Electron and photon spectroscopies of quantum materials

Wednesday, 11.09.2024, Room ETF E 1

Time	ID	Electron and photon spectroscopies of quantum materials I *Chair: Luc Patthey, PSI Villigen*
14:30	501	**Fast and furious: the fate of quasiparticles at high temperature** *Anna Tamai, DQMP, University of Geneva* Strongly interacting Fermi liquids often turn into bad metals at elevated temperature. How this crossover proceeds is largely unknown, as is the nature of the bad metal state. Here, we address this question by studying the temperature dependence of quasiparticles in the model Fermi liquid Sr_2RuO_4. In contrast to common ARPES beliefs, our experiments show that quasiparticles do not disappear via a vanishing quasiparticle residue Z. To the contrary, we find that the residue Z increases with increasing temperature. Quasiparticles eventually disappear not by losing spectral weight but by dissolving via excessive broadening. These findings are in semi-quantitative agreement with dynamical mean field theory calculations.
15:00	502	**Interfacial electron-phonon coupling at a WS_2/hBN interface** *Gianmarco Gatti [1], Felix Baumberger [1,2], Christophe Berthod [1], Julia Issing [1], Salony Mandloi [1], Michael Straub, Anna Tamai [1]* *[1] Department of Quantum Matter Physics, University of Geneva, 24 Quai Ernest-Ansermet, CH-1211 Geneva* *[2] Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI* The interfacial coupling between electronic states in a two-dimensional system and bosonic excitations in an adjacent substrate are still poorly characterized in van der Waals heterostructures. Here, we investigate the nature of such interactions in the electronic states of a WS_2/hBN stack via angle-resolved photoelectron spectroscopy. We resolve dispersing satellites separated from the intense quasiparticle WS_2 valence band by energies comparable to Γ phonon modes in hBN. We derive a spectral function model to describe the interfacial coupling between charges in the WS_2 layer and the lattice vibrations of the polar hBN substrate, which we employ to provide a qualitative estimation of the interaction strength.
15:15	503	**Electronic band structure of strained germanium: bridging theory with direct experimental evidence** *Enrico Della Valle [1,2], Gabriel Aeppli [2], Miki Bonacci [2], Nicola Colonna [3], Andrea Hofmann [4], Nicola Marzari [3], Arianna Nigro, Michael Schüler [2,5], Vladimir Strokov [2], Ilaria Zardo [4]* *[1] ETH Zürich, [2] PSI, [3] EPFL, [4] Uni Basel, [5] Uni Fribourg* Planar Ge/SiGe heterostructures are integral to quantum technologies, particularly as platforms for quantum computation using hole-spin qubits. Compressive strain applied to germanium alters the energy dispersion of holes at the Γ-point, lifting the degeneracy between heavy and light holes by 130 meV. This results in two two-fold degenerate bands, characterized by effective spins $\|j_z\| = 3/2$ and $\|j_z\| = 1/2$. We confirm this energy diagram using soft X-ray ARPES, providing direct access to momentum-resolved energy levels. First-principles calculations quantitatively reproduce the experimental band structure and energy splittings, enhancing our understanding of the quantum functionality of Ge/SiGe heterostructures. Additionally, we explore the utility of soft X-ray ARPES in studying semiconductor/superconductor heterostructures, such as Al/Ge/SiGe.

