ÉCOLE DE
PHYSIQUE DES HOUCHES

SUCCESS-2025

School on UV and X-ray spectroscopies of correlated electron systems

15-26 September 2025
Les Houches
France

	Mon 15/9	Tue 16/9	Wed 17/9	Thu 18/9	Fr 19/9	Sat 20/9	Sun 21/9	Mon 22/9	Tue 23/9	Wed 24/9	Thu 25/9	Fr 26/9
7h45 8h45		Brkfst	Brkfst	Brkfst	Brkfst	Brkfst	Brkfst	Brkfst	Brkfst	Brkfst	Brkfst	Brkfst
8h45 10h15		Intro 15 min **PES-EXP-1** **Claessen**	**PES-EXP-2** **Claessen**	**2D spin detection** **Schönhense**	**XPS-SCES-1** **Elnaggar**	**ARPES correlated systems** **Santander-Syro**	**Free**	**PES-TH** **Minar**	**XR(E)S/RIXS** **Giringhelli**	**XR(E)S/RIXS** **Giringhelli**	**Laser-PEEM** **Taniuchi**	**PARTICIPANTS TALKS** **8:45 – 10:00**
10h15 10h45		Coffee	Coffee	Coffee	Coffee	Coffee		Coffee	Coffee	Coffee	Coffee	Coffee 10:00 – 10:15
10h45 12h15		**SCES-1** **Biermann**	**SCES-3** **Biermann**	**HHG-UV lasers** **Barreau**	**XPS-SCES-2** **Elnaggar**	**Oxide thin-films** **Baeumer**		**Hands-on: Calculation Methods** **Minar**	**Hi-Res ARPES** **Ishizaka**	**Spin-ARPES** **Okuda**	**PARTICIPANTS TALKS** **10:45 – 12:15**	**PARTICIPANTS TALKS** **10:15 – 11:30** Closing 30min
12h30 14h00		Lunch	Lunch	Lunch	Lunch	Lunch	Lunch	Lunch	Lunch	Lunch	Lunch	Lunch
14h00 16h00	Arrival	**Free**	**Free**	**Free**	**Free**	**Free**	**Free**	**Free**	**Free**	**Free**	**Free**	Departure
16h00 17h30		**Light-Src-1 Synchrotron** **Le Fèvre**	**PES-EXP-3** **Claessen**		**Light-Src-2 Synchrotron** **Le Fèvre**	**Oxides' electronic structure** **Kumigashira**		**Topological Insulators 1** **Carpentier**	**PARTICIPANTS TALKS** **16:00 – 17:30**	**TR-ARPES** **Gierz**		
17h30 17h45		Coffee	Coffee		Coffee	Coffee		Coffee	Coffee	Coffee		
17h45 19h15		**SCES-2** **Biermann**	**K-space Analyzers** **Schönhense**		**HAX-PEEM** **Müller**	**Soft X-ray PES in functional materials** **Kobayashi**		**Topological Insulators 2** **Carpentier**	**Electronic Moiré Systems** **Bascones**	**PARTICIPANTS TALKS** **17:45 – 19:15**		
		19h00 Pot d'accueil										
19h30 20h30	Dinner	Dinner	Dinner	Dinner	Dinner	Dinner	Dinner	Dinner	Dinner	Dinner	Dinner	
					POSTERS + snacks/drinks					**POSTERS + snacks/drinks**		

Lectures

Photoelectron Spectroscopy: The Joys And Pitfalls Of The Photoelectric Effect

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Photoelectron spectroscopy (PES) in its many variants is the most direct and powerful experimental tool to probe the microscopic electronic structure of condensed matter. Although its basic principles can be readily understood from the physics of the photoelectric effect, a number of assumptions and approximations are involved, before a PES signal can be converted into useful information. Assuming that the attendants of the School have already some basic knowledge of the method (as practitioner or as theorist), my introductory lectures will try to provide an overview of the central concepts and ideas underlying the PES methodology and prepare the grounds for the subsequent SUCCESS lecture program. Besides the obvious essentials I will also try to touch upon some special issues, which are not treated often in the standard literature but may become relevant as the technique progresses into novel regimes of photon intensity and/or energy. Among the topics I plan to cover are:

- PES instrumentation: past, present, future
- Fermi's Golden Rule and the dipole approximation
- Photoemission final states and the $k_\perp$ problem
- Surface photoemission: the $div\vec{A}$ term
- Many-body theory of PES: Sudden Approximation and Spectral Function
- Probing depth issues: from low to high energy PES
- Resonant photoemission: quantum interference at work

The focus of my lectures will be mostly on conceptual physics, with more room for comprehensive theory and detailed research examples left to the following, more specialized lectures.

Strongly Correlated Materials

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The field of electronic structure calculations for correlated materials has witnessed tremendous progress in recent years due to the development of combined electronic structure and many body theories. We will give an introduction to the concept of electronic correlations and the modeling thereof. Then we will give an overview of density functional theory (DFT), the workhorse of modern electronic structure calculations, and discuss some of its successes as well as failures.

Having evidenced the need of going beyond DFT, we will summarize some of the main strategies of many-body theory and their combination with realistic electronic structure techniques. We will describe the ideas and formalism of dynamical mean field theory, and discuss its application in the electronic structure context. Finally, we will comment on current questions in the field and open challenges. The lectures will thus be structured as follows:

1. Correlation effects in condensed matter - Brief overview
2. Spectroscopic signatures of correlations
3. Modeling correlated electron behavior
4. Tools of many-body theory – survival kit
5. Density Functional Theory (DFT) - An introduction
6. Successes and failures of DFT: the need of going beyond
7. Dynamical mean field theory
8. Electronic structure calculations for correlated materials: the present status
9. What about U?
10. Perspectives and open questions

Synchrotron Radiation

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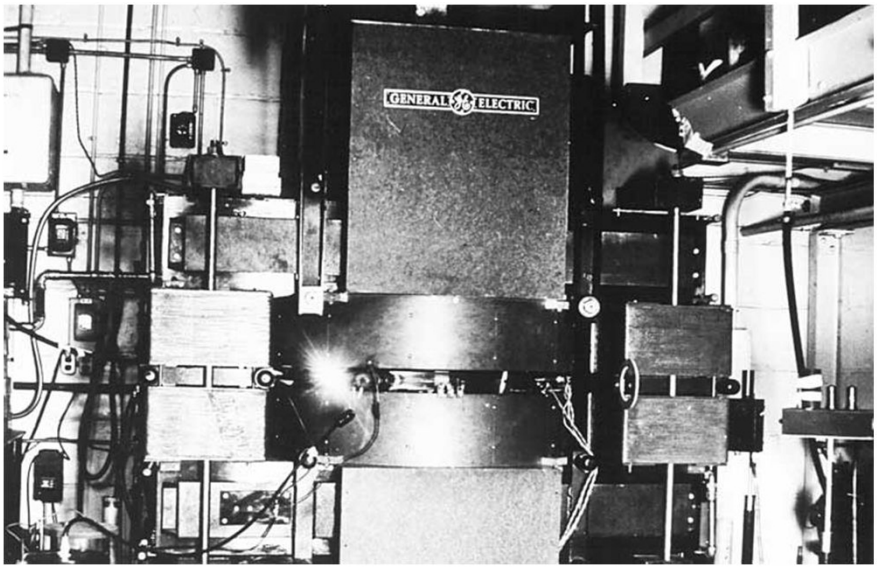
Synchrotron radiation has been the ultimate photon source for countless experimental techniques for nearly 50 years. It is emitted by electric charges (usually electrons) traveling at a speed close to the speed of light in circular storage rings. When their trajectory is bent in a magnetic field, electrons radiate an intense, brilliant and polarized light which contains all the wavelengths from infrared to X-rays. This so-called synchrotron radiation, was first considered as undesirable by high energy physicists who first built these kind of machines since it was limiting the energy of the stored particles. A handful of pionneering experimentalists then realized that it could be useful as an unprecedented photon source and were allowed to work on the accelerators as parasitic users. Today, there are more than 60 facilities fully dedicated to the production of synchrotron radiation all over the world.



The first observation of synchrotron radiation, made in 1947 at General Electric laboratory in Schenectady (NY, United States of America). According to G. C. Baldwin and D. W. Kerst, in "Origin of synchrotron radiation" (Physics Today ***28****, 9 (1975)), "...it was made possible by a trivial design change [the removal of the silver coating of the glass vaccum chamber in which the electrons were circulating] and by a conscious disregard for the rules of radiation safety".*

In this lecture, I will try to give some simple pictures of the physics involved and we will derive the main useful results from (more or less...) short and basic calculations.

We will start from a simple accelerated electric charge and see how it radiates an electric field. We will then see how this field behaves when the charged particle becomes relativistic. This will lead us to the main characteristic of synchrotron radiation emitted by bending magnets, the magnets that connect two consecutive straight sections of a storage ring. These were the first sources used by pionneering experimentalists who discovered the joy and happiness of spending their nights on capricious beamlines in noisy and dark experimental halls, while high energy physicists were enjoying a well-deserved rest.

We will then describe the insertion devices which were developped to produce light in the storage ring's straight sections. They consist in periodic arrays of magnets, placed above and below the electron beam trajectory, creating a sinusoidal magnetic field in which the particles wiggle, producing light at each bend. They are now the most efficient sources on storage rings as we will demonstrate it by calculating their main characteristics.

At the end of the lecture, we will focus on the ongoing evolutions of the field by discussing the so-called ultimate storage rings and free electron lasers.

k-Space Analyzers

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This lecture will address the basics of photoelectron momentum microscopy (MM), briefly k-space microscopy. This novel method is an alternative approach to angle-resolved photoelectron spectroscopy (ARPES) and photoelectron diffraction (PED). MM has proven superior for "photon-hungry" experiments, like soft- and hard-X-ray ARPES, spin-resolved ARPES and time-resolved pump-probe experiments studying ultrafast processes in the fs-range. MM makes use of a basic concept of microscopy: In each imaging optical system the reciprocal image (in mathematical language Fourier image) represents the distribution of the transversal momentum components. Owing to $k_{\|}$-conservation in photoemission, the observed k-distribution of photoelectrons formed in the backfocal plane of the objective lens (top left inset in Figure 1; from [1]) directly relates to the band structure inside the crystal. The intensities are determined by the photoemission matrix elements and symmetry selection rules for polarized light. A momentum microscope can be understood as a "magnifying glass" looking directly into k-space, with k-field diameters ranging between a fraction of a Brillouin zone (BZ) for maximum resolution and diameters of up to 15 Å^{-1}, yielding PED patterns with many Kikuchi lines for structural analysis. High energies can access true bulk electronic structures [2].

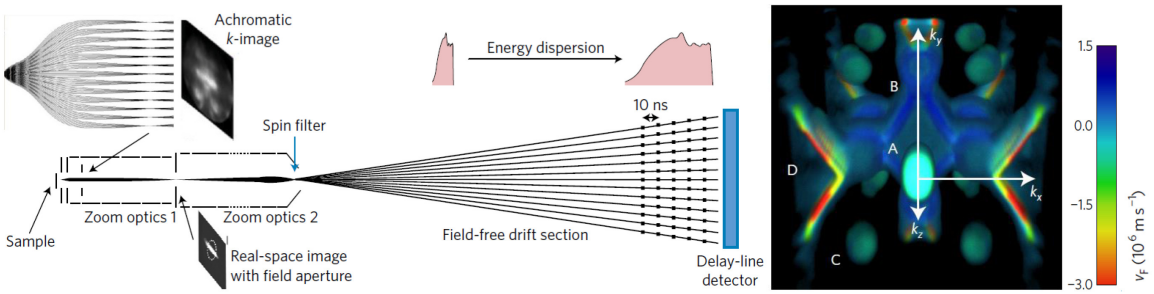

Figure 1: Left: *Schematic cross section of a* ***time-of-flight momentum microscope*** *with details of the ray paths between sample and first k-image (top left), the first real image with adjustable field aperture (bottom left), zoom optics 2, the field-free drift section (with 10 ns time markers on the rays) and the time-resolving imaging unit (delay-line detector).* ***Right:*** *View of the measured Fermi surface of tungsten; the Fermi velocity* $\boldsymbol{v_F(k)}$ *is quantified by the color bar, in* 10^6 *m/s. (from* [1]*).*

Different approaches of energy discrimination have been developed. The first one employs double or single hemispherical analyzers (HSAs) as energy filter. These instruments capture 2D k-patterns I(k_x,k_y) directly in reciprocal space on a linear k-scale at the selected energy. For comparison, conventional ARPES experiments record in real-space polar coordinates. The

transversal momentum $k_{\parallel}$ is related to the kinetic energy E_{kin} and the polar emission angle θ by the relation:

$$k_{\parallel} = 0.512 \sqrt{E_{kin}} \sin\theta \quad (1)$$

A high-performance instrument of the double-HSA type has been developed at the Max-Planck Institute in Halle [3, 4], adopting the concept of an earlier design (NanoESCA) [5], originally developed for spectroscopic real-space imaging exploiting chemical information from core levels [6]. Later, a single-HSA MM has been developed in Mainz [7, 8]. The HSA-based instruments in Halle and Mainz have shown benchmarking performance with respect to k-resolution and energy resolution, 0.0042 Å^{-1} [3] and 4.2 meV [8], respectively.

The second way of energy discrimination is based on time-of-flight (ToF) detection, facilitating parallel recording of a certain energy band of up to 6 eV, yielding 3D data arrays I(k_x, k_y, E_B) [1]. The ToF-MM solution emerged from earlier work on ToF-PEEM [9]. Fig. 1 (left) shows a schematic cross section of the ToF k-microscope. The objective lens generates a largely achromatic (∼10 eV) k-image in its backfocal plane. A subsequent first zoom optics yields a real-space (Gaussian) image in a plane, where an array of field apertures (different sizes selectable via piezomotors) is located. This field aperture allows the selection and positioning of analyzed regions on the sample surface with sizes down to the range of 1 μm, without the need for a small photon spot. A second zoom optics projects the k-image of the electrons passing the field aperture to the detector located behind a low-energy drift section. A key element is the 3D $I(k_x, k_y, t)$-resolving image detector (delay-line detector) with 145 ps time resolution and a maximum count rate of ∼5 Mcps. The intriguing advantage of the ToF-method lies in the simultaneous recording of >6 eV energy band and a k-range of up to 12 Å^{-1}, exceeding the size of typical BZs (full half-space above the sample surface up to E_{kin} ∼100 eV).

For **mapping of the full 4D bulk electronic structure**, the third momentum coordinate k_z is scanned by stepwise variation of the photon energy. After finishing the photon-energy sequence, the series of 3D data arrays corresponding to different k_z is concatenated to the 4D I($\boldsymbol{k}$,E_B) array. Examples of this approach are shown in [1]. Figure 1 shows a schematic section of a ToF-MM and the Fermi surface of tungsten. Shape and topology of the Fermi surface, velocity of the electrons at the Fermi energy $\boldsymbol{v_F(k)}$ and spin texture $\boldsymbol{P(k)}$ are key features for the design of materials with tailored electronic properties. The binding energy E_B is recorded via time of flight τ; transversal momentum (k_x,k_y) via imaging of the Fourier plane of the cathode lens and k_z by scanning the photon energy, exploiting the concept of direct transitions.

