New prospects in ARPES for quantum materials

Tuesday, 05.09.2023, Room 115

Time	ID	NEW PROSPECTS IN ARPES FOR QUANTUM MATERIALS I *Chair: Felix Baumberger, Université de Genève*
14:00	501	**2D with a twist** *Neil Wilson, Department of Physics, University of Warwick, UK* A new parameter space to explore has been added to the beautiful world of 2D materials (2DMs); the twist angle between neighbouring layers. This is exemplified by 'magic-angle' twisted graphene, engineering strongly correlated behaviour through moire interactions, an effect also used to trap ordered arrays of excitons in transition metal dichalcogenide (TMDC) heterobilayers. Moire effects conventionally require a moire wavelength much longer than the atomic scale. But for larger lattice mismatch, Umklapp processes can result in unexpected electronic structure changes. Here, I will present our recent studies of twisted 2DMs, including twisted graphenes and TMDCs. I will discuss initial-state and final-state effects, and the twist-angle dependence of inter-layer interactions.
14:30	502	**Different electronic phases on the surface of bulk 1T-$TaSe_2$** *Michael Straub, Yann Alexanian, Gianmarco Gatti, Catherine Witteveen, Fabian von Rohr, Felix Baumberger, Anna Tamai, Université de Genève* Recent STM experiments revealed a variety of different correlated states to coexist on the surface of bulk 1T-$TaSe_2$. The different regions have the same in-plane charge density wave ordering, yet range from insulating to strongly correlated metal. By utilizing microfocus ARPES, we have resolved the quasiparticle dispersion in the different spatial domains. In the metallic regions, we found heavy quasi-particles forming a chiral Fermi surface, whereas, in the insulating domains our measurements are consistent with a band insulator. We will discuss the origin of this spatial inhomogeneity in terms of the interplay between electron-electron interactions and interlayer coupling.
14:45	503	**Observing Electronic Band Structure of Antiferromagnetic Phase in Topological Weyl Semimetal $Co_3Sn_2S_2$** *Sandy Adhitia Ekahana [1], Felix Baumberger [2], Dariusz Jakub Gawryluk [1], Satoshi Okamoto [3], Loïc Roduit [1], Yona Soh [1], Anna Tamai [2]* *[1] Paul Scherrer Institute, [2] Université de Genève, [3] Oak Ridge National Laboratotry* $Co_3Sn_2S_2$ has been reported to be a magnetic Weyl semimetal expanding our understanding of topological materials. This material is considered to be ferromagnetic as demonstrated experimentally and also by DFT calculations. However, recent muon measurement suggests a co-existence of antiferromagnetism and ferromagnetism around the magnetic transition temperature, which has been neglected previously in the discussion of $Co_3Sn_2S_2$. In this talk, we present our micro-ARPES measurement revealing the presence of an antiferromagnetic phase co-existing as a minority phase with the majority ferromagnetic phase. We confirm the magnetic nature of the phase by studying the temperature dependence of the electron band. Our result provides the first spatial visualization of the aforementioned co-existence.
15:00	504	**First micro-ARPES measurements of encapsulated monolayer Td-$MoTe_2$** *Julia Issing, Ignacio Gutiérrez-Lezama, Fabian von Rohr, Alberto Morpurgo, Anna Tamai, Felix Baumberger, University of Geneva* Bulk orthorhombic Td-$MoTe_2$ is a type-II Weyl semimetal with topological Fermi arc surface states and becomes superconducting at a critical temperature of T_c = 0.1 K. Remarkably, superconductivity becomes far more robust in the 2D limit, contrary to generic models and the established trend in ultrathin metal films. Recent transport measurements reported an increase in T_c for decreasing thickness with T_c reaching 7.6 K in the monolayer. The reasons for the strong increase in T_c as well as the nature of the superconducting state remain unknown. To address the opened questions, we will present the electronic structure of exfoliated monolayer $MoTe_2$ encapsulated between graphite and graphene probed by micro-focused ARPES.

