O 84: Electronic Structure of Surfaces I: Spectroscopy, Surface States

Time: Thursday 10:30–13:00 Location: MA 144

O 84.1 Thu 10:30 MA 144

A new beamline at the ASTRID2 synchrotron for spatially resolved ARPES — •Alfred Jones, Paulina Majchrzak, Zhihao Jiang, Klara Volckaert, Deepnarayan Biswas, Chakradhar Sahoo, Marco Bianchi, Nykola Jones, Søren Hoffmann, Philip Hofmann, Jill Miwa, and Søren Ulstrup — Aarhus University, Denmark

Increased scientific interest in 2D materials, heterostructures, and operational devices that incorporate quantum materials necessitates measurement techniques capable to isolating clear signals from such small and complex systems. Here, we present our new spatially resolved ARPES beamline at the ASTRID2 synchrotron, SGM4, where a <4 μm beam spot is produced using an elliptical capillary optic. We demonstrate the capability of this beamline using nanoARPES measurements on several example systems, such as in-operando ARPES from a 2D device.

O 84.2 Thu 10:45 MA 144

Recent progress in ToF-XPEEM and Momentum Microscopy: Theory and Experiment — •O. Tkach[1,2], Q. Nguyen[3], O. Fedchenko[1], S. Chernov[4], D. Kutnyakhov[4], F. Pressacco[4], J. Dilling[4,5], L. Bruckmeier[4,5], F. Scholz[4], M. Scholz[4], M. Hoesch[4], K. Rossnagel[4,5], H.-J. Elmers[1], and G. Schönhense[1] — [1]Univ., Mainz — [2]SumDU, Ukraine — [3]SLAC Nat. Accel. Lab., USA — [4]DESY, Hamburg — [5]CAU Kiel

Cathode-lens instruments (PEEM, LEEM, momentum microscopes MM) usually have a strong accelerating electric field in front of the sample. Here we present an alternative route towards good performance in k-imaging mode. It is based on *field shaping* in the region close to the sample by planar concentric ring electrodes. Ray-tracing reveals: (i) An accelerating lens in front of the sample reduces spherical aberration and field curvature, enabling large k-fields of view. (ii) A retarding lens can tune the field to zero, enabling studies of non-planar objects in zero field. (iii) Stronger retarding fields direct all slow electrons back to the surface, reducing space-charge effects in pump-probe experiments. Simulations are confirmed by first experiments at PETRA-III and FLASH.

O 84.3 Thu 11:00 MA 144

Control of the asymmetric band structure in Mn_2Au by a ferromagnetic driver layer — •Y. Lytvynenko[1,2], O. Fedchenko[1], S. Chernov[1,3], S. Babenkov[1], D. Vasilyev[1], O. Tkach[1], A. Gloskovskii[3], T. R. F. Peixoto[3], C. Schlueter[3], V. Grigorev[1], M. Filianina[1,4], S. Sobolev[1], A. Kleibert[5], M. Kläui[1], J. Demsar[1], G. Schönhense[1], M. Jourdan[1], and H.-J. Elmers[1] — [1]JGU Mainz, Germany — [2]Institute of Magnetism of the NAS and MES of Ukraine — [3]DESY, Germany — [4]Stockholm University, Sweden — [5]SLS, PSI, Switzerland

In this work, the hard X-ray angle-resolved photoemission spectroscopy (HARPES) reveals the momentum-resolved band structure in an epitaxial Mn_2Au(001) film capped by a 2 nm thick ferromagnetic Permalloy (Py) layer. By magnetizing the Py layer, the exceptionally strong exchange bias aligns the Néel vector (NV) in the Mn_2Au film leading to changes in the electronic properties. Uncompensated Mn interfacial magnetic moments in Mn_2Au are identified as the origin of the exceptional exchange bias using XMCD in combination with PEEM. Using time-of-flight momentum microscopy, we measure the asymmetry of the band structure in Mn_2Au resulting from the homogeneous orientation of the NV. Comparison with theory shows that the NV, determined by the magnetic moment of the top Mn layer, is oriented antiparallel to the Py magnetization. Our experimental results demonstrate that HARPES can measure the band structure of epitaxial layers beneath a metallic capping layer. We thus confirm that the ferromagnetic capping layer controls the bulk band structure of the AFM film.

O 84.4 Thu 11:15 MA 144

Surface atomic and electronic structure of multiferroic GeTe(111) — •Martin Heinrich[1,2], Juraj Krempasky[1], Gunther Springholz[3], and Matthias Muntwiler[1,2] — [1]Paul Scherrer Institute, Photon Science Division, 5232 Villigen PSI, Switzerland — [2]Swiss Nanoscience Institute, University of Basel, 4056 Basel, Switzerland — [3]Institute of Semiconductor Physics, Johannes Kepler University Linz, 4040 Linz, Austria

Multiferroic materials combine multiple coupled ferroic orders in the same system which could be used to bridge the gap between traditional electronics and spintronics. GeTe is a IV-VI semiconductor with multiple existing applications in optoelectronics and thermoelectrics. It recently gained renewed attention due to the discovery of a large Rashba spin splitting in both bulk and surface states that couples to the ferroelectric polarization. A detailed study of its surface atomic and electronic structure is therefore of high relevance towards a deeper, atomic scale understanding of the relevant interactions.