The Fermi surface is projected from the 4D data stack as the isosurface at $E = E_F$ in 3D k-space. $\boldsymbol{v_F(k)}$ is determined from the k-distance of adjacent energy isosurfaces (E_F, $E_F - \Delta E$). $\rho(E_B$,$\boldsymbol{k})$ contains all information on the electronic structure, *i.e.* band dispersions, energy isosurfaces, total and partial band gaps, effective mass and inner potential; for further reading, see [1, 2, 10].

In Figure 1, the Fermi surface contour is decorated by the corresponding Fermi velocity [group velocity $\boldsymbol{v_F(k)}$], defined by the gradient of the 3D energy dispersion $E(\boldsymbol{k})$ in momentum space. When extending this experiment to excitation by circularly polarized radiation, the corresponding circular dichroism texture of the 4D data array can be determined [10]. For the corresponding CDAD movie in 3D k-space as function of binding energy, see link [11]. The Circular Dichroism in the Angular Distribution of photoelectrons CDAD is usually quantified in terms of the asymmetry

$$A_{CDAD} = I_{RCP} - I_{LCP}/(I_{RCP} + I_{LCP}) \quad (2).$$

Due to the three-dimensional recording scheme, the ToF-approach bears the advantage of higher recording efficiency and hence higher data throughput. Naturally, it requires sources with defined time structure, while the hemisphere instruments can be operated with cw-sources like discharge lamps. Luckily, all modern high-performance photon sources like Synchrotrons, free-electron-lasers (FELs) or high-harmonic-generation (HHG) based lab sources have well defined time structures. We will show and discuss examples of rapid recording of a full 4D spectral density function $\rho(E_B,\boldsymbol{k})$ (with matrix-element-weighted intensities) and Fermi-velocity distribution. The 4D data array comprises twenty 3D-arrays with $\sim 10^6$ (E_B, k_x, k_y)-voxels each, measured in short time at the high-brilliance soft-X-ray beamline P04 of PETRA III.

The third and most recent approach of energy discrimination combines the two earlier methods, establishing a HSA & ToF hybrid MM, with an imaging ToF analyzer behind the exit slit of a large single HSA. The first prototype was installed at beamline I09 of the Diamond Light Source, UK [12]. This combination circumvents the problem that the pure ToF-MM approach cannot be performed at Synchrotron sources operated at 500 MHz pulse rate. Given a time resolution of the image detector of 145 ps, the 2 ns period of the photon pulses would not allow recording a full ToF spectrum. However, when the HSA selects a suitable bandpass, e.g. 0.5 eV, the subsequent ToF drift section and delayline detector can analyze this bandpass further. A schematic view of this instrument is shown in Figure 2; we will discuss the functioning scheme. A key

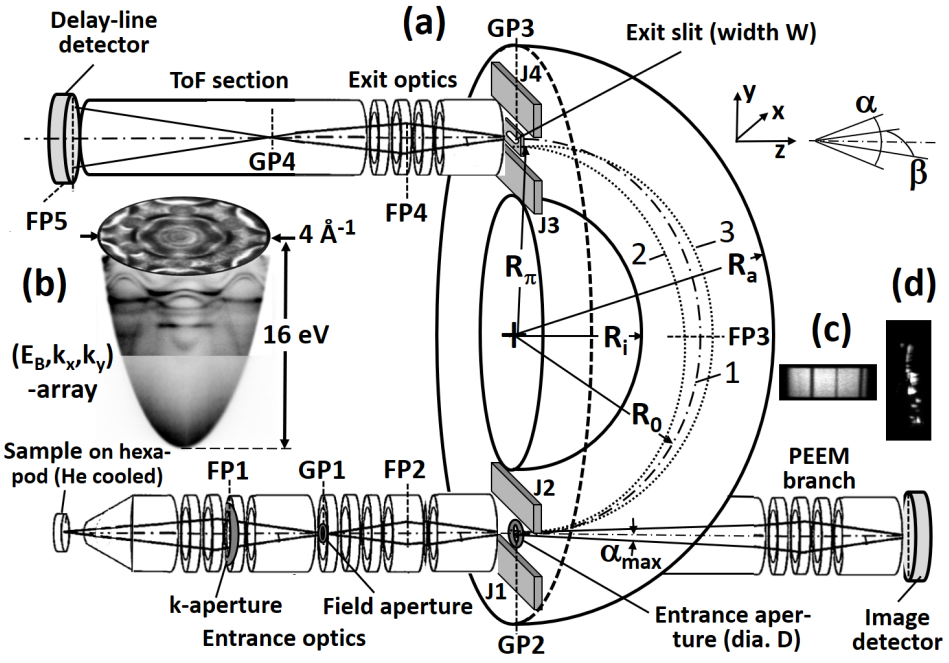

Figure 2: *Schematic view illustrating the basic principle of the hybrid single-hemisphere & ToF momentum microscope. (a) Set-up comprising entrance zoom optics, straight branch for real-space imaging (PEEM), hemisphere and exit optics with time-of-flight discrimination behind the exit slit. Electrons entering the analyzer at $\alpha = 0$ travel on a circular path (ray 1) with radius R_0. GP1-GP4 denote the Gaussian (real-space) image planes, FP1-FP5 the Fourier (momentum) image planes. (b) Data array recorded with He I radiation, (c) PEEM image of entrance aperture and calibration-grid and (d) hot-spot emission along a scratch on a smooth single-crystal surface. (from* [12]*)*

application of the hybrid MM will be ARPES at sources with high pulse rates like Synchrotrons with 500 MHz time structure; a first example is a study of the Kagome metal CsV_3Sb_5 [13].

The "ToF-booster" of this instrument captures 3D data arrays I(E_B, k_x, k_y), yielding a gain in recording efficiency of presently 24. Without the booster it can be operated with cw sources; excitation by an unfocused He lamp yielded an energy resolution of 10 meV. The α^2-*aberration term* (α: entrance angle in the dispersive plane) and the transit-time spread of electrons in the spherical field have been studied in detail and can be corrected numerically. Time- plus k-resolved detection circumvent the pre-conditions of previous theoretical work on the limitation of time- and energy-resolution due to α^2-term and transit-time spread. The paradigmatic claim that an inverting lens and second hemisphere are required for aberration correction had been questioned already in a theoretical treatment by Tusche et al. [4].

A second key application will be **PhotoElectron Diffraction (PED)**. PED was first developed in the 1970s [14, 15] and has become a powerful technique for analyzing the structure of solids. Recording efficiency has been greatly improved by a full-field imaging approach, and extending into the hard X-ray region provides access to true bulk information [16]. In these experiments a benchmarking angle resolution of 0.03° was achieved in PED mode. We will present a novel application of PED at extremely low kinetic energies, within the range of the minimum inelastic mean free path curve [17].

A full-field PED pattern with a diameter of $\sim$7 Å^{-1} is typically acquired in 5-10 minutes. This high recording speed enables ***PED movies*** to be captured with small kinetic energy steps down to 2 eV. Such movies have been recorded for Si-2p, Ge-3d and Ge-3p core-level photoelectrons at final state energies between 45 and 400 eV (kinetic energy inside the material). Thanks to a novel type of objective lens [18], these patterns correspond to polar angle ranges of 0-90° up to 80 eV and 0-30° at 230 eV. The richness in detail is incompatible with the low IMFP in this energy range. Figure 3 shows different sections through such a 3D stack for Si-2$p_{3/2}$; the image contrast is CDAD. Understanding these patterns requires new concepts to describe the core-level photoemission process, particularly with regard to the nature of the final state. In

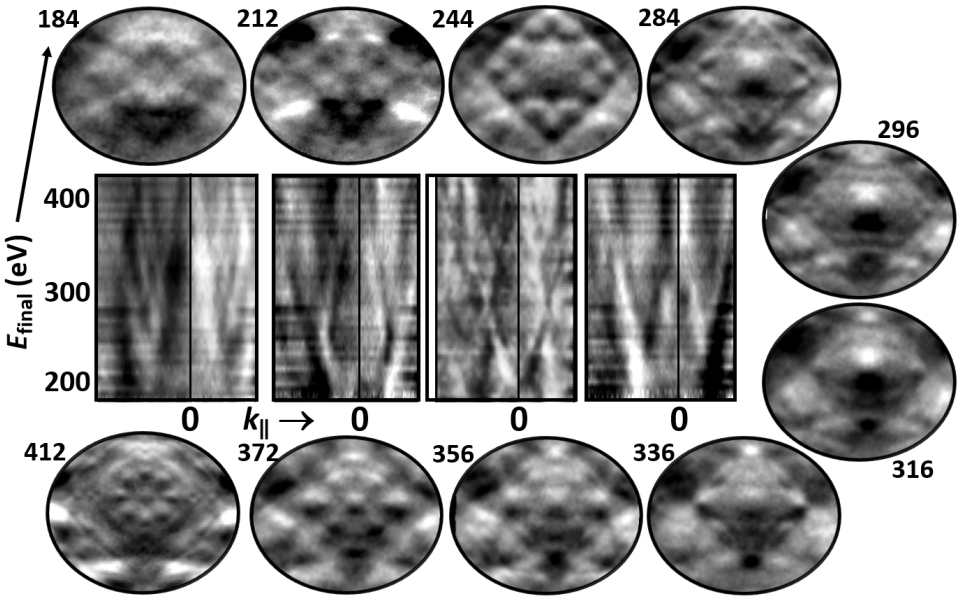

Figure 3: *PED measurement (CDAD contrast) for Si-2$p_{3/2}$, recorded in a photon energy range from 270 to 500 eV using the hybrid HSA&ToF-MM SAMMy at the Diamond Light Source, Didcot, UK. The outer panels show k_x−k_y sections, the inner ones E_B-vs-$k_{\|}$ sections at different positions. $E_{final} = h\nu - E_B + V_0$ is the kinetic energy inside of the solid.*

the last part of the lecture, I will address the application of ToF-MM with the steepest gradient, *i.e.* femtosecond time-resolved photoemission. In this type of experiment, a pump-probe

technique is used to excite an electronic system by a fs pump pulse and the ultrafast dynamics of the system is probed by a fs probe pulse. Observing the full photoelectron distribution in an energy band of several eV width, ToF-MMs can capture the hot-electron dynamics and the hole dynamics simultaneously. Several groups are using this approach and have published an amazing number of high impact papers in a few years. The 'HEXTOF' [19], is installed at the PG2 soft X-ray beamline of the free-electron laser FLASH. The high photon energies allowed to precisely observe the correlation between core-level and conduction-band dynamics [20]. This work was followed by real-time observation of the metamagnetic phase transition in FeRh [21], the first ultrafast core-level and photoelectron diffraction experiments [22], and capturing the phonon-electron energy flow in laser-heated nickel [23]. An emerging application of ToF-MM is ultrafast orbital tomography. The first experiments, performed at FLASH [24] and using HHG sources [25, 26], suggest that time-resolved tomography of molecular wave functions during chemical reactions will be possible in the near future.

High-harmonic generation (HHG)-based ToF-MM experiments are performed by several groups in Germany, Japan, France and the USA. These experiments focus on the dynamics and intrinsic timescales at which phase transitions occur in materials [27, 28], on exciton formation and the retrieval of the corresponding excitonic wavefunction [29 – 32], including moiré interlayer excitons in layered materials [33, 34]. In addition to providing deep insight into ultrafast dynamics, ToF-MM is particularly well-suited for studying time-resolved dichroism phenomena in photoelectron patterns, as demonstrated for time-reversal and Fourier dichroism [35, 36]. An emerging field is Floquet physics and other light-induced topological phenomena. The first experiments on 2H-WSe_2 [37] and graphene [38] have been successful.

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Multichannel Spin Filters

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Multichannel photoelectron recording, introduced in the 1970s in hemispherical analyzers (HSAs), see e.g. [1], gains 4 orders of magnitude in detection efficiency relative to single-channel recording. Transferring the basic idea of the multichannel approach to spin-analysis has led to a substantial increase of the effective figure-of-merit (FoM) of spin filters in conventional HSAs and momentum microscopes (MMs). This lecture will address the basics of *multichannel spin filters*, in microscopy also termed *imaging spin filters*.

The following spin-detection schemes will be discussed: in HSAs ($E_B-\theta$ *spin detection scheme*, 2D), HSA-based MMs (k_x-k_y *scheme*, 2D) and time-of-flight (ToF) MMs ($k_x-k_y-E_B$ *scheme*, 3D). Combining concepts of spectroscopy and microscopy, the latter two provide gains in FoM of 2-3 orders of magnitude compared with single-channel spin detectors.

Early spin polarimeters yielded typical values of FoM=$P^2\ \frac{I}{I_0}\ \sim 10^{-4}$ (for an overview, see [2]). Exploiting exchange-scattering asymmetries from ferromagnetic films at very low scattering energies (pioneered in [3]) improved the FoM to $\sim 10^{-2}$. The fairly slow improvement over several decades turned into a steep increase with the advent of multichannel spin detection. The ToF-Mott [4] and ToF-SPLEED-detector [5] constituted the first multichannel spin filters with parallel energy recording (1D). The idea of 2D parallel spin detection by spatially-resolved diffraction or scattering [6] was first realised in Mainz and Halle. In the $E-\theta$ detection mode of a HSA the imaging spin filter detects an energy band and a range of emission angles in parallel [7], in a HSA-based MM a spin-filtered (k_x, k_y)- or real-space image is recorded [8] and the ToF-based MM adds parallel recording of a certain energy band, yielding a spin-filtered (k_x, k_y, E_B)-data stack [9]. Early experiments used W(001) [7, 8]. With Ir(001) [10] and Ir(001)-Au(1×1) [11] spin-filter surfaces with high figure-of-merit and long lifetime in UHV have been found.

The functioning principle is illustrated in Figure 1. The left panel shows a schematic section of the $E-\theta$ approach, omitting the electron lens system for sake of simplicity. Instead of a single beam, a complete 2D electron distribution is analyzed simultaneously. The figure shows the case of specular diffraction from a single-crystal surface, it could as well be Mott-scattering at a Au foil at higher energies [12]. The energy coordinate (in the drawing plane) and angular coordinate (perpendicular to the plane) are retained by the diffraction/scattering process.