15:15	**505**	**Strain tuning the band structure in a charge-order Kagome system** *Chun Lin [1], Julia Küspert [1], Armando Consiglio [2], Ola Forslund [1], Wojciech Pudelko [3], M. Michael Denner [1], Hechang Lei [4], Youguo Shi [5], Zurab Guguchia [3], Qisi Wang [1], Gerardina Carbone [6], Mats Leandersson [6], Craig Polley [6], Balasubramanian Thiagarajan [6], Alex Louat [7], Matthew Watson [7], Timur Kim [7], Cephise Cacho [7], Giorgio Sangiovanni [2], Titus Neupert [1], Johan Chang [1]* *[1] University of Zurich, [2] University of Würzburg, [3] Paul Scherrer Institut, [4] Renmin University of China, [5] Chinese Academy of Sciences, [6] MAX IV Laboratory [7] Diamond Light Source* Kagome-lattice investigations are growing vigorously owing to the simultaneous realisation of topologically non-trivial electronic structure including Dirac fermions, flat bands, and Van Hove singularities (VHS). As an effective external stimulus, uniaxial strain manifested in a form of physical pressure, is playing an increasingly important role in engineering the band structure and hence physical properties of quantum materials. Utilising high-resolution ARPES, we have successfully applied uniaxial strain and tuned the energy gaps as well as the VHSs in the charge-order state of a Kagome superconductor CsV_3Sb_5.
15:30	**506**	**Photoemission Orbital Tomography for Pump-probe Photoelectron Spectroscopy** *Christian S. Kern, Andreas Windischbacher, Peter Puschnig, University of Graz* In order to interpret and simulate recent time- and angular-resolved photoemission spectroscopy (tr-ARPES), we extend the successful method of photoemission orbital tomography (POT) to excited states. Our theory retains the intuitive orbital picture of POT, while respecting both the entangled character of the electron-hole exciton wave function and the energy conservation in the photoemission process. Going beyond simple HOMO-LUMO transitions in organic molecules, we classify generic exciton structures and give an intuitive interpretation of tr-ARPES data in terms of natural transition orbitals. It is further shown how this new method for excited-states POT can be independently validated by real-time simulations of tr-ARPES from time-dependent density functional theory.
15:45	**507**	**Circular Dichroism and Orbital Angular Momentum in chiral Weyl semimetals PdGa/PtGa** *Yun Yen [1,2], Jonas A. Krieger [3], Niels B. M. Schröter [3], Maia G. Vergniory [4], Iñigo Robredo [5], Michael Schüler [1,6], Qun Yang [7], Mengyu Yao [5]* *[1] Paul Scherrer Institute, [2] EPFL, [3] Max Planck Institute of Microstructure Physics [4] Donostia International Physics Center, [5] Max Planck Institute for Chemical Physics of Solids [6] Department of Physics, University of Fribourg, [7] Weizmann Institute of Science* In this work, we show that circular dichroism angle resolved photoemission spectroscopy (CD-ARPES) can map topology in chiral Weyl semimetals PdGa/PtGa, where multifold nodes host large Chern number. We successfully simulate the CD intensity using our in-house code dynamics- w90. The correspondence between local OAM and dipole matrix elements depends on orbital characters and experimental geometry. Pd/Pt local OAM can be measured by CD, where d orbital contribution is dominated by $m = \mp 2$ complex orbitals. Although the total CD signal consists of interatomic interference terms, they still exhibit radial structure. We conclude that one can see the reminiscence of radial OAM structure, which comes from the topological nature of the Weyl nodes.
16:00	**508**	**Band topology induced by strain in $SrNbO_3$** *Victor Rosendal [2], Alla Chikina [1], Hang Li [1], Mads Brandbyge [3], Eduardo Bonini Guedes [1], Marco Caputo [1], Dirch Hjorth Petersen [2], Felix Baumberger [4], Milan Radovic [1], Nini Pryds [3]* *[1] Paul Scherrer Institute* *[2] Department of Energy Conversion and Storage, Technical University of Denmark* *[3] Department of Physics, Technical University of Denmark* *[4] University of Geneva* Transition metal oxides could also be a platform for conceiving novel quantum properties, such as nontrivial topology induced by crystal structure modification. In this study, we investigate the effect of strain on the electronic structure and band topology of ultra-thin $SrNbO_3$ films. By employing angle-resolved photoemission spectroscopy (ARPES) and density functional theory (DFT)

		calculations, we gain insight into band structure of $SrNbO_3$ strained tetragonal phases. We will discuss a formation of nontrivial Dirac band crossings in $SrNbO_3$ films originating from in-phase and out-of phase octahedral tilting. Our study provides direct evidence and proves that heteroepitaxial strain can be effectively used for engineering quantum phases in transition metal oxides.