15:30	**504**	**New Developments in Deflector Analyzer Technology for ARPES** *Saumya Mukherjee, Stefan Böttcher, Michael Meyer, Sven Mähl, Thorsten Kampen, Oliver Schaff* *SPECS Surface Nano Analysis GmbH, Voltastrasse 5, 13355 Berlin, Germany* Electron-optical deflectors in the lenses of hemispherical analyzers have been changing the data acquisition strategies of ARPES significantly. Among other benefits, keeping the experimental conditions constant (the sample light geometry stays fixed) and enhanced acquisition precision (no mechanical movement is involved) have increased the data quality and acquisition speed. However, several aspects of the electron-trajectory manipulation have been unaddressed so far, such as field inhomogeneities in the deflector sections and distortions induced by deflecting the angular image. We present a new type of deflector technology for APRES measurements, enhancing the deflector precision and simultaneously overcoming existing limitations of deflector analyzers, such as angular acceptance, reliability of mechanical parts and electron optical distortions. We have characterized the analyzer in lab-based environments using well established standard samples and compared the results to cutting edge literature from synchrotron experiments.
15:45	**505**	**Doping and temperature dependence evolution of the electronic properties of electron-doped Sr_2IrO_4 seen by ARPES** *Yann Alexanian [1], Robin Perry [2,3], Anna Tamai [1], Felix Baumberger [1,4]* *[1] Department of Quantum Matter Physics, University of Geneva, 24 Quai Ernest-Ansermet, CH-1211 Geneva* *[2] ISIS Pulsed Neutron and Muon Source, STFC Rutherford Appleton Laboratory, Harwell Campus, Didcot, Oxon OX11 0QX, United Kingdom* *[3] London Centre for Nanotechnology and Department of Physics and Astronomy, University College London, London WC1E 6BT, United Kingdom* *[4] Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI* Sr_2IrO_4 is a layered perovskite isostructural to the cuprate 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. Theses 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, the antinodal pseudogap persists up to highest doping and up to high temperature, in contrast to previous results on surface doped Sr_2IrO_4.
16:00	**506**	**Unveiling the Electronic Properties of α-SnTe: From Ferroelectric Distortion to Unexpected Topological Surface State** *Frédéric Chassot [1], Hugo Dil [2,3], Geoffroy Kremer [4], Juraj Krempaský [3], Jan Minár [5], Claude Monney [1], Aki Pulkkinen [5], Gunther Springholz [6], Chennan Wang [1]* *[1] Université de Fribourg, CH-1700 Fribourg, [2] EPFL, [3] Paul Scherrer Institut, 5232 Villigen PSI* *[4] Institut Jean Lamour, CNRS-Université de Lorraine, FR-54011 Nancy* *[5] New Technologies-Research Center University of West Bohemia, CZ-30614 Pilzen* *[6] Johannes Kepler Universität, AT-4040 Linz* α-SnTe(111), a semiconducting and ferroelectric material, exhibits unique topological behavior. At room temperature, its rocksalt structure enables a metallic topological surface state. However, below a critical temperature, a structural distortion suppresses this state, leading to a macroscopic ferroelectric polarization and significant Rashba splitting. Firstly, using ARPES, we can follow the thermal evolution of the Rashba splitting as an indicator of the distortion to provide insights into the ferroelectric transition. Secondly, using time-resolved ARPES, we can also restore an ultrashort-lived topological state while the atomic structure remains distorted, photoinducing this way a topological state that coexists with a ferroelectric structure.

16:15	**507**	**Characterization of Excitons for bulk Black Phosphorus** *Juan F. P. Mosquera [1,2], Geoffroy Kremer [2,3], Claude Monney [2], Michael Schüler [1,2]* *[1] Paul Scherrer Institut, Laboratory for Materials Simulations (LMS)* *[2] University of Fribourg, Centre for Nanomaterials* *[3] Institut Jean Lamour, CNRS-Université de Lorraine* Excitons (coupled electron–hole pairs) in semiconductors can form collective states that exhibit spectacular nonlinear properties and possible applications in future optoelectronic devices. We present here some theoretical methods and a workflow for determining the excitonic wave functions and the corresponding excitonic binding energies for bulk Black Phosphorus. We solve the Bethe-Salpeter equations for coherent and incoherent excitations. The theoretical/numerical results are compared to the experimental ones of angle resolved photoemission spectroscopy (ARPES) to understand the nature and characteristics of these two-particle bound states, being challenging due to the stronger screened potential for 3D materials, resulting in short time excitations.
16:30		***Coffee Break***
		ELECTRON AND PHOTON SPECTROSCOPIES OF QUANTUM MATERIALS II *Chair: Claude Monney, Université de Fribourg*
17:00	**511**	**Exciton dynamics in two-dimensional quantum materials in space and time** *Stefan Mathias, I. Physical Institute, University of Göttingen, Germany* In 2D semiconducting quantum materials, organic semiconductors and their heterostructures, the energy of absorbed light is stored in Coulomb-bound electron-hole pairs, i.e. excitons. In our research, we have built a new photoemission-based experiment that is capable studying excitons at the space-time limit (nanometers and femtoseconds). In my talk, I will present the ultrafast formation dynamics of dark interlayer excitons in twisted WSe_2/MoS_2 heterostructures in space and time. Furthermore, I will present photoemission exciton tomography that allows us to study multiorbital contributions in the exciton formation in an organic semiconductor.
17:30	**512**	**The Balance Between Independent and Correlated Electron Dynamics in Transition Metals** *Erik de Vos [1], Shunsuke Sato [2], Sergej Neb [1], Marko Hollm [1], Florence Burri [1], Lukas Gallmann [1], Ursula Keller [1]* *[1] Department of Physics, ETH Zürich, 8093 Zürich* *[2] Center for Computational Sciences, University of Tsukuba, Ibaraki 305-8577, Japan* Attosecond transient absorption spectroscopy studies are presented to provide a systematic overview of the electronic and phononic response of optically excited thin-film transition metals on timescales ranging from a few femtoseconds to hundreds of picoseconds. Special emphasis is placed on understanding the balance between independent-electron population dynamics and correlated electron dynamics. It is found that collective effects dominate the response in first-row transition metals through a modification of local screening dynamics. However, due to the more delocalised nature of the valence orbitals of third-row transition metals, independent-electron phenomena such as Pauli state-blocking become most prominent in this class of materials.