The effective FoM is given by the average single-channel FoM times the number N of resolved pixels (i,j) or voxels in the ToF spin filter:

$$\mathrm{FoM}_{eff} = \mathrm{N} <\mathrm{FoM}_{(i,j)single}>$$

Although FoM_{single} stays in the range of 10^{-3} to 10^{-2}, FoM_{eff} exceeds 1 (being the value for a perfect, Stern-Gerlach-type single-channel spin filter) due to the factor N; for details and the evolution over some decades, see [13]. The $k_x - k_y$ detection scheme reached a value of FoM=37 with the optimized double-HSA MM in Halle [14]. This instrument delivers stacks of spin-resolved full-field $k_x - k_y$ momentum images comprising $\sim 10^5$ resolved data pixels in each image. In Mainz we pursued the combination of the imaging spin filter with ToF parallel energy

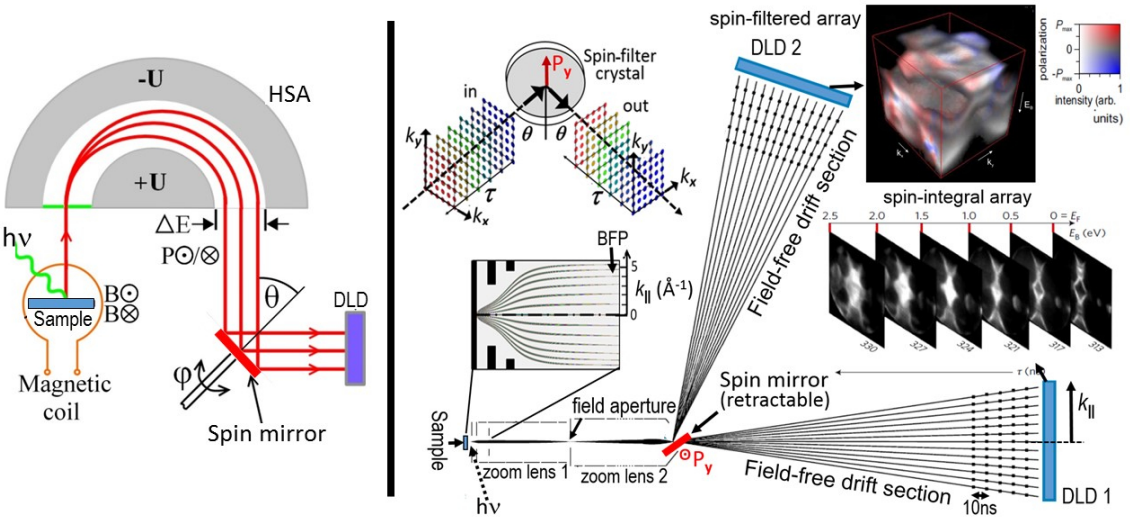

Figure 1: *Strategies for 2D and 3D parallel spin detection using a hemispherical analyzer (left, from* [7]*) and a ToF-type momentum microscope (right). The top centre inset illustrates the scheme of 3D spin filtering, the top right inset the spin texture of anomalous surface states on W(110) (from* [15]*). Objective and zoom lens 1 focus the electrons from the sample via the first k-image in the backfocal plane (BFP) to the first real image with adjustable field aperture, zoom lens 2 focuses the beam to the spin filter. The diffracted beam passes the field-free drift section to the time- and space-resolving delay-line detector (DLD2). The straight branch with DLD1 records spin-integral stacks.*

recording, making up a 3D $k_x - k_y - E_B$ detection scheme and another gain factor of 10. Figure 1 (right panel) shows a schematic cross section of the spin-filtered ToF k-space microscope. The spin filter scheme is illustrated in the inset: The momentum coordinates (k_x, k_y) are encoded in the lateral position (or scattering angle); the energy coordinate is encoded in the time-of-flight τ.

The spin-filter arrangement sketched in Figure 1 (right panel) records one spin component simultaneously as function of three coordinates, here $P_y(k_x, k_y, E_B)$. As example, the top right inset shows the spin texture of the surface states on W(110) (from [15]) and the image sequence below shows cuts through the measured array $I(k_x, k_y, E_B)$. This data set covering the complete Brillouin zone revealed the existence of a time-reversal invariant surface state in a local bandgap of W, showing Dirac-type spin texture like a topological surface state. The example in Figure 2 shows the spin texture of the ferroelectric bulk Rashba system α-GeTe(111) [16]. The complex texture with Rashba-split surface and bulk states requires a full 3D analysis as provided by the spin-filtered ToF k-microscope.

Finally, we will discuss the capability of vectorial multichannel spin detection [17]. Several problems still need to be solved, like the energy-dependence of the spin asymmetry or the chromatic aberration of the electron-optical system. For a review, see [18].

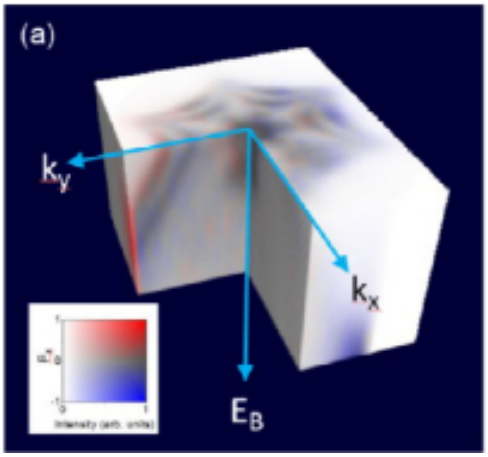

Figure 2: *Spatial view of the spin-polarization texture for the ferroelectric bulk Rashba semiconductor α-GeTe(111). The color code shows spin up and down in red and blue and unpolarized intensity in grey. (from* [16]*)*

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High-Order Harmonic Generation Sources For Ultrafast X-ray Spectroscopies

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In the context of time-resolved spectroscopy, one important advance was the discovery of high-order harmonic generation (HHG), a strong-field interaction between a femtosecond laser pulse and a gas or solid medium. This phenomenon proved to be able to produce pulses of light of attosecond duration (1 as = 10^{-18} s) with wavelengths in the extreme ultraviolet and soft X-ray domains, on a table-top setup. This discovery, together with the characterization of attosecond pulses, have been awarded the 2023 Nobel Prize in Physics. HHG has now become a widely used tool to observe ultrafast dynamics in molecules and materials.

In this lecture, the fundamentals of high-order harmonics generation will be presented. Current strategies to increase the photon energy towards the soft X-ray domain will be discussed. Finally, I will present a few examples targeting correlated materials.

Probing Correlated Electron Systems with Core-level X-ray Spectroscopies

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Transition metal and rare earth compounds exhibit a remarkable range of physical and chemical properties—including superconductivity, ferroelectricity, and magnetism—that make them central to technologies like data storage, ultrafast electronics, and sensing. This rich behavior stems from the low-energy degrees of freedom associated with partially filled d- and f-electron shells. However, strong local interactions in these open-shell systems make them challenging to understand and model.

Core-level spectroscopies provide powerful tools to probe these materials. In the first lecture, I will introduce X-ray Absorption Spectroscopy (XAS) as a method for element- and site-specific insight into electronic structure. I will explain why electron-electron interactions in correlated systems must be treated beyond mean-field approaches, and how this is addressed within Ligand Field Multiplet Theory (LFMT) [1].

We will then examine how polarization control in XAS experiments—specifically through dichroism—enables the determination of ground-state spin and orbital magnetic moments using the famous sum rules [2, 3]. We will also discuss how to construct the full complex conductivity tensor—experimentally and theoretically—with an example from Fe_3O_4 [4]. These approaches can be extended spatially using X-ray Photoemission Electron Microscopy (X-PEEM), which enables nanoscale mapping of magnetic domains. I will present examples including antiferromagnetic domains in engineered perovskite thin films [5], as well as recent advances in visualizing altermagnetic domains [6].

In the second lecture, I will discuss the limitations of XAS, showing how even dichroism may not unambiguously identify the ground state, using the example of $FePS_3$, a van der Waals antiferromagnet that retains long-range order down to the monolayer limit [7]. I will then introduce Resonant Inelastic X-ray Scattering (RIXS), which provides access to low-energy excitations. I will explain how RIXS reveals subtle distortions in $FePS_3$ and how its cross-section is computed within LFMT. We will see that the RIXS process involves a higher-rank tensor, giving rise to complex polarization-dependent selection rules and unexpected dichroism effects [8].

Finally, I will briefly introduce how RIXS can resolve elementary excitations such as magnons and preview emerging capabilities in femtosecond time-resolved RIXS at X-ray free-electron lasers (XFELs) [9], which will be covered in more detail during the dedicated RIXS sessions

later in the program.

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Hard X-ray Photoelectron Spectroscopy (HAXPES) – An introductory Guide

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X-ray photoelectron spectroscopy has been developed as one of the most powerful tools to explore the chemical composition and electronic structure of solids. While the probing depth of classical XPS using laboratory x-ray sources is well suited for studying the subsurface region of an ultrathin film (about 3–5 nm), the photoelectron information depth is significantly enhanced to tens of nanometers by performing photoelectron spectroscopy in the hard x-ray regime (HAXPES). The strongly reduced photoelectron cross sections at high photon energies are compensated by high brilliance beamlines optimized for HAXPES, and provides the opportunity to element-selectively monitor chemical states, electronic and electrostatic properties with bulk sensitivity.

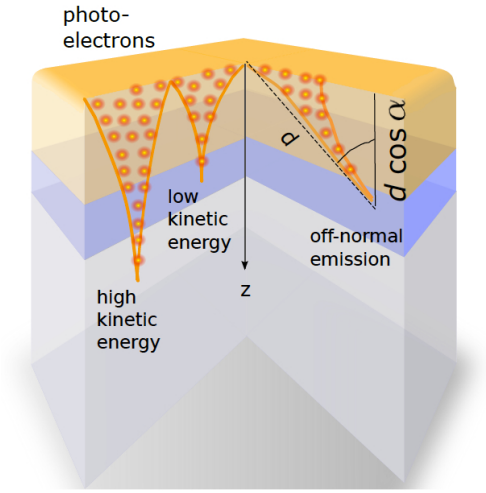

Figure:*Photoelectron yields for low and high kinetic energy and off-normal emission. In case of a high kinetic energy of the photoelectrons, the information depth is large due to less probable inelastic scattering. Low-kinetic energy electrons experience inelastic scattering more likely on their escape paths, such that the depth of unscattered photoelectrons is smaller. Off-normal emission reduces the information depths by cos α and makes this configuration more surface sensitive.*

In addition, HAXPES allows for a nondestructive depth profiling by varying either the photon excitation energy or photoelectron emission angle. A quantification of stoichiometry via chemical binding energy shifts is possible down to a few percent, which permits uncovering for example redox processes by valence changes. Spectroscopic signatures of indirect nature, like defects or

vacancies, become apparent by rigid binding energy shifts of core levels, which are caused by changes of the Fermi level position in an altered local electric potential. This approach is also used in the so-called Kraut method, which can be applied to derive the band alignment at materials interfaces, provided that there are no chemical reactions. For such samples, the variant of *in operando* HAXPES becomes applicable, which serves as a powerful tool to determine the band alignment and the chemical state of interfaces under operation conditions of an electric device in a single measurement.

This lecture highlights research examples for which synchrotron-based hard X-ray photoelectron spectroscopy emerged as the key experimental probe to uncover chemical, electrostatic and magnetic phenomena in multilayers. In particular, emerging interface states and their tunability in ferro(i)magnetic and ferroelectric oxide heterostructures — covering both fundamental aspects and exploring application-relevant devices — are discussed.

Further readings:

Hard X-ray Photoelectron Spectroscopy– Joseph C. Woicik (Edt.) Springer 2018.
W. Drube (Edt.), *Recent advances in Hard X-ray photoelectron spectroscopy*, J. Electron Spectroscopy, Vol. **190**, p.125-314 (2013).
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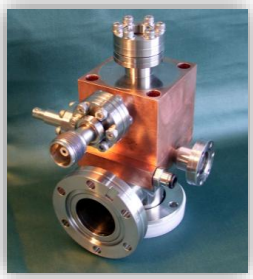

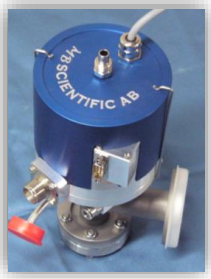

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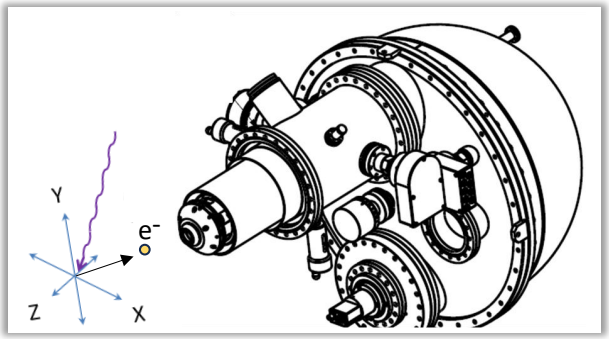

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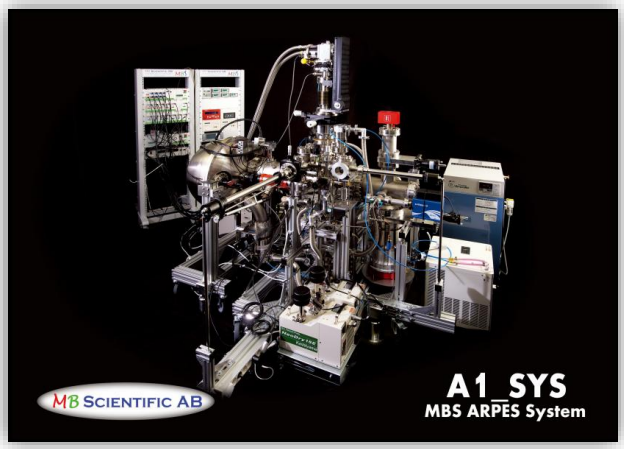

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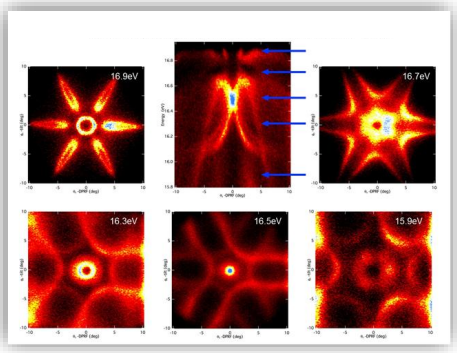
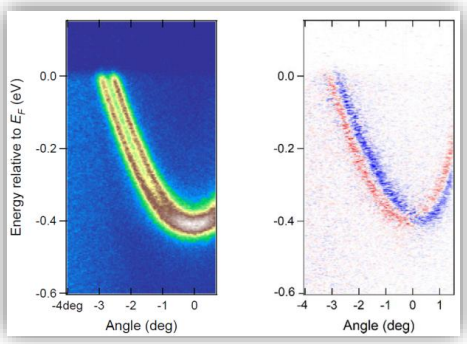
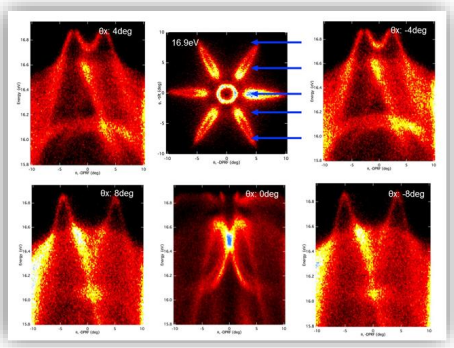
A-1 Performance

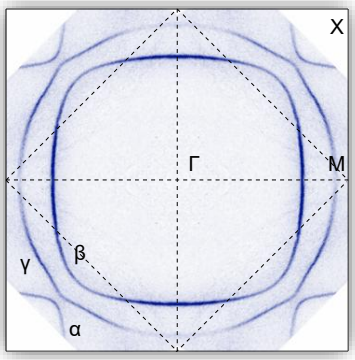




Data of Prof. Dr. Kiyohisa Tanaka at UVSOR. Fermi surface Au111 acquisition using of MBS A-1 Spin system including the and MBS Spin Manipulator.