16:15	**509**	**Photoemission matrix element correction for accurate quantification of electronic spectral functions: the case of TiO_2-terminated $SrTiO_3$** *Tom van Waas [1], Igor Sokolovic [2], Martin Setvín [2], Eduardo Bonini Guedes [3], Hugo Dil [4], Samuel Poncé [1]* *[1] Université catholique de Louvain, [2] TU Vienna, [3] PSI Villigen, [4] EPFL* In ARPES, access to the electronic spectral function $A(E, \mathbf{k})$ is obscured by the photoemission matrix elements $M_{k,k}$. We provide a heuristic approach based on the sum rule to obtain the momentum dependence of these elements. We show how matrix element correction (MEC) enables extraction of the Eliashberg spectral function from both light band branches of a TiO_2-terminated $SrTiO_3$ surface state. Finally, we illustrate how the MEC allows for direct comparison of $A(E, \mathbf{k})$ from ARPES and first principles.
16:30		***Coffee Break***
		New prospects in ARPES for quantum materials II *Chair: Claude Monney, Université de Fribourg*
17:00	**511**	**ARPES of quantum confined semiconductor and topological insulator heterostructures grown by molecular beam epitaxy** *Gunther Springholz, Johannes Kepler Universität, Linz* Angle resolved photoemission spectroscopy (APRES) has emerged as a powerful tool to assess the electronic band structure of quantum materials. Here, it is applied to study quantum confined states in IV-VI semiconductor and topological insulator heterostructures produced by molecular beam epitaxy. This allows to study a large variety of low dimensional structures revealing the electronic spectra with high resolution, as is exemplified for zero gap Dirac quantum wells, double quantum wells, as well as Volkov-Pankratov heterojunctions. We reveal the significant probing depth of APRES stemming from the emergent wave functions, which opens up a new realm for ARPES applications.
17:30	**512**	**Persistent Rashba splitting in the bulk bands of SnTe in the paraelectric phase** *Frédéric Chassot [1], Aki Pulkkinen [2], Geoffroy Kremer [3], Hugo Dil [4], Juraj Krempasky [5], Ján Minár [2], Gunther Springholz [6], Claude Monney [1]* *[1] Department of Physics and Fribourg Center for Nanomaterials, Université de Fribourg, CH-1700 Fribourg* *[2] New Technologies-Research Center, University of West Bohemia, Plzeň, Czech Republic* *[3] Institut Jean Lamour, UMR 7198, CNRS-Université de Lorraine, Nancy, France* *[4] Institute of Physics, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne* *[5] Photon Science Division, Paul Scherrer Institut, CH-5232 Villigen PSI* *[6] Institut für Halbleiter-und Festkörperphysik, Johannes Kepler Universität, Linz, Austria* SnTe is a ferroelectric semiconductor with similar properties as GeTe, which has already been extensively studied, notably for applications in spintronics. However, the lower critical temperature of SnTe (around 100K) makes it an ideal candidate to investigate the ferroelectric transition. Here we present a study of its bandstructure with photoemission spectroscopy. We follow the evolution of the Rashba splitting induced by the ferroelectric distortion in the bulk and discover drastic deviations from a mean-field-like transition. In particular, the persistence of a splitting at room temperature supports an order-disorder type of transition, questioning the topological nature of surface states. We conclude by showing ongoing work on time-resolved photoemission spectroscopy.

17:45	**513**	**Are high-energy photoemission final states free-electron-like?** *Vladimir N. Strocov [1], Fatima Alarab [1], Procopious Constantinou [1], Leonid L. Lev [2], Jan Minár [3], Lorent Nicolaï [3], Jan Očenášek [3], Thorsten Schmitt [1], Taylor J. Z. Stock [4]* *[1] Swiss Light Source, Paul Scherrer Institute, [2] Moscow Institute of Physics and Technology* *[3] University of West Bohemia, Plzeň* *[4] London Centre for Nanotechnology, University College London* Three-dimensional (3D) electronic bandstructure is fundamental for a vast diversity of physical phenomena in solid-state materials, including topological phases, interlayer interactions in van-der-Waals materials, etc. Interpretation of ARPES data in terms of 3D bandstructure is commonly based on the free-electron approximation for the photoemission final states. Our soft-X-ray ARPES data on various metals and semiconductors reveal, however, that even at high excitation energies the final states can be quite complex, where several Bloch waves with different out-of-plane momenta form a complex structure of the spectral peaks. Our findings are essential for accurate determination of the 3D bandstructure from the ARPES experiment over a wide range of materials and excitation energies.
