# O 76: Electronic structure of surfaces: Spectroscopy, surface states II

Time: Thursday 10:30–12:15 Location: HSZ/0201

O 76.1 Thu 10:30 HSZ/0201

**Angle-resolved photoemission spectroscopy study on AgTe/Ag/Au(111) heterostructures.** — •Muthu P. T. Masilamani, Sophia Munne, Begmuhammet Geldiyev, Maximilian Ünzelmann, and Friedrich Reinert — Experimental Physics VII and Würzburg-Dresden Cluster of Excellence ctd.qmat, Universität Würzburg, Germany

We report a comprehensive angle-resolved photoemission spectroscopy (ARPES) study on the electronic band structure of AgTe/Ag/Au(111) heterostructures. We systematically explore the interplay between Rashba-like spin-split surface states (SS) of AgTe [1] and quantum well states (QWS) of Ag/Au(111) [2] by epitaxially varying the Te coverage and the Ag spacer-layer thickness. This allows us to address the influence of epitaxial composition on the electronic structure. Our measurements reveal decoupling of the Rashba-like SS and QWS, with no observable hybridisation, attributed to their distinct orbital symmetries. Furthermore, we investigate the emergence of moiré reconstruction in the AgTe/Ag/Au(111) heterosystem.

[1] Ünzelmann, M. et al. PRL. 124, 176401 (2020)
[2] Forster, F. et al. PRB. 84, 075412 (2011)

O 76.2 Thu 10:45 HSZ/0201

**One-step investigation of the electronic tapestry of 2H-WSe2** — •Ridha Eddhib[1], Samuel Beaulieu[2], Aki Pulkkinen[1], and Jan Minar[1] — [1]New Technologies Research Centre, University of West Bohemia, 301 00 Pilsen, Czechia — [2]Université de Bordeaux-CNRS-CEA, CELIA, UMR5107, F33405 Talence, France.

Angle-resolved photoemission spectroscopy (ARPES) is a powerful tool for unraveling the electronic band structure of crystalline solids. However, the intricate and multifaceted electronic structures of complex materials often require complementary measurement strategies and careful experimental design. In our research, we employed the one-step model of photoemission, as implemented in the SPRKKR code[1], supported by experimental studies. We combined circular dichroism in photoelectron angular distributions (CDAD) with the layer-dependent symmetry properties of 2H-WSe2, which enables a time-reversal operation (TRCDAD)[2]. This approach quantifies the modulation of photoemission intensity across a wide energy range, providing detailed insight into the material's fine electronic structure while suppressing extrinsic contributions to the photoemission cross section to some extent. We present the monolayer, bilayer, and trilayer contributions to the photocurrent alongside the bulk response, while accounting for final-state effects using both time-reversed low-energy electron diffraction and a free-electron-gas final-state. [1]Ebert, H., Koedderitzsch, D., & Minar, J. (2011). Reports on Progress in Physics, 74(9), 096501. [2]Beaulieu, S., Schusser, ... & Ernstorfer, R. (2020). Physical Review Letters, 125(21), 216404.

O 76.3 Thu 11:00 HSZ/0201

**Spin-orbital signatures and topological evolution in the $Mo_x W_{1-x} Te_2$ alloy** — •Sarath Sasi[1], Aki Pulkkinen[1], Raphaël Salazar[1], Jakub Schusser[1], Laurent Nicolaï[1], Christine Ritcher[2,3], and Karol Hricovini[2,3] — [1]New Technologies Research Centre, University of West Bohemia, Pilsen, Czech Republic — [2]LPMS, CY Cergy Paris Université, Neuville-sur-Oise, France — [3]Université Paris-Saclay, CEA, CNRS, LIDYL, Gif-sur-Yvette, France

We examine how compositional disorder modifies the electronic structure of the transition-metal dichalcogenide alloy $Mo_x W_{1-x} Te_2$[1], with particular attention to the evolution of band topology and the persistence of Type-II Weyl features. Using high-resolution spin-polarized ARPES and circular-dichroism ARPES provides complementary insights into the spin and orbital character of the electronic states. These measurements give insight into its intrinsic spin-orbital properties compared to $WTe_2$[2], and for identifying how alloying is affecting its properties, like Berry curvature. Together with fully relativistic one-step photoemission calculations within the SPR-KKR[3] framework, we yield a detailed picture of how alloying tunes the electronic structure and topological responses in this family of quantum materials.

[1] Belopolski, I., Sanchez, D., Ishida, Y., et al. Nat. Commun. 7, 13643 (2016).
[2] Heider, T., Bihlmayer, G., Schusser, J., et al. Phys. Rev. Lett. 130, 146401 (2023).
[3] Braun, J., Minar, J., Ebert, H. Physics Reports, 740 (2018).

O 76.4 Thu 11:15 HSZ/0201

**electronic properties observation of kagome lattice Nb3X8 by angle-resolved photoemission spectroscopy** — •Xiaojing Liu[1], Antonija Grubisic-cabo[1], Joost aretz Aretz[2], Sergii Grytsiuk[2], Marco Bianchi[3], Malte Rosner[2,4], Mazhar Ali[5], Philip Hofmann[3], Zhiying Dan[1], Giovanna Feraco[1], Chrystalla Knekna[1,6], Muhammad Waseem[1], and Mikhail Katsnelson[2,7] — [1]University of Groningen, Groningen, The Netherlands — [2]Radboud University, Nijmegen, The Netherlands — [3]Aarhus University, Aarhus, Denmark — [4]Bielefeld University, Bielefeld, Germany — [5]Delft University of Technology, Delft, the Netherlands — [6]University of Amsterdam, Amsterdam, The Netherlands — [7]Constructor University, Bremen, Germany

The Nb3X8 family (X=Cl, Br, I) is a novel group of breathing kagome materials. Despite interest in these materials, their electronic properties are still unclear and are likely to differ among the family members. For instance, they could exhibit characteristics of either a strongly correlated Mott insulator or a weakly correlated obstructed atomic insulator. Moreover, the kagome lattice can naturally host flat bands, which give rise to exotic properties such as spin-liquids and high-temperature superconductivity. Here, I will present our recent experimental investigation of the band structure in bulk Nb3X8 kagome materials by means of angle-resolved photoemission spectroscopy (ARPES). With ARPES we directly image the flat bands in the Nb3X8 systems, and are able to verify their strong correlation character with the support of theoretical calculations.