Bi (111) Angular Mapping Data taken by Dr. M. Imamura & Prof. Dr. K. Takahashi at Saga University Synchrotron Light Application Centre using MBS A-1_#0004.



Fermi surface of Sr_2RuO_4 11 eV Lumeras laser and MBS A1 analyzer (A1_#0021). Dr. Anna Tamai and Prof. Felix provided this data which was taken by rotating the sample and is symmetrized.

Data Acquisition

MBS A-1 provides an integrated data acquisition system that maps the kinetic energy and emission angles of electrons. The analyser is controlled via LabView software, enabling real-time visualization and flexible control over lens modes, detector settings, and acquisition parameters. The system supports both 2D (see in the data above) and 3D data mapping.

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Angle-resolved photoemission spectroscopy for the study of the electronic structure of correlated materials

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Angle-resolved photoemission spectroscopy (ARPES) gives direct access to the electronic structure of a material, providing valuable information about the many-body interactions and/or phase transitions affecting it.

This lecture will review some recent applications of ARPES to the study of the electronic structure of paradigmatic correlated systems. Time permitting, topics to be discussed include:

- Brief overview of many-body effects and how to study them using ARPES.
- Electron-phonon coupling (and similar electron-boson couplings).
- High-T_C Superconductivity.
- One-dimensional systems and spin-charge separation.
- 2D electron systems at oxide surfaces and interfaces.
- Heavy fermions and exotic phase transitions.
- Metal-to-insulator transition.

Operando X-ray Spectroscopy of Complex Oxide Electrocatalysts – Bridging Surface Dynamics and Water Electrolysis Performance

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The transition to sustainable energy systems demands electrocatalysts that combine high activity, stability, and elemental abundance for reactions like the oxygen evolution reaction (OER) in water electrolysis. A central challenge lies in the dynamic restructuring of catalyst surfaces under operational conditions, where the *true active phase* often diverges from the as-synthesized material. This complexity is amplified in strongly correlated oxides, such as perovskite heterostructures and high-entropy oxides (HEOs), where synergistic interactions between multiple transition metal cations and epitaxial strain effects govern interfacial electronic states.

In this talk, I will discuss how **operando X-ray photoemission (XPS)** and **X-ray absorption spectroscopy (XAS)** enable direct probing of electronic structure, surface composition, and ligand environments during electrocatalysis. Using epitaxial thin films of model systems like $LaNiO_3$ and multi-cation HEOs (e.g., $LaCr_{0.2}Mn_{0.2}Fe_{0.2}Co_{0.2}Ni_{0.2}O_{3-\delta}$), we decouple the roles of surface termination, oxidation states, and subsurface correlations in OER activity. For instance, atomic-layer-controlled $LaNiO_3$ films reveal that Ni-terminated surfaces exhibit 2× higher activity than La-terminated analogs, linked to Ni^{2+}/Ni^{3+} redox dynamics and formation of highly active sites via surface transformations [1]. In $La_{0.67}Sr_{0.33}MnO_3$, we demonstrated that the presence of ferromagnetic ordering below the Curie temperature enhances OER activity [2].

A key focus is the **high-entropy design strategy**, where configurational disorder in HEOs promotes cooperative redox transitions. X-ray photoemission studies reveal a synergistic effect of simultaneous oxidation and reduction of different transition metal cations during adsorption of reaction intermediates, leading to the hypothesis that neighboring sites may contribute to the formation of different reaction intermediates, thus optimizing the overall efficiency [3].

Finally, I will address technical advances in liquid-phase operando XPS [4], which enhance surface sensitivity to track surface transformations, even with laboratory-based XPS instruments like the **MESA+ operando HAXPES user facility** [5]. Overall, these operando approaches enable insights into the true active surface phase, making them essential for the rational, predictive design of next-generation energy materials.

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In Situ Photoemission Spectroscopy Combined With Oxide Molecular Beam Epitaxy

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Understanding the unique quantum states appearing at interfaces is crucial for designing functionalities in oxide nanostructures. These functionalities arise from strong mutual coupling among the spin, charge, and orbital degrees of freedom in the interface region between two different oxides [1]. Therefore, to control such functionalities, it is necessary to clarify the interfacial electronic, magnetic, and orbital structures. We are therefore using synchrotron radiation spectroscopic techniques having elemental selectivity to probe these structures in the nm-scale at oxide heterointerfaces. For example, the electronic structure at the interfaces is determined by angle-resolved photoemission spectroscopy (ARPES) and X-ray absorption spectroscopy (XAS), the magnetic structure by magnetic circular dichroism of XAS, and the orbital structure by linear dichroism of XAS. We aim to design and create novel quantum materials by optimally combining such advanced analysis techniques using synchrotron light with sophisticated oxide growth techniques using laser molecular beam epitaxy (MBE). This approach unveils the relationship between the nanostructures and functionalities. In my lecture, I will explain how synchrotron-radiation spectroscopy provides important insights for functionality design of oxide nanostructures by introducing our recent activities, as listed below:

1. Development of an in situ photoemission spectrometer- oxide MBE system which is installed at an undulator beamline [2]
2. Creation and control of two-dimensional liquid states in oxide quantum well structures by visualization of quantization states using *in situ* ARPES [3]
3. Resonant-tunneling Mott transistor designed by synchrotron-radiation analysis [2,4]
4. Control of interfacial charge transfer based on the common-anion rule [5]

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Soft X-Ray Photoemission Spectroscopy Applied To Functional Electronic Materials

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The semiconductor technology used for the electrical products has been made progress through miniaturization of the devices, realizing for example handy seized high-performance smartphone in the modern era. However, effective transistor size becomes 5 nm or less has been achieved, which is the size at which quantum mechanical effects become pronounced, and the production costs are a problem for further miniaturization. Thus, the improvement of the device performance through the miniaturization is approaching its physical limit. On the other hand, as the Novel Prize was recently awarded to generative AI, the development of the information society including IoT, big data, and supercomputing has been remarkably progressed. Additionally, the evolution of the hardware to support is desirable to sustain the development of the information society. Then, next-generation electronics based on new scientific principles following the conventional semiconductor engineering are indispensable for future electronics.

Quantum materials show extraordinary physical properties beyond the conventional materials such as superconducting, metal-insulator transition, colossal magnetoresistance, high mobility quantum transport, and so on. Indeed, semiconductor spintronics, oxide electronics, and topological electronics using quantum materials are being studied as candidates for next-generation electronics. One possible approach for such electronics would be to combine quantum materials with the state-of-the-art semiconductor engineering to create new functionalities and extend the contemporary semiconductor technology.

In the semiconductor engineering, the devices have developed based on band theory with rigid band picture, which describe the electronic properties of the conventional materials. Then, there has been little demand for direct experimental observation of the electronic structure (band structure) of semiconductor materials and heterostructures. However, in quantum properties such as superconductivity, metal-insulator transition, ferromagnetism and high-mobility topological surface states, where electron correlation, spin and orbital degrees of freedom and topology are relevant, *the band theory based on the one-electron approximation itself cannot describe the electronic properties of semiconductor quantum-material heterostructures.*

X-ray spectroscopies are very useful experimental tools to investigate electronic and magnetic states of the quantum material heterostructures. In particular, angle-resolved photoemission spectroscopy (ARPES) is one of the most powerful experimental tools to observe band dispersion in a crystalline thin film. X-ray absorption spectroscopy (XAS) allows us to study chemical

states of transition metals, and X-ray magnetic circular dichroism (XMCD) allows us to study element-specific magnetic states. Then, ARPES can study the band dispersion and electronic structure near the Fermi level of metals and semiconductors, and XAS/XMCD can elucidate the local electronic structure of transition metals.

In this lecture, I would like to explain the scientific background of the semiconductor technology and principles of the soft X-ray spectroscopy, share recent highlight data of the soft X-ray spectroscopy, and give a perspective for future electronics.

Theoretical Description Of ARPES: One Step Model Of Photoemission

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Spectroscopy is an extremely important experimental tool providing information on the electronic structure of the probed system that has to be seen as a stringent benchmark for the success of any electron structure theory. Photoemission spectroscopy (PES) or its inverse – the Bremsstrahlen isochromat spectroscopy (BIS) – in their angle-integrated form should reflect the density of states (DOS) rather directly, in particular in the high photon energy regime (XPS). For that reason it is quite common to check the ab-initio calculations by comparing the calculated DOS directly to PES spectra. However, this approach ignores the influence of the specific PES matrix elements that in general will introduce an element- and energy-dependent weight to the partial DOS.

In case of angle-resolved photo emission (ARPES) the situation is even more severe as the surface as well as dipole selection rules may have a very pronounced impact on the spectra demanding for a coherent description within so called one-step model of photoemission.

In the first lecture, I will present a general theoretical description of the ARPES by means of one-step model of photoemission. After the historical overview of this method, I will discuss how to solve the Fermi golden rule for semi-infinite surface. This is done by multiple scattering Green's function KKR method.

In the second lecture, I will present recent developments of the one-step model of photoemission as, for example, inclusion of correlation effects by means of dynamical mean field theory (DMFT), description of disordered alloys by so called coherent potential approximation (CPA) and inclusion of electron-phonon coupling. All developments will be followed by corresponding examples covering the wide photon energy window, e.g. from laser photoemission up to soft and hard-X-ray regime.

In the third lecture, I will present features of the Munich SPR-KKR package including graphical user interface xband. This package includes possibility to calculate various spectroscopic methods, in particular ARPES.

Topological Insulators For Dummies

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Topological Insulators are new states of matter. At first sight, these are just ordinary band insulators : an energy gap separates the energy of states occupied by electrons from unoccupied states. However, the ensemble of occupied electronic states possesses a non-intuitive property, known in mathematics as a topological property. Its existence is at the origin of the main physical characteristic of topological insulators : the existence or metallic states at their surface.

Hence from a phenomenological point of view the topological insulators are insulating materials surrounded by a metallic surface. Moreover these surface metals are rather unique : their electrons behave as if they were massless relativistic particles. More precisely their motion is described by a Dirac equation usually associated with relativistic particles. This leads to several unique physical properties, some of them reminiscent of those of graphene. Recently, this relation between relativistic excitations and topological property triggered a large amount of work to identify other phases with analogous properties.

In these lectures I will introduce in a simple and pedagogical way the notion of topological property of an insulator, and the constraints it imposes on its surface properties.

Resonant Spectroscopies (XAS, RXS, RIXS) For The Study Of Strongly-Correlated Materials

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Modern synchrotrons offer brilliant, intense and tunable sources of x-rays with a full control of polarization. In particular, in the 450-1000 eV photon energy range we can find all the $L_{2,3}$ absorption edges of $3d$ transition metals, from Ti to Cu, so that the highly resonant $2p \rightarrow 3d$ transition can be exploited to study the $3d$ states in $3d$-TM oxides, even in very thin films or diluted systems. Moreover oxygen K edge and lanthanides' $M_{4,5}$ edges fall in the same energy range. That is why high resolution resonant spectroscopies have blossomed particularly in the soft x-rays, although remarkable developments have taken place in the hard x-rays for $4d$ and $5d$ transition metals.

XAS (x-ray absorption spectroscopy) is a well established technique at the $L_{2,3}$ edges. XAS is also the first of the two steps giving rise to resonant x-ray scattering, a second order process that can reveal a variety of properties of the electronic and magnetic structure of materials. The elastic scattering (RXS), a sort of resonant diffraction technique, is used to study spin, charge and orbital ordering phenomena. The inelastic scattering spectra (RIXS) are rich with information about local and collective excitations.

When measured with high energy resolution (better than 50 meV), the $2p \rightarrow 3d \rightarrow 2p$ RIXS process can provide a wealth of information with chemical and site selectivity. Being an energy loss spectroscopy, RIXS is akin to optical Raman, electron energy loss spectroscopy or inelastic neutron scattering. It can provide access to orbital, spin, lattice and charge excitations, of local or collective character. Its strength is in the selectivity, where the polarization dependence of the excitation and de-excitation steps adds further information on the symmetry of the excitation left in the sample. I will introduce the basic concepts of the technique and provide some key information on the instrumentation. Then I will present recent results, where RIXS has been used to study localized dd excitations, spin wave dispersion, electron-phonon coupling and charge order phenomena. High T_c superconducting cuprates will provide most of the examples of significant RIXS results.

Introduction to XAS and resonant spectroscopy in general will take approximately 1 hour. The remaining 2 hours will be devoted to high resolution RIXS.

Recent Advances In Probing Excited States Of Solids By Time-Resolved ARPES

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In strongly correlated systems, electron, spin, and phonon degrees of freedom are intricately intertwined, and various symmetry breaking phenomena occurs. These systems exhibit condensed states reflecting the interactions, thereby acquiring peculiar anisotropy and/or hierarchical structures which show unique dynamics in non-equilibrium states. Recently we have been working on observations of these dynamics by using new measurement techniques such as time- & angle-resolved photoelectron spectroscopy and ultrafast electron microscopy.

In this talk, I will introduce our works on several correlated materials e.g. nematic iron-based superconductor FeSe, trimer-ordered "charge-density-wave" material VTe_2 and room-temperature magnetic skyrmion CoZnMn system. In FeSe, through the time-, energy-, momentum- and orbital-resolved photoelectron spectroscopy, we detected the ultrafast dynamics of the Fermi surface anisotropy, and found the short-lived nematic oscillation appearing right after the strong perturbation by light [1]. In VTe_2, we first clarified the electronic structure and found that the trimer formation is intimately related with the band inversion and the Dirac surface state located at the Brillouin zone boundaries [2]. In addition, by using the ultrafast electron diffraction and imaging, we found the peculiar phononic responses related to the trimer dissolution by optical irradiation [3], suggesting the possibility of ultrafast control of band inversion. Finally, we introduce our recent work on CoZnMn system, where the hierarchical spatiotemporal behavior of magnetic skyrmions are visualized by nanosecond × nanometer magnetic imaging [4].

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Electronic Correlations In Moiré Materials

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A major breakthrough in the field of correlated materials happened in 2018 with the discovery of gate-tunable superconductivity and correlated insulating states in magic angle twisted bilayer graphene (TBG), two layers of graphene with a relative rotation angle of 1°, opening the fields of twistronics and moiré materials. Stacking two similar, but non-identical, lattices creates a moiré pattern with a very large unit cell, up to several thousand atoms, which alters the electronic structure of the material and controls its properties. Combining 2D materials of diverse functionalities and lattices, with different moiré realizations, including a variety of twisted geometries or selective alignment with the substrate, opens endless possibilities for the design of quantum materials. Under certain conditions very narrow electronic bands, highly sensitive to electronic interactions, with very unconventional topological properties form.

Since 2018, an incredible variety of correlated quantum states and phenomena have been found in TBG and other moiré materials. Remarkably, the properties of these materials are highly tunable with gate electrodes (which alter doping and displacement field), magnetic field, substrate alignment, strain, pressure, etc...

In the talk I will first give an overview of flat band moiré materials and of some of the electronic states that have been found. Then I will discuss how the interplay of strong correlations and topology shape the spectrum and electronic properties of twisted bilayer graphene, described in terms of topological heavy electron models.