18:00	**514**	**Observing and manipulating orbital textures in quantum materials** *Michael Schüler [1,2], Samuel Beaulieu [3], Ralph Ernstorfer [4], Rupert Huber [5], Ulrich Höfer [6], Suguru Ito [6], Niels Schröter [7], Michael Sentef [8], Yun Yen [1]* *[1] Paul Scherrer Institute, [2] University of Fribourg, [3] University of Bordeaux, [4] TU Berlin, [5] University of Regensburg, [6] University of Marburg, [7] MPI Halle, [8] University of Bremen* Angle-resolved photoemission spectroscopy (ARPES) provides an unprecedented “zoom” into the electronic degrees of freedom. Besides mapping the band structure, fingerprints of wave-function aspects such as the orbital texture, associated orbital angular momentum (OAM) and Berry curvature are contained in ARPES. Extracting such wave-function information is a challenge due to the complexity of the photoemission process. Based on accurate theory, we discuss the principles of how exploiting the photon polarization degree of freedom and the crystal orientation can provide wave-function information. We will demonstrate these principles by joint experimental and theoretical work on the transition metal dichalcogenide WSe_2 and the topological chiral semimetal PdGa.
18:30	**515**	**Real-time pump-probe simulations within time-dependent density functional theory** *Dominik Brandstetter, Christian S. Kern, Peter Puschnig, University of Graz* Real-time time-dependent density functional theory provides an ab-initio framework to directly simulate (sub-)femtosecond pump-probe ARPES experiments. Incident light field(s) of any shape and magnitude can be incorporated, electron correlations are considered at a mean-field level and no assumptions regarding the final state of the escaping electron are required. In this contribution, we study a resonantly driven HOMO-LUMO transition of an organic rod-line molecule to study the intra-molecular charge transfer upon the optical excitation. We simulate the oscillatory behavior in the population of the frontier orbitals resembling detuned Rabi oscillations and study the characteristics of the intramolecular charge transfer by simulating photoemission momentum maps to be compared with time-resolved-ARPES experiments.
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18:45	**517**	**Photon-energy-dependence of the circular dichroic ARPES with InAs(110)** *Anna Hartl [1], Dmitry Usanov [1], Enrico Della Valle [1], Ján Minár [2], Vladimir Strokov [1]* *[1] Paul Scherrer Institut, [2] University of West Bohemia, Plzeň* In ARPES, coupling of polarized light to the valence-band states contains valuable information about their orbital and spin texture. This information, however, is distorted by non-trivial behavior of the photoemission matrix elements. We explored the circular dichroism in InAs(110) over a broad photon-energy range from VUV to soft X-rays, focusing on the Fermi-surface maps. Supported by ARPES computations based on the multiple-scattering Green’s function approach (SPR-KKR), we analyzed the experimental data in terms of photon-energy-dependent final states and dichroic matrix elements. Our methodology paves the way towards ARPES investigations of the orbital and spin texture in complex quantum materials.
19:00		***END; Postersession with Apéro***

ID	New prospects in ARPES for quantum materials Poster
531	**Momentum-space imaging and chemical gating of the novel polarization induced two-dimensional electron and hole gases on AlN single crystals** *Enrico Della Valle [1,2], Debdeep Jena [3], Guru Khalsa [3], Thai-Son Nguyen [3], Vladimir Strokov [2], Zexuan Zhang [3]* *[1] ETH Zürich, [2] PSI Villigen, [3] Cornell* Lattice-matched interfacing of two large band-gap semiconductors such as AlN, AlGaN, and GaN can induce high-mobility electron and hole charge carriers without addition of dopants. Determining this phenomenon are the pseudomorphic strain and the spontaneous polarization along the (0001) direction. To access the physics of the interfacial charge carriers confined in quantum-well states, we have measured their k-resolved band structure with soft-X-ray ARPES. Additionally, we have experimentally demonstrated how deposition of atoms with different electron affinities can move the Fermi level within the heterostructure and eventually increase or deplete the concentration of interfacial electrons and holes.
~~532~~	*moved to talk 517*
533	**Doping and temperature dependence evolution of the electronic properties of electron-doped Sr_2IrO_4 seen by ARPES** *Yann Alexanian [1], Anna Tamai [1], Felix Baumberger [1], Robin Perry [2]* *[1] University of Geneva, Department of Quantum Matter Physics* *[2] London Centre for Nanotechnology Faculty of Maths & Physical Sciences* Sr_2IrO_4 is a layered perovskite isostructural to the cuprate superconductor La_2CuO_4. The combination of strong spin-orbit coupling inherent to Ir^{4+} ions and modest Coulomb interaction induces a Mott insulating ground state with Heisenberg spin dynamics. Theses striking similarities with cuprates extend to the unusual metallic state of lightly doped Sr_2IrO_4 characterized by Fermi arcs and a pseudogap. Here, I will present new ARPES data on bulk crystals with higher doping than reached previously. Our results show that nodal states become more coherent with increased doping. At the same time, an antinodal pseudogap persists up to the highest doping, in contrast to previous results on surface doped Sr_2IrO_4.
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