In this contribution, we discuss synchrotron based photoelectron diffraction (XPD, PhD) data combined with multiple scattering calculations, which indicate a contracted surface layer structure of GeTe(111) compared to its bulk structure. Additionally, scanning tunneling microscopy (STM) measurements reveal triangular island growth and a hexagonal atomic surface structure. dI/dV spectroscopy probes the local density of states, which we compare to spatially averaged photoelectron spectra. We identify the Rashba split surface states and resolve their spatial distribution.

O 84.5 Thu 11:30 MA 144

Spin Texture in Honeycomb Monolayers AgTe/Ag(111) and CuTe/Cu(111) — •Begmuhammet Geldiyev[1], Maximilian Ünzelmann[1], Philipp Kagerer[1], Jakub Schusser[1], Hendrik Bentmann[2], and Friedrich Reinert[1] — [1]Experimentelle Physik 7 and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg — [2]Center for Quantum Spintronics, Department of Physics, NTNU, Norway

In this contribution we will investigate the spin texture of honeycomb monolayers CuTe and AgTe [1] grown on Cu(111) and Ag(111), respectively. In case of both materials, our spin-resolved ARPES measurements suggest the existence of Rashba-like spin texture, which originates from the broken inversion symmetry at the surface. Moreover, we here for the first time observe the Rashba-like spin splitting in CuTe/Cu(111). Prior, it could not be seen in spin-integrated ARPES and we deduce a value of 0.25 ± 0.05 eV Å for the Rashba constant. It is approximately a factor of 4 smaller compared to the case of AgTe, almost equal to the relative factor between Rashba constants of Cu_2Bi and Ag_2Bi alloys [2]. In addition, we elaborate on the formation of out-of-plane spin polarization which can be induced by the underlying honeycomb lattice structure.

[1] M. Ünzelmann et al., Phys. Rev. Lett. 124, 176401 (2020)
[2] H. Bentmann et al., EPL 87, 37003 (2009)

O 84.6 Thu 11:45 MA 144

Exploring the topologically dark surface of a layered weak 3D topological insulator — •Johannes Hessdörfer[1,2], Maximilian Ünzelmann[1,2], Eduardo Carillo-Aravena[2,3], Armando Consiglio[2,4], Michael Ruck[2,3], Domenico Di Sante[5], and Friedrich Reinert[1,2] — [1]Experimentelle Physik VII, Universität Würzburg, Germany — [2]Würzburg-Dresden Cluster of Excellence ct.qmat, Germany — [3]Anorganische Chemie II, Technische Universität Dresden, Germany — [4]Theoretische Physik I, Universität Würzburg, Germany — [5]University of Bologna, Italy

Weak three-dimensional (3D) topological insulators (TI) can be considered as a stack of 2D TIs separated by insulating spacer layers. In the family of $Bi_{14}Rh_3I_9$ based [1] weak TIs, the electronic properties can be modified by altering the spacer layer through substitution. Here, we investigate the compound $Bi_{12}Rh_3Ag_6I_9$, by means of photoemission experiments and density functional theory band structure calculations. The results indicate the presence of surface states within the projected bulk band gap of the topologically dark surface which might alter the topological properties there. These states can be assigned to originate from the two different types of layer terminations. By analyzing the I 4d peak in the X-ray core level spectra, we show how the surface termination can be controlled, e.g. by the cleaving temperature.

[1]Rasche et al., Nat. Mater, 12, 422-425 (2013)

O 84.7 Thu 12:00 MA 144

Novel electronic structures from anomalous stackings in transition metal dichalcogenides — •Mihir Date[1,2], Alex Louat[1], Niels Schroeter[2], and Matthew D. Watson[1] — [1]Diamond Light

Source, Diamond Light Source, Harwell Science and Innovation Campus, Didcot, United Kingdom — [2]Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

Advances in photoemission spectroscopy, especially in terms of spatial resolution, have opened a plethora of possibilities in probing variations in the local electronic structure, which are elusive in traditional angle -resolved photoemission spectroscopy (ARPES) experiments. In our experiments, we have shown that in some "2H"-bulk transition metal dichalcogenides (TMDCs), MoS2, NbS2 and TaS2, minority regions on the sample show spectral signatures of quantum well states. Furthermore, we observe subtle differences in the spectral weight and band splitting in the hole-like pockets around M- and K-points in anomalously stacked MoS2, compared to the bandstructures of its 2H- and 3R-phases. We speculate such electronic structures are derived from local lattice imperfections, where the periodicity of the 2H stacking is broken along the c-axis. We propose that these stacking faults offer a convenient plane for sample cleaving and therefore, are easily captured in a surface sensitive technique like ARPES. Our work not only presents novel electronic structures of traditional TMDCs, but also highlights the strength and importance of spatially resolved ARPES measurements.