Spin- and Angle-Resolved Photoelectron Spectroscopy

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Angle-resolved photoelectron spectroscopy (ARPES) is one of the most powerful tools for investigating the electronic structure of solids as it allows direct experimental access to the band structure. Spin- and angle-resolved photoelectron spectroscopy (SARPES) is the method adding the capability of resolving the spin of electrons to the ARPES measurement, which is realized by combining a spin detector with an electron analyzer in a standard ARPES setup.
Since spin polarized states arising in the Rashba systems or topological materials is **k**-dependent, the observation of **k**-resolved spin polarization — i.e., spin-resolved band structure — is essential for understanding the spin texture of such a new class of materials, and SARPES is the only method that can directly provide this information.

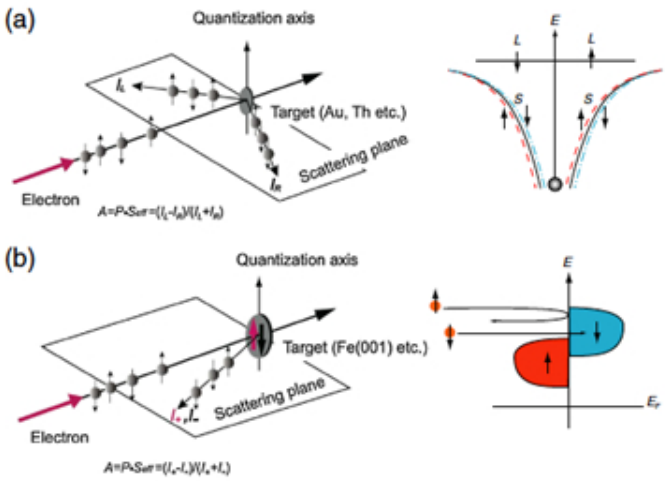

Figure: *Principles of the electron spin-detection. (a) Mott detector utilizing the spin-dependent electron scattering by spin-orbit interaction. (b)VLEED detector utilizing spin-dependent electron reflectivity by exchange split bands.*

As shown in Figure, spin detectors currently in practical use utilize spin-dependent electron scattering. Among them, the Mott detector is the most widely used detector, in which the spin

polarization of incoming electrons is deduced from the intensity asymmetry of scattered electrons detected by the left and right electron counters after scattering off a heavy metal target (e.g., Au, Th), due to the spin-orbit interaction (see Figure(a)). One of the advantages of the Mott detector is its ability to simultaneously measure two orthogonal components of spin polarization (e.g., S_x and S_z) with stable performance. However, the low efficiency of spin detection (figure of merit: FOM$\simeq 10^{-4}$) limits its applicability to high-resolution measurements. The efficiency can be improved by employing an alternative method of spin detection. As shown in Figure(b), spin-dependent electron reflection (or absorption) by the unoccupied bands of a ferromagnetic material—where the spin-up and spin-down bands are energetically shifted due to exchange interaction—can be utilized for spin detection. A spin detector using this principle is called a VLEED (Very Low Energy Electron Diffraction) detector, as it operates with electron energies around 10 eV, which is much lower than that of the Mott detector (>20 keV). Owing to the approximately 10 times higher reflectivity of low-energy electrons and enhanced spin sensitivity in this method, the VLEED detector achieves about 100 times higher efficiency than the Mott detector.

The recent discovery of Weyl semimetals, altermagnets, and related materials has driven the demand for much higher energy, angular, and spatial resolutions, along with improved efficiency in SARPES measurements. Multi-channel spin detection (see Gerd Schönhense's lecture) and laser-based SARPES are among the promising approaches to meet these demands. In this context, this lecture will present recent developments in SARPES techniques and their applications in current research.

Time and Angle Resolved Photoemission Spectroscopy

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Time- and angle-resolved photoemission spectroscopy (trARPES) is a pump-probe technique that provides a direct view on the energy- and momentum-resolved non-equilibrium carrier dynamics as well as the transient band structure of various photoexcited solids. In my lecture I will

1. introduce the technical basics such as the generation of (extreme) ultraviolet probe pulses and variable wavelength pump pulses,
2. address common problems including space charge effects and laser assisted photoemission that need to be understood when measuring and interpreting trARPES data, and
3. highlight a few applications of the technique including ultrafast charge transfer in van-der-Waals heterostructures [1], light-induced phase transitions [2], the formation of photon-dressed states [3], and the visualization of light-wave driven currents [4].

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Laser-PEEM: A Tool For Electronic Structure Imaging With Temporal And Spatial Resolutions

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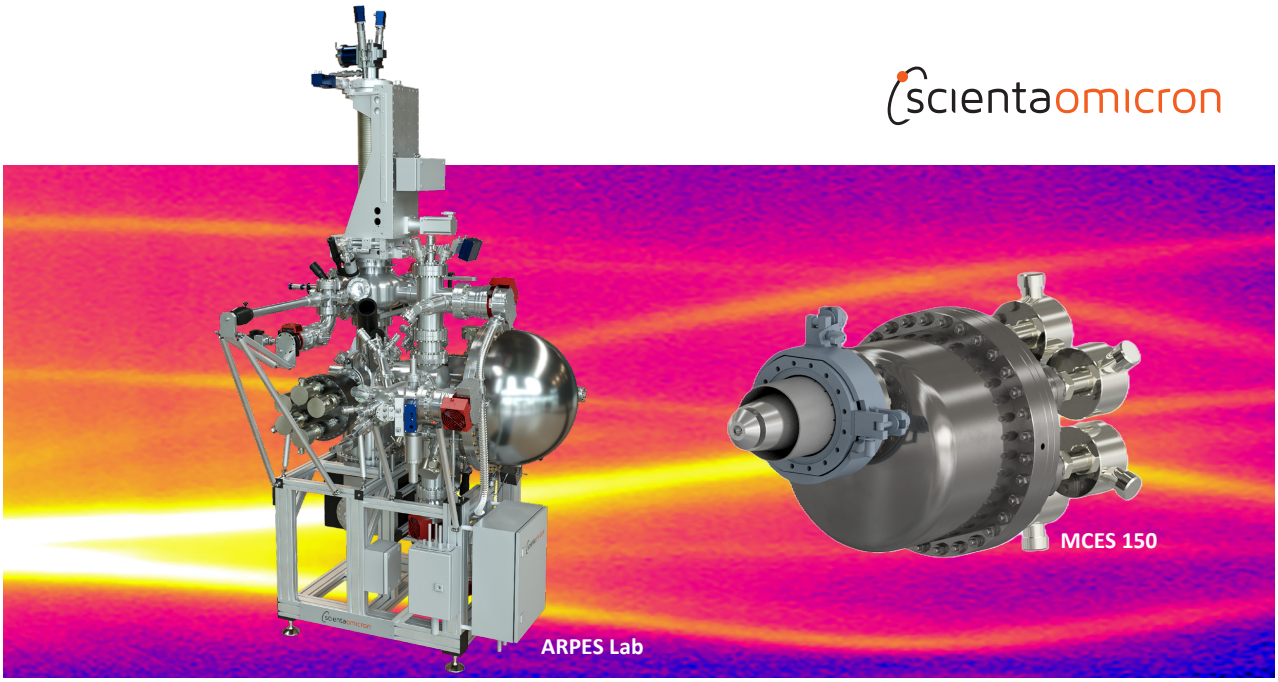
Photoemission electron microscopy (PEEM) is an imaging method based on a cathode objective lens, which enables non-scanning and high-resolution imaging of electrons emitted from sample surfaces. Synchrotron radiation PEEM (XPEEM) has evolved into a powerful spectromicroscopy characterization tool, which enables us to map local difference in the emitter chemical state, site location or valence state as well as magnetic order. Thanks to femtosecond pump–probe techniques, laser-based PEEM (laser-PEEM) has been emerging as a temporally resolved microscopy tool. In the recent decade, this technique has been established mainly for the observation of surface plasmons: collective charge density fluctuations that can be excited by external optical fields at metal-vacuum interfaces.

Another technical feature of laser-PEEM is very high spatial resolution. Combination of continuous wave laser and aberration correction technique in electron optics has significantly improved its spatial resolution, because it is able to avoid space charge effect and compensate the spherical and chromatic aberrations. With ultraviolet laser excitation, photoemission yield (threshold photoemission yield) strongly depends on density of states, work function and magnetic order of samples. Therefore laser-PEEM is expected to be one of the most powerful tools for ultrahigh resolution chemical and magnetic imaging.

After an introduction into the basic concept of PEEM, the lecture will describe the history and present situation of laser-PEEM technique with some of its unique use cases such as temporal and/or spatial resolved imaging of surface plasmons, electron carriers, magnetism, and so on. The lecture will close with some views on its future possibilities.

Participants Talks



From electrons to collective excitations: The ARPES-HREELS synergy

High Resolution Electron Energy Loss Spectroscopy (HREELS) is a method for investigating the collective excitations of quantum materials.

The Scienta Omicron ARPES Lab now features a high-intensity, narrow-bandwidth electron source for HREELS measurements, seamlessly integrated into a single, cutting-edge system.

Combined with VUV and X-ray excitation sources and the groundbreaking DFS30 analyzer, featuring electrostatic 3D focus adjustment, the lab empowers researchers to explore a wide range of quantum properties on a single sample, including:

- Electronic band structure
- Chemical composition
- Vibrational modes
- Dispersion of collective excitations (phonons, plasmons, excitons, magnons)

This unified setup makes the investigation of quantum materials more accessible and feasible than ever before!

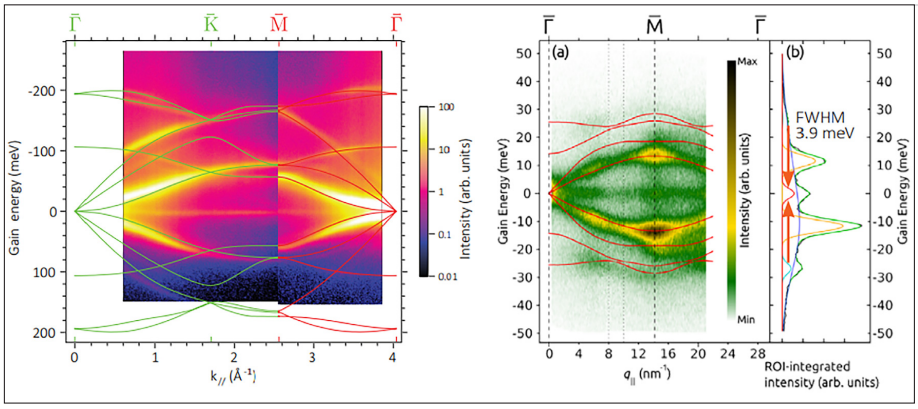


Figure 1, Left: Phonon dispersion of single crystal graphite, measured along the Γ-M direction. Single spectrum, primary energy 110 eV.

Data courtesy: Dr. F. C. Bocquet and Prof. F. S. Tautz, PGI-3 @ FZJülich, Dr. S. Tanaka, Osaka Univ.

Right: Dispersion of Cu(111) surface phonons, acquired in merely 7 minutes (private communication).
The experimental resolution after multi-phonon background subtraction is 3.9 meV.

Data: Ibach et al, Review of Scientific Instruments, 88(2017)033903.

Explore now at *www.scientaomicron.com/Arpes-Lab*

Tuesday, September the 23^{rd} – 16h00

A Pedagical Introduction To The Measurements Of 2D Materials: Two-Dimensional To Bulk Crossover Of The WSe_2 Electronic Band Structure

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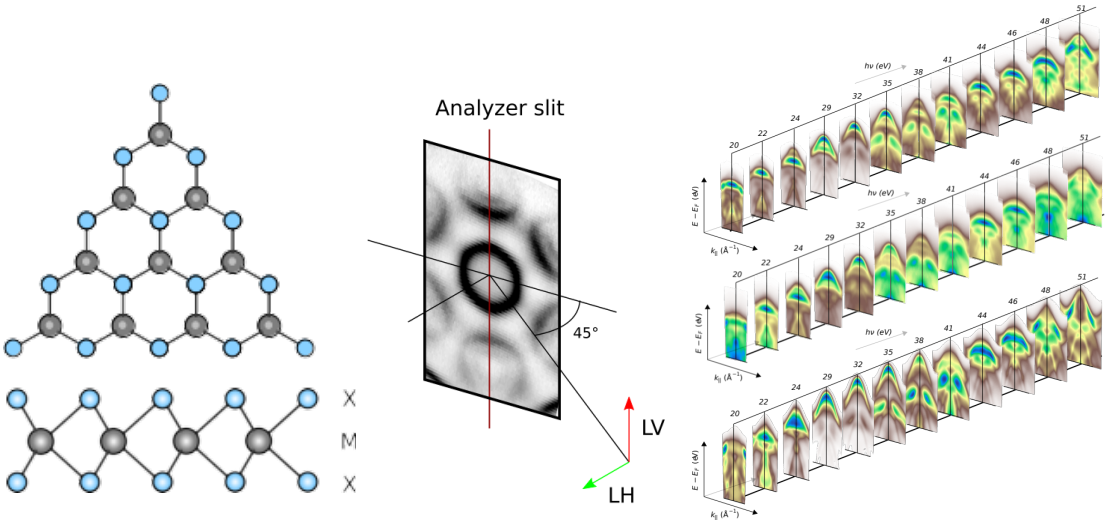

Figure: *Structural, electronic structure and measurement geometry of bi-,tri-layer and bulk WSe_2.*

Transition metal dichalcogenides (TMDs) are layered materials obtained by stacking two-dimensional sheets weakly bonded by van der Waals interactions. In bulk TMD, band dispersions are observed in the direction normal to the sheet plane (z-direction) due to the hybridization of out-of-plane orbitals but no k_z-dispersion is expected at the single-layer limit. Using angle-resolved photoemission spectroscopy, we precisely address the two-dimensional to three-dimensional crossover of the electronic band structure of large area epitaxial WSe_2 thin films.

*Speaker

Increasing number of discrete electronic states appears in given k_z-ranges while increasing the number of layers. The continuous bulk dispersion is nearly retrieved for 6-sheet films. These results are reproduced by calculations going from a relatively simple tight-binding model to a sophisticated KKR-Green's function calculation.