17:45	**513**	**Anomalous magnetic excitations in the half-filled Tl-based cuprate** *Izabela Biało [1], Qisi Wang [2], Julia Küspert [1], Karin von Arx [1], Chun Lin [1], Wojciech Radoslaw Pudelko [3], Davide Betto [4], Nicholas Brookes [4], Nicholas Clark Plumb [3], Kaori Tanaka, Johan Chang [1]* *[1] University of Zurich, [2] The Chinese University of Hong Kong, [3] Paul Scherrer Institut* *[4] European Synchrotron Radiation Facility, Grenoble, FR* Manifestations of quantum fluctuations on ground states and their excitations are at the heart of condensed matter physics. Electronic two-dimensional square-lattice systems are in the moderate coupling limit extremely complex. Here, we introduce an ultra-clean half-filled cuprate system with moderate correlation strength. Using high-resolution resonant inelastic x-ray scattering, we probe the magnon excitations and their dispersion. We show that the dispersion is associated with a discontinuous “band” velocity. Within a Heisenberg-Hubbard model, this discontinuity is assigned to the presence of strong quantum fluctuations.
18:15	**514**	**Exploring Low-Energy Excitations and Magnetic Dichroism in Resonant Inelastic X-ray Scattering of the Ferromagnetic van der Waals Material VI_3** *Yuan Wei [1], Wenliang Zhang [1], Zhen Tao [1], Teguh Citra Asmara [1], Tianlun Yu [1], Mirian Garcia-Fernandez [2], Cedomir Petrovic [3], Ke-Jin Zhou [2], Thorsten Schmitt [1]* *[1] Paul Scherrer Institut, [2] Diamond Light Source, UK, [3] Brookhaven National Laboratory, USA* The ferromagnetic van der Waals Material VI_3 is proposed as a Mott insulator with S = 1 state. A distinct symmetry breaking indicative of the FM transition is observed in the Raman spectra of monolayer samples. This study investigates low-energy excitations in VI_3 using high-resolution resonant inelastic X-ray scattering (RIXS). We identify the spin wave, revealing insights into the spin dynamics and exchange interactions, and unveil an orbital redistribution through the RIXS magnetic circular dichroism (MCD), underscoring the significance of orbital degrees of freedom in the magnetism. Our findings illustrate the sensitivity of RIXS-MCD in probing ferromagnetic van der Waals materials.
18:30	**515**	**Spin-orbital correlations in the van der Waals magnet $CrPS_4$ revealed by resonant inelastic X-ray scattering** *Zhijia Zhang, Yuan Wei, Carlos Galdino, Wenliang Zhang, Tianlun Yu, Thorsten Schmitt, Paul Scherrer Institut* Exfoliable magnetic van der Waals (vdW) materials have enabled the study of magnetism at the true two-dimensional limit. Bulk $CrPS_4$ is an A-type vdW antiferromagnet with strong correlation between the electronic, orbital, structural properties and the magnetic state. I will present our temperature-dependent resonant inelastic X-ray scattering (RIXS) data: the linear-dichroic RIXS intensity of one of the orbital excitations shows an order-parameter-like temperature dependence around the Néel temperature (38 K). I will discuss this temperature-dependent orbital asymmetry in relation to our multiplet simulations, and how the RIXS dichroism of this orbital excitation will allow access to the magnetic state in future RIXS investigations of exfoliated flakes of this topical material.
18:45	**516**	**Altermagnetism at mangantite/cuprate interface** *Yurii Pashkevich [1,2], Subhrangsu Sarkar [1], Christian Bernhard [1], Davide Betto [3], Nicholas Brookes [3], Roxana Capu [4], Jarji Khmaladze [1], Jonas Knobel [1], Kurt Kummer [3], Claude Monney [1], Abhishek Nag [5], Marli R. Cantarino [3], Roberto Sant [3], Christhoper W. Nicholson [1], Ke-Jin Zhou [6]* *[1] University of Fribourg* *[2] O. O. Galkin Donetsk Institute for Physics and Engineering NAS of Ukraine* *[3] European Synchrotron Radiation Facility: Grenoble, FR* *[4] West University of Timisoara, Romania, [5] Technische Universität Dresden (DE)* *[6] Diamond Light Source, Oxford, UK* We report a resonant inelastic X-ray scattering study of multilayers made from a cuprate high-T_c superconductor and a magnetic perovskite manganite. Our study reveals combined spin and orbital order at the interfacial cuprate monolayer constituting a 2D altermagnetic state. Our findings significantly advance state of the art in the field of altermagnets that are of great current interest since they enable new kinds of spintronic and magnonic devices.