O 84.8 Thu 12:15 MA 144

Utilizing matrix element effects to study the orbital texture of Dirac surface state in $PtTe_2$ — •Muthu P. T. Masilamani[1], Jakub Schusser[1], Mohammed Qahosh[2], Lukasz Plucinski[2], Begmuhammet Geldiyev[1], and Friedrich Reinert[1] — [1]Experimentelle Physik VII and Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Würzburg, Germany — [2]Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich GmbH, Jülich, Germany

In this work, we study the matrix element effect of the ARPES intensity to deduce k-space initial state orbital texture featuring different symmetries in type-II Dirac semimetal $PtTe_2$. Our spin- and angle-resolved photoemission data were augmented by the one-step model of the photoemission within the spin-polarized relativistic Korringa-Kohn-Rostoker (SPR-KKR) Green's function method of the Munich band structure software package. In order to extract information about the different contributions to the resulting spectral weight and spin-polarization, the matrix element used in our one-step model of photoemission calculations includes all experimental parameters such as photon energy, light polarization and geometry configurations. Via such control over the experimental parameters, in order to investigate the orbital wavefunction above and below the Dirac point, we performed polarization-dependent ARPES calculations where we varied the angle of the crystal mirror plane with respect to the experimental mirror plane.

O 84.9 Thu 12:30 MA 144

Observation of Chiral Surface State in Superconductor NbGe — •Mengyu Yao[1], Martin Gutierrez-Amigo[2,3], Subhajit Roychowdhury[1], and Claudia Felser[1] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany — [2]Departamento de Física, Facultad de Ciencia y Tecnología, Universidad del País Vasco (UPV/EHU), Apartado 644, 48080 Bilbao, Spain — [3]Centro de Física de Materiales (CSIC-UPV/EHU), Manuel de Lardizabal pasealekua 5, 20018 Donostia/San Sebastián, Spain

The interplay between topology and superconductivity in quantum materials harbors rich physics ripe for discovery. In this work, we investigate the topological properties and superconductivity in the nonsymmorphic chiral superconductor NbGe2 using high-resolution angle-resolved photoemis- sion spectroscopy (ARPES), transport measurements, and ab initio calculations. Our ARPES data reveals exotic chiral surface states on the (100) surface, stemming from the inherent chiral crystal structure. Supporting calculations indicate NbGe2 likely hosts elusive Weyl fermions in the bulk electronic structure. Furthermore, we uncover signatures of van Hove singularities that could engen- der enhanced many-body interactions. Additionally, transport measurements demonstrate NbGe2 exhibits superconductivity below 2 K. Taken together, our comprehensive results provide the first concrete evidence that NbGe2 is a promising platform for investigating the interplay between non- trivial band topology, possible Weyl fermions, van Hove singularities, and superconductivity in chiral quantum materials.

O 84.10 Thu 12:45 MA 144

Mode selectivity in electron mediated vibrational relaxation of adsorbed hydrogen on metal surfaces. — •Nils Hertl[1], Connor L. Box[1], and Reinhard J Maurer[1,2] — [1]Department of Chemistry, University of Warwick, Gibbet Hill Road, CV4 7AL, Coventry, United Kingdom — [2]Department of Physics, University of Warwick, Gibbet Hill Road, CV4 7AL, Coventry, United Kingdom

Vibrational relaxation induced by electron-hole pair (ehp) excitations is a common phenomenon in gas-surface experiments on metallic surfaces. Specific adsorbate vibrational degrees of freedom can be more strongly coupled to ehps at metal surfaces than others, which opens an opportunity for mode-selective energy transfer processes that can activate chemical dynamics. In order to promote mode-selective chemical reactions at solid interfaces a detailed understanding of the coupling of the individual vibrations of adsorbates with the electrons and phonons of the metal substrate is essential. To shed light on the mechanisms involved in energy transfer processes present in gas-surface systems, we study adsorbed hydrogen on single crystalline surfaces. Herein, we calculate the lifetimes of vibrational modes of hydrogen adsorbed on the (100) and (110) surfaces of Mo and W via first-principles first-order perturbation theory based on Density Functional Theory (DFT). Our results show a strong mode dependency on the electron-driven relaxation rates of the vibrations. For the vibrations with a Fano-lineshape, our predicted lifetimes are in good agreement with experiments, indicating that the relaxation of those vibrations is dominated by ehp excitations.