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Tuesday, September the 23^{rd} – 16h18

Disorder Effects In The Band Structure Of Transition Metal Dichalcogenide Alloys $A_xB_{1-x}Se_2$ (A, B= Cr, Mo, W)

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Among the plenty of two-dimensional (2D) materials emerged in the research scenario after the discovery of graphene, transition metal dichalcogenides (TMDCs) attract huge interest as potential functional material candidate for electronic and optoelectronic applications. Various TMDCs with the general formula MX_2 (M=Mo, W; X=S, Se, Te) usually exhibit a distinct bandgap and spin polarized bands. There are many artificial methods put forward to engineer the bandgap and spin polarized bands such as chemical doping, induction of strain or external electric field etc. Recent developments in the synthesis of TMDCs open up a new family of materials called 2D TMDC alloys [1]. Here we are studying the band structure of $Mo_xW_{1-x}Se_2$ single crystals with various stoichiometric ratio x in comparison with WSe_2. The structural characterisation of samples was analysed using Low energy electron diffraction[LEED] and Scanning Electron Microscopy (SEM) with Energy Dispersive X-Ray Analysis (EDX). The core level spectra of the samples were obtained using X-ray photoemission spectroscopy (XPS). We study the band structure evolution in $Mo_xW_{1-x}Se_2$ alloys (x= 0 to 1) utilizing a blend of Angle-Resolved Photoemission Spectroscopy (ARPES)experimentally and is complemented by theoretical one-step model photoemission calculations employing the SPR-KKR package [2]. Furthermore, circular dichroism [3] ARPES measurements provide an insight into the orbital characteristics, revealing Mo concentration-dependent effects that are substantiated through photoemission calculations using the coherent potential approximation(CPA). For homogeneous random alloys, CPA effectively models average scattering properties in alloys and, within the KKR formalism, ensures no extra scattering when embedding an alloy component. Studying these disordered systems uncovers fundamental insights, enhancing their potential applications.

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*Speaker

Tuesday, September the 23^{rd} – 16h36

Uniaxial Strain As a Probe Of The Superconducting Order Parameter Structure And Symmetry In $4Hb$-TaS_2

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$4Hb$-TaS_2 is a layered, highly two-dimensional transition metal dichalcogenide (TMD) that undergoes both a charge-density wave (CDW) and a superconducting transition. Some evidence exists of time-reversal symmetry breaking (TRSB) below the superconducting transition temperature, and other measurements suggest a two-component superconducting order parameter (OP), with experimental results differing from those observed in other, "trivial" superconductors.

Uniaxial strain serves as a powerful, non-destructive, and reversible probe for breaking crystal symmetry, enabling its use as a tuning parameter for phenomena that are highly sensitive to symmetry, such as superconductivity [1].

In this talk, I will demonstrate how I utilize uniaxial strain as a tool to investigate the properties of superconductivity and related phenomena in $4Hb$-TaS_2. Specifically, I aim to demonstrate the evolution of transition temperatures associated with the superconducting phase under uniaxial strain, as well as propose further methods to explore the critical field anisotropy characteristic of this material, and, in conjunction with angle-resolved photoemission spectroscopy (ARPES) measurements, probe the strain-induced changes in the band structure. This approach will provide new insights into the interplay between symmetry, superconductivity, and electronic structure in $4Hb$-TaS_2.

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*Speaker

Tuesday, September the 23^{rd} – 16h54

Low Temperature Specific Heat Of The 1T-TaS_2 Polymorph

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Transition metal dichalcogenides (TMDs) have garnered significant attention in recent years, owing to their polymorphism and the diverse range of physical phenomena they exhibit. Structured as stacks of two-dimensional layers held together by weak van der Waals forces, TMDs exhibit rich phase diagrams and are promising candidates for hosting exotic ground states.

In this talk, I will present my master's thesis work on the low-temperature specific heat of three TaS_2 polymorphs: 1T, 2H, and 4Hb. Specific heat was measured over a broad temperature range, from $400, \mathrm{K}$ down to a few tens of milli-Kelvin, using a dilution-refrigerator-mounted calorimeter. Measurements were performed in magnetic fields ranging from 0 to 14T. These extreme conditions allowed us to probe the low-energy excitations of the ground states in the different polymorphs. At sub-Kelvin temperatures and under high magnetic fields, the large nuclear spin of Ta leads to a pronounced nuclear Schottky effect, which dominates the specific heat signal. This effect arises from energy-level splitting of the hyperfine Hamiltonian.

The main focus of the talk is the 1T-TaS_2 polymorph. The 1T undergoes a sequence of temperature-dependent charge density wave (CDW) transitions. The ground state of 1T-TaS_2 is considered to be a realization of a Mott insulator on a triangular lattice, and it's a candidate host of a quantum spin liquid ground state [1]. The extended temperature range of our measurements enables a separation of the nuclear Schottky contribution from previously reported low-temperature Schottky and field-dependent Sommerfeld-like terms [2]. I will discuss the implications of these results for the nature of the 1T-TaS_2 ground state. Notably, we observe an unusual field dependence of the nuclear Schottky contribution, which we attribute to the effect of long nuclear spin relaxation times in a relaxation calorimetry measurement. I will also address the absence of a clear thermodynamic signature for the nearly-commensurate to commensurate CDW transition. By estimating the associated entropy change, we show that the expected signal is indeed below our detection threshold.

The 2H polymorph is an s-wave superconductor with a critical temperature of $0.7, \mathrm{K}$. On the other hand, the 4Hb-TaS_2 polytype, whose unit cell is composed of a stack of weakly coupled 1T-1H layers, is an unconventional SC, with a possible chiral SC ground state. Both the 2H and 4Hb polymorphs also display a strong nuclear Schottky effect. indicates that the spin excitations in 1T are gapped at low temperatures, casting doubt on the proposed gapless spinon Fermi surface picture of the 1T-TaS_2 ground state.

*Speaker

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Tuesday, September the 23^{rd} – 17h12

Probing Resonant Photoemission And Coulomb Effects In Transition Metal Dichalcogenides

Yashasvi Mehra[1,2,3] *, Aki I. O. Pulkkinen[3], Samuel Beaulieu[4], Mauro Faniculli[1,2], Sotirios Fragkos[4], Olivier Heckmann[1,2] Marchin Rosmos[5], Natalia Olszowska[5], Tomasz Sobol[5], Edyta Beyer[5], Karol Hricovini[1,2], Jan Minar [3] and Maria Christine Richter[1,2]

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We investigate the complex interplay between various decay mechanisms under resonant conditions [1], focusing on radiation-less Raman Auger and Classical Auger emissions in transition metal dichalcogenides (TMDs). By performing resonant angle resolved photoemission spectroscopy (ARPES) measurements and complementary SPR-KKR photoemission calculations, we explore the role of the Coulomb interaction U, a crucial parameter governing electron correlations in these materials. The Coulomb interaction is particularly pronounced in low-dimensional systems, such as quasi-2D TMCs, where it induces a variety of electronic phases, including Charge Density Wave (CDW) order, the coexistence of CDW with superconductivity, and topologically non-trivial phases. We apply the method of Cini [2]and Sawatzky [3, 4]to determine the on-site Coulomb interaction for each element.We compare the resonant spectrum and the self-convolution of single-hole states derived from non-resonant photoemission, to measure the on-site Coulomb energy[5]. On the theoretical front, the SPR-KKR calculations, based on a one-step model, incorporate the full matrix elements of the photoemission process, allowing us to probe the underlying electronic structure with high precision. We further examine the computed ARPES, X-ray Absorption Spectroscopy (XAS), orbital- and element-resolved band structures, and density of states (DOS). The theoretical results show excellent agreement with the experimental data, offering valuable insights into the electronic properties of TMDs and their complex many-body interactions.

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*Speaker

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Wednesday, September the 24^{th} – 17h45

Layered Multiple Scattering Approach To X-Ray Photoelectron Diffraction: Theory And Application

Trung-Phuc Vo[1,2*], Olena Tkach[3,4], Aki Pulkkinen[1], Didier Sebilleau[5], Aimo Winkelmann[6], Olena Fedchenko[3], Yaryna Lytvynenko[3,7] Dmitry Vasilyev[3], Hans-Joachim Elmers[3], Gerd Schonhense[3] and Jan Minar[1†]

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Photoelectron diffraction (PED) is a powerful experimental technique for determining the lattice structure near surfaces with sub-ångström resolution. The strong energy dependence of Kikuchi patterns [1, 2] complicates their interpretation further, necessitating advanced theoretical approaches. In the high-energy regime, PED effects are observed in angle-resolved photoemission spectroscopy (ARPES) measurements alongside other challenges, such as low cross-sections, large photon momentum transfer, and significant phonon scattering). To improve structural analysis and distinguish these PED effects, we present a comprehensive theoretical study [3] of fine diffraction patterns and how they evolve with energy. This study involves simulating core-level emissions from Ge(100) and Si(100) [4]. Using multiple-scattering theory and the fully relativistic one-step photoemission model [5, 6], we simulated faint pattern networks for various core levels across different kinetic energies (106 eV - 4174 eV), avoiding cluster size convergence issues inherent in cluster-based methods. We discuss broadening in patterns via the inelastic scattering treatment. Experimental results from a time-of-flight (ToF) momentum microscope (MM) are reproduced. For the first time, we observe and successfully reproduce circular dichroism in the angular distribution of Si(100)-1s, revealing detailed features and asymmetries of up to 31%. Notably, we successfully replicate both bulk and surface-sensitive diffraction patterns, further validating the robustness of our simulations. The results show remarkable agreement with the experimental data obtained using circularly polarized radiation, demonstrating the potential of this methodology for advancing high-energy PES investigations.

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*Speaker
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3D Mapping Of Valence Bandstructure, Circular Dichroism Texture And Photoelectron Diffraction In A Novel Momentum Microscope

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The 3D recording scheme of time-of-flight momentum microscopes (ToF-MMs) is advantageous for fast mapping of the photoelectron distribution in (E,$\boldsymbol{k}$) parameter space over one or several Brillouin zones. However, the 2 ns pulse period of most synchrotrons is too short for pure ToF photoelectron spectroscopy. At the soft X-ray branch of beamline I09 at the Diamond Light Source we have set up the first HSA & ToF hybrid MM (SAMMy) using a hemispherical analyzer (HSA) as a pre-filter, enabling ToF-MM at such high pulse rates [1].

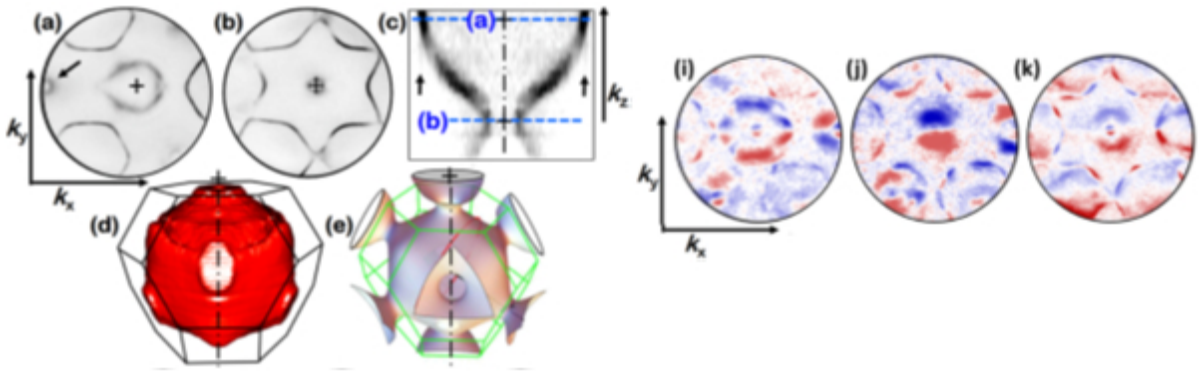

Figure: *3D mapping of the Fermi surfaces of Cu (a-e) and CDAD texture of the Au Fermi surface (i-k).*

The photon energy at I09 ranges from 105 eV to 2 keV, with circular polarization available for h$\nu \geq$145 eV. The HSA reduces the transmitted energy band to typically 0.5 eV, which is

*Speaker

then further analyzed by ToF recording. The overall efficiency gain when switching from the standard 2D (k_x,k_y) mode to the 3D (k_x,k_y,E_{kin}) hybrid mode is about 24. Recently, a new type of entrance lens was installed that substantially reduces the electric field strength at the sample surface, thus mitigating the risk of field emission or flashovers [2].

After introducing the instrument, a few examples will be shown: The 3D mapping of the Fermi surfaces of Cu and Au (Figure), capturing the circular dichroism texture for their *sp* valence bands and an example for photoelectron diffraction (PED). Full-field k-imaging offers an efficient way of recording PED patterns [3], including the core-level CDAD [4].

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Wednesday, September the 24^{th} – 18h21

Advancing Photoemission Orbital Tomography Towards Absolute Electron Density Reconstruction

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Photoemission orbital tomography (POT) is a technique that measures emitted photoelectrons from molecular orbitals (MOs) of adsorbed molecules in momentum space and links them to the underlying molecular electron density distributions in position space, as established for the two-dimensional case [1]. This momentum-position space connection is enabled by approximating the emitted photoelectron as a simple plane wave, allowing for a straightforward mathematical relationship by a Fourier transformation. Despite its success in two dimensions, POT also faces criticism due to this simplistic plane wave approximation, leading to inaccuracies for example in the three-dimensional case [2].

In this work, we aim to improve POT by addressing these limitations. We adapt the plane wave approximation of POT to the photoemission from atomic orbitals, using well-known data from the noble gas neon as a benchmark. Next, we test this adaptation on the molecular gas methane, chosen for its similar electronic structure to neon. To obtain reliable photoemission data for this molecule, we employ photoelectron spectroscopy using radiation between the ultraviolet (UV) and the X-ray spectrum. These data are then used to validate the adapted POT method on the molecular example of methane.

Our findings indicate that refining the description of the emitted photoelectron within the POT formalism beyond the plane wave approximation results in more accurate reconstructions of electron densities in real space. This advancement holds significant implications for studying more complex molecular systems with POT, which are relevant in material science, catalysis, and surface chemistry.

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*Speaker

Wednesday, September the 24^{th} – 18h39

Control Of Intervalley Scattering In Bi_2Te_3 Via Temperature-Dependent Band Renormalization

Akib Jabed[1,2*], Francesco Goto[1], Benson F. Kwaku[1], Dario Armanno[1], Adrien Longa[1], Matteo Michiardi[3], Andrea Damascelli[3] Philip Hofmann[4], Gaëtan Jargot[1], François Légaré1[1], Nicolas Gauthier[1], Samuel Beaulieu[2] and Fabio Boschini[1]

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Three-dimensional topological insulators (3D TIs) exhibit spin-momentum–locked surface states within a bulk bandgap, making them prime candidates for next-generation quantum technologies. However, leveraging these properties requires a deeper understanding of out-of-equilibrium carrier dynamics, more specifically the microscopic interaction between surface and bulk electronic states. As an example, recent work by Mori et al. [1,2] reported a long-lived topological exciton in 3D TIs, arising from the interaction between an electron in the surface states and a hole in the bulk bands. Here, we employ high-resolution time- and angle-resolved

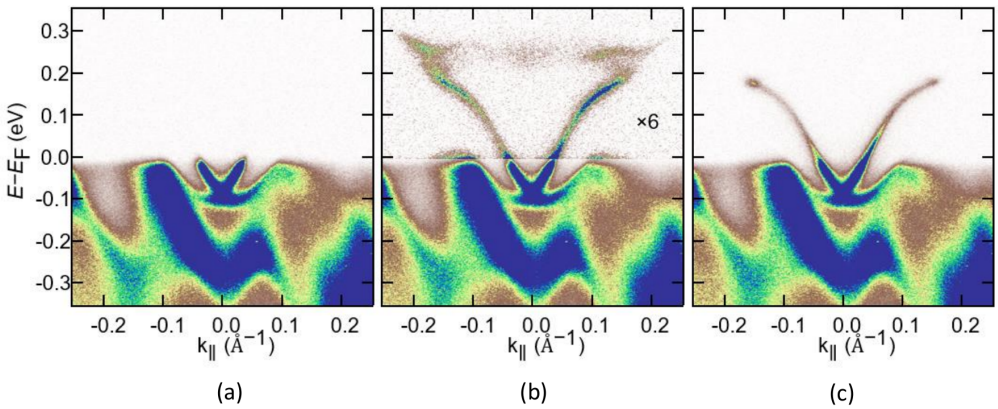

Figure: *Time- and angle-resolved photoemission spectra of p-doped Bi_2Te_3 along the $\bar{\Gamma}$-$\bar{M}$ direction, measured at pump probe-probe delay of (a) <0 ps, (b) 0.5 ps and (c) 22 ps.*

photoemission spectroscopy (TR-ARPES) [3] to examine ultrafast out-of-equilibrium electron

*Speaker

dynamics in p-doped Bi_2Te_3 under mid-infrared optical excitation. We observe a long-living (>20 ps) intensity build-up above the Fermi level, in agreement with Mori et al. [1]. Our experimental findings reveal how a modest (15 meV) renormalization of the conduction band can significantly alter surface and bulk scattering rates [4]. Supported by a kinetic Monte Carlo toy-model, we showed that temperature-induced changes in the bulk band structure modulate the intervalley electron-phonon scattering rate, thus reshaping the out-of-equilibrium response. Our findings suggest that the long-lasting intensity buildup does not necessarily involve the emergence of a spatially indirect topological exciton1, but its formation is well captured by the temperature-induced change in the intervalley scattering efficiency within the conduction band [4]. This work establishes temperature as an effective control knob for engineering scattering pathways in topological insulators.