19:00	**517**	**Charge order fluctuations in a stripe-ordered cuprate superconductor** *Xunyang Hong [1], Karin von Arx [1], J. Choi [2], Yasmine Sassa [3], S. Pyon [4], T. Takayama [4], H. Takagi [4], M. Garcia-Fernandez [2], Ke-Jin Zhou [2], Johan Chang [1], Qisi Wang [5]* *[1] University of Zurich, [2] Diamond Light Source, [3] Chalmers University of Technology* *[4] University of Tokyo, [5] The Chinese University of Hong Kong* This study reports direct observation of charge order fluctuations in the unconventional superconductor $La_{1.675}Eu_{0.2}Sr_{0.125}CuO_4$ (LESCO) using resonant inelastic x-ray scattering (RIXS). Charge order is linked to and competes with superconductivity in cuprates, making its fluctuations key to understanding the low-energy physics in these materials. Past studies mainly focused on indirect methods, but this study uniquely separates out these fluctuations directly. We used numerical simulations to isolate charge order fluctuations from other low-energy signals. Our findings enhance the understanding of these fluctuations in superconductivity and introduce a new method for studying quantum materials.
19:15		***END***

ID	Electron and photon spectroscopies of quantum materials Poster
531	**Quantum Material Dynamics Under Pressure** *Zia Macdermid, Elsa Abreu, Tim Suter, ETH Zürich* This poster showcases development of an experimental setup for time-resolved THz time-domain spectroscopy with tunable temperature and pressure capabilities, down to 10 K and up to 10 GPa. Ultrafast dynamics experiments typically excite materials from their equilibrium ground state to investigate various properties. Pressure control enables direct manipulation of this state. Combining tunable pressure with THz TDS is challenging due to the large THz beam spot size and small sample sizes in diamond anvil cells. To optimize signal acquisition, we investigated parameters like pressure medium and aperture size. We further added an 800 nm optical pump for optical pump-THz probe measurements, enhancing our ability to study phase transitions with sub-picosecond resolution.
532	**Probing mono- and few-layer 1T-$TaSe_2$ with ARPES** *Salony Mandloi [1], Felix Baumberger [1,2], Anna Tamai [1]* *[1] Department of Quantum Matter Physics, University of Geneva, 24 Quai Ernest-Ansermet, CH-1211 Geneva* *[2] Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI* Physical properties can change significantly when bulk materials are thinned down to a few atomic layers. Here, we study the intriguing example of the metallic charge density wave system 1T-$TaSe_2$. Previous transport experiments on 1T-$TaSe_2$ found a metal to insulator transition at a thickness of 5 layers. Monolayer 1T-$TaSe_2$ was proposed to be a Mott insulator and is a candidate quantum spin liquid. We perform Angle resolved photoelectron spectroscopy (ARPES) measure- ments on ultra clean exfoliated few layer 1T-T aSe_2 to study this intriguing phase of matter.
533	**Electronic structure of encapsulated mono-, bi- and trilayer Td-$MoTe_2$** *Julia Issing [1], Ignacio Gutiérrez-Lezama [1], Fabian von Rohr [1], Alberto Morpurgo [1], Marco Gibertini [2], Anna Tamai [1], Felix Baumberger [1]* *[1] University of Geneva, [2] University of Modena and Reggio Emila* Bulk Td-$MoTe_2$ is a type-II Weyl semimetal 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 the trend in ultrathin metal-films. Recent transport measurements reported an increase in T_c for decreasing thickness, with T_c = 7.6, K in the monolayer. The reasons for the strong increase in T_c remains unknown. Here, we present the electronic structure of exfoliated mono-, bi- and trilayer Td-$MoTe_2$ probed by ARPES. The electron pocket of monolayer $MoTe_2$ shows signatures of strong coupling to optical phonons with $\lambda \approx 1.5$. In bi- and trilayer $MoTe_2$ electron-phonon coupling is weaker consistent with thickness dependence of T_c.

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Integrated Synchrotron X-ray and Raman Techniques for the Determination of the Fill Factor and Thickness of III-V Semiconductor Nanowire Layers grown on a Substrate

Dimitrios Sapalidis [1], Maria Katsikini [2], Eleni Paloura [2], Eleni Pavlidou [2], Fani Pinakidou [2], Matthew Zervos [3]
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The primary objective of this study is to propose a methodology for determining the fill factor and thickness of III-V semiconductor nanowire layer grown on a substrate. To achieve this goal, we utilized the surface phonon-peak positions in the Raman spectra, which correspond to the perturbation of the GaN nanowire (NW) surface, to model the dielectric environment near the surface and thus estimate the fill factor of the layer. The average radii of the nanowires were obtained through Small-Angle X-ray Scattering modeling, and employing the effective medium approximation, a quantitative analysis using Synchrotron X-ray Fluorescence was performed to ascertain the thickness of the nanowire layer. SEM images verified the results.