sanber Vizcaya, Rolando Esparza, and Patricio Häberle — Departamento de Física, Universidad Técnica Federico Santa María, Valparaíso, Chile

Inverse photoemission spectroscopy (IPES) offers direct access to the unoccupied electronic structure of solids and is particularly well suited for investigating layered transition-metal dichalcogenides such as MoS_2. We present momentum-resolved IPES measurements on a bulk 2H-MoS_2 single crystal, performed with a normal-incidence grating spectrometer operated at a fixed electron kinetic energy of 25.6 eV. The sample was prepared by ex-situ exfoliation and subsequently annealed, in UHV, up to 400°C to remove surface contaminants. By recording the photon intensity as a function of emission energy and incidence angle, we constructed two-dimensional maps of the unoccupied states along the ΓK and ΓM directions of the Brillouin zone. The data reveal several dispersive features whose energy-momentum dependence closely matches density-functional theory (DFT) band-structure calculations. In particular, the conduction-band minimum is experimentally found away from high-symmetry points, consistent with theoretical predictions. These results highlight the capability of momentum-resolved IPES to characterize the unoccupied band structure of MoS_2 and provide a benchmark for future studies of two-dimensional materials.