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Wednesday, September the 24^{th} – 18h57

Chemical-Potential Tuning In The Type-II Dirac Semimetal $PtBi_xTe_{2-x}$

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Type-II Dirac semimetals are topological semimetals featuring Lorentz-violating Dirac fermions in their electronic band structures, leading to unique transport properties and novel quantum effects due to tilted Dirac cones. The first direct experimental identification of a type-II Dirac semimetal was achieved in $PtTe_2$ single crystals by means of angle resolved photoemission spectroscopy (ARPES) [1]. Nevertheless, the deep-lying energy position of the type-II Dirac cone hinders exploitation of its exotic properties.

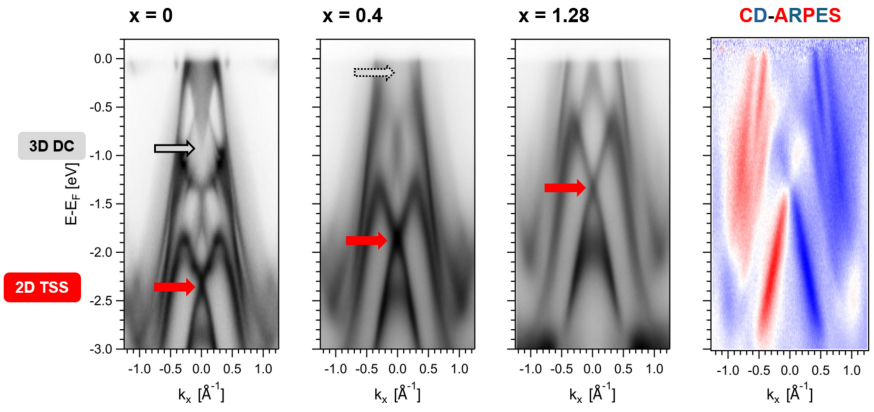

Figure: *ARPES data in the $PtBi_xTe_{2-x}$ series obtained for x=0, x=0.4, and x=1.28. The type-II 3D Dirac cone and the 2D topological surface states are highlighted with grey and red arrows, respectively. On the right-hand side, CD-ARPES data for x=1.28 indicate that it may be possible to engineer the band structure while maintaining its topologically non-trivial properties.*

*Speaker

In this talk, I will discuss the approach of tuning the chemical potential of $PtTe_2$ by Bi doping to bring the bulk Dirac cone closer to the Fermi level. I present our latest ARPES data in the series of $PtBi_xTe_{2-x}$ single crystals and discuss the evolution of the electronic structure. Interestingly, our data - supported by DFT calculations - highlight that Bi doping not only shifts the chemical potential closely to what theory predicts, but also that it opens *further* a giant (> 1 eV) inverted bulk gap in Bi-rich samples. Our latest CD-ARPES data indicate that the band structure in the $PtBi_xTe_{2-x}$ series can be significantly engineered while preserving a topologically non-trivial band structure (see Figure).

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Thursday, September the 25^{th} – 10h45

Influence Of Strong Correlations On Impurity-Induced TRSB In A $s+id$-wave Superconductor

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In numerical simulations of the extended Hubbard model with nearest-neighbor attraction, which is an actively investigated model for high-Tc-superconductors, there has been made observations of time reversal symmetry breaking in the form of loop currents in the last few years [1][2]. Those loop currents emerge mainly in the vicinity of an $s + id$-state when nonmagnetic disorder is present in the superconductor. While previous work has focused on the investigation of this phenomenon within the Bogoljubov-de Gennes approximation, we will discuss here the influence electronic correlations on the stability of the loop currents. This is accomplished via the time-dependent Gutzwiller approximation extended towards the inclusion of pairing correlations.

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*Speaker

Thursday, September the 25^{th} – 11h03

Phonon Softening Induced By Charge Density Fluctuations In $YBa_2Cu_3O_{7-\delta}$: Uncovering The Role Of Electron-Phonon Coupling In High-T_c Superconductivity

Martina Fedele [1] *, Giacomo Merzoni [1,2], Marco Moretti Sala[1], Francesco Rosa[1], Nicholas B. Brookes[3], Lucio Braicovich[1,3] Floriana Lombardi[4], Giacomo Ghiringhelli[1,5], Riccardo Arpaia[4,6]

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The discovery of high-temperature superconductors (HTS) has driven significant progress in condensed matter physics and their potential for technological applications has further fueled research efforts to elucidate the microscopic mechanisms underlying this unconventional phenomenology.

While the BCS theory successfully describes the microscopic properties of conventional superconductors, it indeed fails to account for the intricate phase diagram of HTS such as cuprates.

In the electron pairing mechanism at the core of BCS theory, phonons play a fundamental role as mediators of the interaction with electric charge. Therefore, elucidating their role in high-temperature superconductors can be highly significant, particularly in relation to their interplay with the dominant orders in the complex phase diagram of these materials. Among these orders, charge modulations, in the form of long-ranged charge density waves (CDWs) and more short-ranged charge density fluctuations (CDFs), are particularly prevalent in HTS and have been widely studied over the past two decades with increasingly advanced experimental techniques, such as Resonant Inelastic X-ray Scattering (RIXS) [1][2][3].

Furthermore, recent studies have also succeeded in tracking the evolution of bond-stretching phonon modes in the CuO_2 planes, which are most involved in the phenomenology of these materials, revealing peculiar characteristics in phonon dispersions across different regions of the phase diagram and suggesting the existence of a relationship between charge modulations and

*Speaker

phonons [4][5].

In [6] we present a parallel study aimed at a comprehensive comparison of the evolution of both CDWs and CDFs contributions and the energy and intensity of the breathing and bond-stretching phonon modes. High-resolution RIXS is employed to investigate $YBa_2Cu_3O_{7-\delta}$ (YBCO) thin films as a function of key parameters such as doping, temperature, and the direction of the transferred momentum relative to the copper-oxygen planes. The detailed analysis highlights a significant phonon energy softening at a momentum value corresponding to the charge order wavevector. The anomaly is robust, persisting up to temperature and doping conditions where only CDFs occur, and suggesting therefore a greater involvement of charge fluctuations in phonon anomalies.

These findings offer novel insights into the coupling between charge dynamics and lattice vibrations in cuprates, highlighting the central role of CDFs, which are known to be more widespread across the phase diagram and have already been implicated in various theories explaining other peculiar phenomena, such as the strange metal phase.

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Thursday, September the 25^{th} – 11h21

Dominant Role Of Disorder In The Magnetic Excitations Of The Hund's Metal Cr-Doped $BaFe_2As_2$

Marli Dos Reis Cantarino[1*†], Rafael M. P. Teixeira[2], K. R. Pakuszewski[3], Wagner R. da Silva Neto[4], Juliana G. de Abrantes[5], Mirian Garcia-Fernandez[6], P. G. Pagliuso[7], C. Adriano[3], Claude Monney[8], Thorsten Schmitt[9], Eric C. Andrade[2] and Fernando A. Garcia[2]

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While $BaFe_2As_2$ is a Hund's metal [1], where Hund's coupling enhances correlations and stabilizes local moments, hole doping toward half-filling is expected to further increase correlations. When doping is achieved through transition metal substitution (Mn, Cr), the substitution directly perturbs the Fe magnetic lattice believed to promote high-temperature superconductivity in these materials [2]. We investigate the impact of Cr substitution on the magnetic excitations and electronic structure of $BaFe_2As_2$ using high-resolution Resonant Inelastic X-ray Scattering (RIXS) and Angle-Resolved Photoemission Spectroscopy (ARPES) for $x = 0$, 0.035, and 0.085. Our RIXS results show that Fe-derived spin excitations are strongly damped by Cr, becoming overdamped at higher doping levels, similarly to the Mn case.

While Cr acts as a hole dopant, evidenced by the expansion of hole pockets seen in ARPES [3], the band reconstruction associated with nematic order in the parent compound disappears at $x = 0.085$. This contrasts with Mn substitution at the same level: Mn does not alter the Fermi surface via hole doping [4], preserves the nematic band splitting, yet still causes strong magnon damping [5]. To explain these observations, we propose a localized spin model that explicitly incorporates substitutional disorder and Cr local spin interactions. The model reproduces the damping of spin excitations, showing that spatial disorder plays a major role. This highlights the importance of localization and disorder when interpreting the evolution of magnetism in

*Speaker
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Fe-based superconductors.

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Orbital-Resolved Correlation Energies For C_{60} Via Photoelectron Coincidence Spectroscopy

Kathrin Plass[1*], Arkamita Bandyopadhyay[1], Robin Kamrla[1] Cheng-Tien Chiang[2], Frank O. Schumann[3], Jamal Berakdar[1] and Wolf Widdra[1],

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Via photoelectron spectroscopy, important insights into the electronic structure of solids were obtained. However, conventional single photoemission (SPE) methods provide only indirect access to electron correlation effects. In contrast, double photoemission spectroscopy (DPE) enables direct insight into these many-body phenomena by detecting pairs of correlated photoelectrons emitted upon the absorption of a single photon [1, 2]. This process is depicted in figure 1. The molecule C_{60} represents an ideal model system for such investigations, as it is

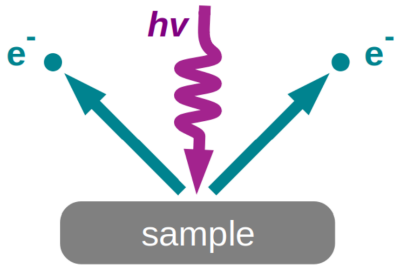

Figure 1: *Pictogram of the DPE process.*

classified as a strongly correlated material with a highly structured valence band spectrum. In our work, we present a comprehensive DPE study of C_{60} thin films deposited on a $SrTiO_3(001)$ substrate, utilizing a laboratory-based high-order harmonic generation (HHG) light source. This source operates at photon energies ranging from 14 to 40 eV and MHz repetition rates, enabling detailed energy-resolved measurements of correlated electron emission [3].

We analyze two-dimensional energy maps of correlated electron pairs and systematically compare the resulting sum energy spectra to theoretical simulations. In particular, we employ a model based on a two-electron density of states [4, 5] to extract orbital-resolved two-electron binding energy shifts - revealing correlation-induced energy renormalizations in the valence band of C_{60} for the first time. In addition, we compare DFT calculations with our experimental spectra and can thus make statements about the spin orientation of the emitted electron pairs. Our findings

*Speaker

mark a significant advancement in the understanding of correlation effects in molecular solids and demonstrate the potential of DPE as a powerful tool for exploring many-body physics in complex materials.

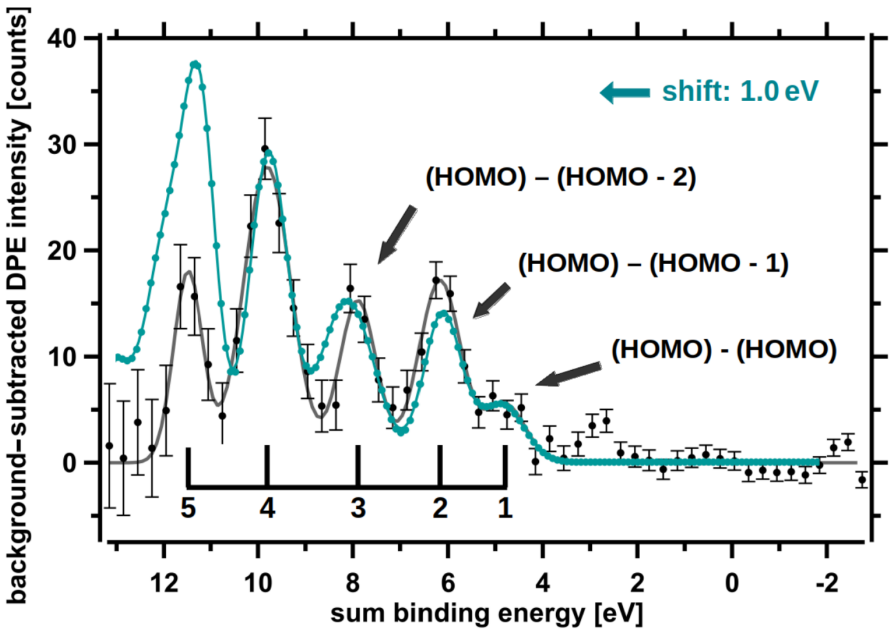

Figure 2: *Background-subtracted DPE spectrum (black) compared to the background-subtracted two-electron density of states (teal). The two-electron density of states has been shifted by 1.0 eV to higher two-electron binding energies. Different molecular orbital combinations of the emitted electron pairs were assigned to the peaks.*

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Also presented as a poster

Thursday, September the 25^{th} – 11h57

Next-Gen ARPES: AI-Controlled Beam Polarization Through Graphene

Ridha Eddhib[1*], Aki Pulkkinen[1], Laurent Nicolai[1], Craig Polley[2], Mats Leandersson[2], Balasubramanian Thiagarajan[2] and Jan Minar [1]

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Angle-Resolved Photoemission Spectroscopy (ARPES) stands as a cornerstone technique in condensed matter physics, offering deep insights into electronic structures and quantum states. However, the precision of ARPES measurements critically depends on the exact calibration of the photon beam's polarization, a challenge that often confronts experimentalists. This study introduces an innovative application of artificial intelligence (AI) to revolutionize ARPES experiments by enabling precise calibration and tuning of photon beam polarization, aiming for the ideal of 100% circular polarization.