O 76.5 Thu 11:30 HSZ/0201

**Studying the polar surfaces of MAX and MAB phases using $\mu$-ARPES** — •Gesa Siemann[1], Gianmarco Gatti[1], Amalie Svaneborg[5], Wu Bing[4], Anders S. Mortensen[1], Charlotte Sanders[2], Naina Kushwaha[2,6], Jenny Rigden[2], Yu Zhang[2], Matthew D. Watson[3], Kristian Thygesen[5], Zdeněk Sofer[4], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Aarhus University, DK — [2]Central Laser Facility, Harwell, UK — [3]Diamond Light Source, UK — [4]University of Chemistry and Technology Prague, CZE — [5]Department of Physics, Technical University of Denmark, Lyngby, DK — [6]School of Physics and Astronomy, St Andrews University, UK

Natural heterostructures with interlayer charge transfer in the bulk can exhibit distinctive surface effects when this transfer is interrupted, such as Rashba splitting and itinerant ferromagnetism, both absent in the bulk. These layered systems therefore provide a platform to study how charge redistribution and symmetry breaking shape the emerging surface electronic structure. Here, we introduce MAX and MAB phases as a promising material family to host similar effects due to their alternating MX and A layers. After cleaving the samples, we used photoemission experiments with a micrometer-scale light spot ($\mu$-ARPES), allowing us to reliably distinguish different surface terminations and their electronic structures. This work furthermore explores how covalency and metallicity govern charge transfer, and thus the surface electronic properties, in layered compounds.

O 76.6 Thu 11:45 HSZ/0201

**Spin-resolved momentum microscopy of $BiX_2$ surface alloys on Cu(111) and Ag(111) using a 2D imaging spin-filter** — •Fabian Göhler, Stefanie Suzanne Brinkman, Xin Liang Tan, Anders Christian Mathisen, Chul-Hee Min, and Hendrik Bentmann — Center for Quantum Spintronics, Department of Physics, Norwegian University of Science and Technology, 7491 Trondheim, Norway

Despite the rapid development of angle-resolved photoelectron spectroscopy (ARPES), measurements of the electron spin over wide regions in momentum space remain challenging with single-channel spin detectors. In this contribution, we present spin-resolved ARPES measurements from a momentum microscope, which gives the photoelectron momentum distribution over the full half-sphere above the sample surface. When combined with a 2D imaging spin filter [1], this allows parallel measurement of the in-plane spin polarization for full constant energy cuts $E(k_x, k_y)$. We acquired data on $BiX_2$/X(111) surface alloys - formed by 1/3 monolayer of Bi atoms arranged in a

$(\sqrt{3}\times\sqrt{3})R30^\circ$ periodicity on Cu(111) or Ag(111) - which are well established model systems for spin-orbit effects and (spin-dependent) photoemission from surfaces [2-4]. Using linearly polarized ($h\nu$ = 6.0 eV) and unpolarized ($h\nu$ = 21.2 eV) light sources, we probe the spin polarization in these systems for varying experimental conditions.

[1] C. Tusche et al., Ultramicroscopy 159, 520 (2015)
[2] R. Noguchi et al., Phys. Rev. B 95, 041111 (2017)
[3] H. Bentmann et al., Phys. Rev. Lett. 119, 106401 (2017)
[4] A. Winkelmann et al., New J. Phys. 14, 083027 (2012)

O 76.7 Thu 12:00 HSZ/0201

**Distinguishing bulk vs surface states from designed cleaving planes in ruthenium dioxide with ARPES** — •Maria Visscher[1,2], Lea Richter[1], Sebastian Buchberger[2], Shu Mo[2], Bruno Saika[2], Mats Leandersson[3], Craig Polley[3], Andrew Mackenzie[1,2], and Phil King[2] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]University of St Andrews, St Andrews, UK — [3]Max IV, Lund, Sweden

Ruthenium dioxide has a rich band structure, giving rise to phenomena like superconductivity under strain and hosting a Dirac nodal line network. Recent studies also found that the material hosts flat band surface states and unusual spin-polarisations. These phenomena motivate the need for more detailed studies into its electronic structure. ARPES would be an ideal probe for this, and there have been several pioneering studies to date. However, the material's strongly three-dimensional structure makes these experiments challenging because of difficulties both in preparing the required atomically flat and clean surfaces, and in disentangling bulk from surface states in the electronic structure. Here, we exploit a fabrication method based on Focused Ion Beam (FIB) structuring to stimulate cleaving along desired crystallographic planes. With this method, we obtained high quality surfaces in two distinct orientations, allowing high-resolution ARPES experiments. From this, and supporting density-functional calculations, we identify a rich hierarchy of bulk and surface states in this system and uncover a strong influence of structural relaxations and surface stoichiometry on the electronic states that form.