At the heart of our methodology is a neural network model, meticulously trained on datasets generated by the sophisticated one-step model of the SPRKKR [1] (Spin-Polarized Relativistic Korringa-Kohn-Rostoker) code, renowned for its accurate ARPES simulation capabilities. This study leverages the ase2sprkkr [2] package for streamlined interfacing with SPRKKR, enriching our AI model's training data with high-fidelity simulations of graphene—a 2D material, serves as the test material for this calibration process, celebrated for its superior electronic properties and pivotal role in advancing material science.

To enhance the efficiency and accuracy of our model training and data analysis process, we've developed and implemented SparkkFLOW [2], a novel workflow specifically tailored for managing and analyzing ARPES simulation data. Coupled with the JobMaster [2] workflow manager, SparkkFLOW enables the automated generation, organization, and sorting of simulation data, significantly reducing the time and computational resources required for model training. This integration of AI with cutting-edge computational tools allows for real-time prediction of optimal ARPES experimental conditions, ensuring each measurement's precision is maximized. By implementing this AI-driven methodology, researchers can dynamically adjust their ARPES setups, ensuring that each measurement is conducted under optimal polarization conditions. This level of precision not only enhances the quality and accuracy of ARPES experiments but also opens new avenues for investigating the electronic behaviors of advanced materials, including novel 2D systems and quantum materials.

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*Speaker

Friday, September the 26^{th} – 8h45

Floquet-Bloch Valleytronics In TMDCs

Quentin Courtade[1*], Sotirios Fragkos[1], Baptiste Fabre[1], Olena Tkach[2,3], Stéphane Petit[1], Dominique Descamps[1] Gerd Schönhense[2], Yann Mairesse[1], Michael Schüler[4,5] and Samuel Beaulieu[1]

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Driving quantum materials out of equilibrium enables the realization of exotic states of matter beyond conventional equilibrium tuning methods. When electrons are periodically driven by electromagnetic fields, Floquet-Bloch states emerge, allowing for the creation of nonequilibrium quantum phases without equilibrium analogs [1,2].

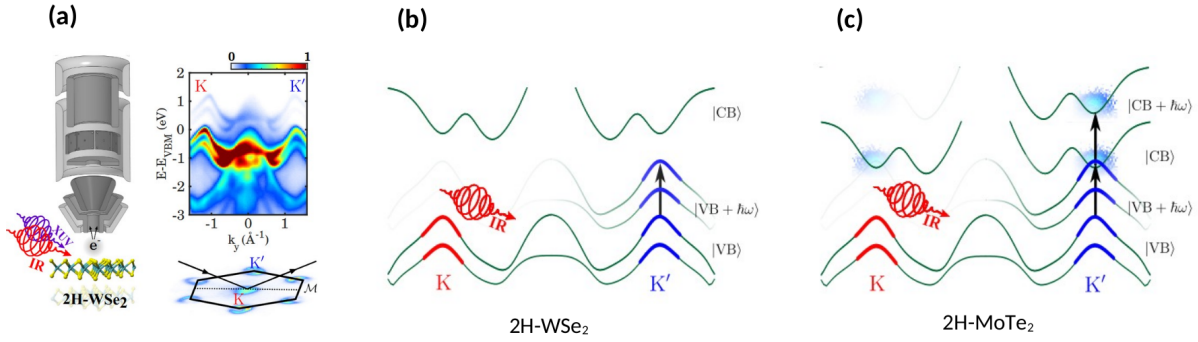

Figure: *Experimental setup and concept of Floquet-Bloch valleytronics.* ***(a)*** *Two polarization-tunable pulses are focused onto the sample (2H-WSe_2) in the interaction chamber of a time-of-flight momentum microscope* [4]*: an IR pump (1.2 eV, 135 fs) and an XUV probe (21.6 eV). The energy-momentum cut along K-Γ-K' at the pump-probe overlap shows the emergence of a sideband at the energy of the valence band plus the pump photon energy. The modulation of the XUV probe polarization allows the creation of Floquet and Volkov states to be investigated, while the modulation of the XUV probe polarization allows circular dichroism of the photoelectron angular distribution from light-driven states to be recorded.* ***(b)*** *Below-bandgap pumping: upon periodic drive using chiral light pulses, time-reversal symmetry is broken and valley-polarized Floquet states are created.* ***(c)*** *Resonant pumping: Floquet and Volkov states are created upon periodic drive from occupied states; light-dressed states are also created from photoinduced excited states.*

*Speaker

In transition metal dichalcogenides (TMDCs), the broken inversion symmetry in monolayers gives rise to a nonzero Berry curvature at the K and K' valleys, leading to chiroptical selection rules central to valleytronics [3]. Here, we establish a connection between Floquet engineering and valleytronics.
First, using below-bandgap pumping, we demonstrate the formation of valley-polarized Floquet-Bloch states in 2H-WSe_2. We reveal quantum path interference between Floquet-Bloch and Volkov states, showing its dependence on valley pseudospin and light polarization. Extreme ultraviolet (XUV) photoemission circular dichroism in this nonequilibrium regime further illustrates the potential for orbital character control in Floquet-engineered states.

Second, under resonant pumping of 2H-$MoTe_2$, we observe the emergence of Floquet-Bloch states not only from the occupied valence band but also from photoinduced excited states. A ∼20 fs delay between the formation of Floquet-Volkov states from valence and conduction bands highlights the interplay between photoexcitation and light-field dressing by the infrared (IR) pump pulse. Furthermore, we demonstrate valley-selective Floquet-Bloch states formation from excited states.

These findings bridge Floquet engineering and quantum geometric light-matter coupling in two-dimensional materials. They provide a pathway toward novel nonequilibrium phases of matter by dynamically breaking symmetries through coherent dressing of Bloch electrons with tailored light pulses.

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Friday, September the 26^{th} – 9h03

Doping-Driven Control Of Charge Density Waves, Doublon Lifetime And Amplitude Mode in $1T$-TaS_2: A Time-Resolved Photoemission Study

J. Jayabalan[1] *, Jiyu Chen[2], Laura Pätzold[3], Florian K. Diekmann[4], Negar Najafianpour[1], Ping Zhou[1] Walter Schnelle[5], Kai Rossnagel[4,6], Tim Wehling[3], Martin Eckstein[3], Philipp Werner[2] and Uwe Bovensiepen[1]

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The quantum material $1T$-TaS_2 enters a Mott insulating state that is intimately coupled to the formation of a commensurate charge density wave (CDW) phase. The material's behavior is governed by a complex interplay of electronic correlations, polaronic distortions, spin excitations, dynamical screening, and the stacking configuration of individual layers-making a fundamental understanding particularly challenging. In this work, we introduce chemical doping as a control parameter to tune the material's response to ultrafast laser excitation. Using time-resolved photoelectron emission spectroscopy (trPES), we investigate the transient electronic dynamics of $1T$-$Ta_{(1-x)}M_xS_2$ (M = Mo, W; $x = 0.02, 0.04, 0.06$). Our experiments, which combine low-energy electron diffraction, electrical transport measurements, and trPES, reveal that the chemical doping modifies both the amplitudon and doublon dynamics through enhanced screening effects and altered carrier-lattice coupling. Tungsten doping leads to a pronounced change in the lifetime of doublon features near the upper Hubbard band energy: whereas the undoped material exhibits a short doublon lifetime of approximately 20 fs [1], the doped samples display significantly extended lifetimes of several hundred femtoseconds, with a subset of carriers persisting for more than a few microseconds. Additionally, the doped samples exhibit weaker and more rapidly decaying CDW amplitudon oscillations compared to pristine $1T$-TaS_2 [2]. By analyzing the doping-induced modifications in the trPES spectra in conjunction with theoretical insights, we offer a microscopic understanding of the intertwined roles of stacking order, electronic correlations, and CDW dynamics. Our results demonstrate that chemical doping provides an effective means to tune interaction strengths and transient electronic structure, opening pathways for controlling the ultrafast dynamics and phase behavior of correlated quantum materials.

*Speaker

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Friday, September the 26^{th} – 9h21

Ultrafast Coherent Dynamics In Open Quantum Systems: Auger-Meitner Decay And Controlled Stearing Of Interactions In SF_6

Sina Shokri [1*], Patrick Rupprecht [2,3], Thomas Pfeifer [4] and Maurits W. Haverkort [1],

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Ultrafast x-ray pump–probe spectroscopy provides a powerful means to study and steer quantum materials on their intrinsic time and length scales. In correlated molecules and solids, theoretical understanding remains challenging due to the interplay of multiple competing interactions. In small molecules, however, it is possible to both experimentally measure and theoretically describe quantum dynamics introduced by strong laser fields. For example one can observe how in SF_6 strong laser fields can modulate exchange interactions via coupling to excited electronic states [1]. Problematic in steering dynamics, especially at x-ray frequencies, is that the coupling to many continuous of degrees of freedom can lead to rapid loss of coherence, leading to a large set of uncontrolled excitations. In core-level spectroscopy, the manner in which coherently driven excitations decay has a direct impact on the spectral line shapes, yet predicting these effects quantitatively remains highly non-trivial.
In this work, we employ nonlinear response theory to predict the transient dynamics and lifetimes of electronic excitations in x-ray absorption spectroscopy (XAS) of SF_6, following excitation by an intense infrared laser field. Our model incorporates the full electronic Coulomb interaction as well as relevant Auger–Meitner decay channels, and is built upon first-principles density functional theory (DFT) calculations.

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Also presented as a poster

*Speaker

Friday, September the 26^{th} – 9h39

Beamline Development Optimized For STARPES : A Bandwidth-Tunable Extreme Ultraviolet Lightsource

P. Nonnon[1,2*†], T. Auguste[2], M. Fanciulli[1,2], R. Geneaux[1,2], O. Heckmann[1,2], J.-F. Hergott[2], K. Hricovini[1,2], F. Lepetit[2], F. Réau[2], M.-C. Richter[1,2], T. Ruchon[2], O. Tcherbakoff[2] and D. Bresteau[2†]

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We present the upgrade of an attosecond beamline, which was previously using a Ti:Sa laser source [1]. We increase the repetition rate from 10 to 100 kHz by using an industrial-grade Yb-doped laser system. Based on the High Harmonic Generation (HHG) process, the beamline is optimized for Spin-, Time-, and Angular-Resolved Photoemission Spectroscopy (STARPES) in solids and gases. Its design allows the switching between the full extreme ultraviolet (XUV) spectrum or monochromatized harmonics down to 200 meV bandwidth.

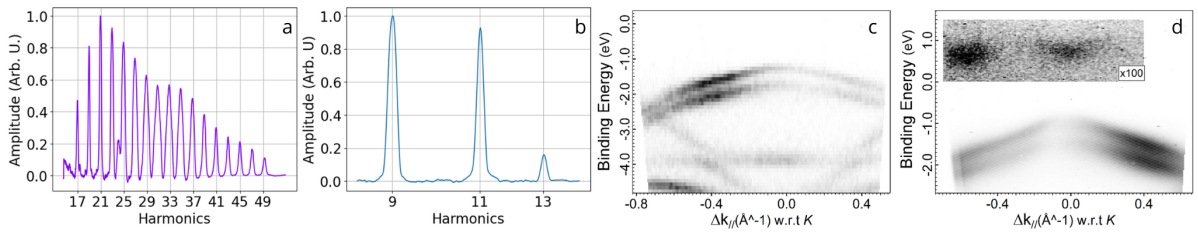

Figure: *Harmonics and Bulk 2H-WSe_2 bandmaps. Harmonics using the 1030 nm (a) and 515 nm (b) drivers. (c) Bulk 2H-WSe_2 ARPES bandmap along the direction perpendicular to $\Gamma - K$ and centered at K using s-polarized XUV light, $h\nu = 26.48 \pm 0.01$ eV. (d) Bulk 2H-WSe_2 tr-ARPES bandmap along the direction perpendicular to $\Gamma - K'$ and centered at K' point using s-polarized probe and a 515 nm p-polarized pump at $\Delta t = 100$ fs and a fluence of 1.5 mJ/cm^2.*

HHG-based STARPES allows the investigation of the momentum-resolved dynamics of electronic spin polarization upon light excitation [2]. Up to now, it has mostly been performed using Ti:Sa sources, which are limited in their repetition rate.

*Speaker
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On the other hand, the advent of Yb-based sources has now allowed for much higher repetition rates. In the context of STARPES, this solves two major limitations: (1) Reduce the acquisition time required by increasing the counts of photoemitted electrons. (2) Mitigate the space charge occurring whenever more than one photoelectron per pulse is emitted into the vacuum. This modifies both the spectral and angular distributions of photoelectrons leading to a loss of resolution in STARPES experiments.

Here we present our implementation of a Yb-doped laser system for STARPES. The laser provides 800 µJ energy per pulse at 100 kHz centered at $\lambda_0 = 1030$ nm with a pulse duration of 350 fs.

The pulses drive a high-harmonic generation process, either directly at 1030 nm, yielding the $q = 17^{th}$ to $q = 49^{th}$ harmonic (Figure 1.a), or with a frequency-doubled beam. Because of the favorable wavelength scaling law [3], the 515 nm driver results in significantly increased XUV flux, at the cost of lower cutoff energy ($q = 9$ to $q = 13$, Figure 1.b).

Varying the delay between a monochromatized harmonic and the fundamental pulse, one can measure the dynamics of the electronic structure. This is known as time-resolved ARPES. First measurements of tr-ARPES have been performed in this configuration on bulk 2H-WSe_2 using the 11^{th} harmonic from the 515 nm driver, showing pump-induced electronic dynamics in the conduction band at the high symmetry points $K'$and Σ points (Figure 1.d).

Further measurements, including STARPES, performed in this configuration will be presented as a complete characterization of the XUV stability, demonstrating the advantage of this new laser source.

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Friday, September the 26^{th} – 10h15

The Effect Of Niobium Doping On Electronic And Atomic Chirality In The Kagome Metal CsV_3Sb_5

Harshit Agarwal[1*], O. Tkach[1,2], Y. Lytvynenko[1,3], P. Yogi[1] M. Schmitt[4,5], D. Biswas[4], J. Liu[4] S. V. Chernov[6], M. Hoesch[6], D. Kutnyakhov[6], N. Wind[6,7] L. Wenthaus[6], M. Scholz[6], K. Rossnagel[7,8] A. Gloskovskii[6], C. Schlueter[6], A. Winkelmann[9], A.-A. Haghighirad[10] M. Merz[10], T.-L. Lee[4], R. Claessen[5] M. Le Tacon[10], J. Demsar[1], G. Schönhense[1], H.J. Elmers[1] and O. Fedchenko[1,11]

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A family of Kagome metals AV_3Sb_5 (A= Cs, K, Rb) has gained significant attention due to its unique properties of charge density wave, superconductivity and electronic structure, characterized by flat bands, Dirac points, and saddle points [1,2]. These features give rise to a diverse range of exotic quantum phenomena [3].

We investigated the changes to the geometric and electronic structure of the Nb-doped CsV_3Sb_5 Kagome metal at low temperatures, particularly at the transition to a charge density wave (CDW) state. Nb doping decreases the CDW transition temperature TCDW, while increasing the critical temperature for superconductivity T_c [4]. X-ray photoelectron diffraction measurements reveal the emergence of a chiral atomic structure in the CDW phase, and circularly polarized X-ray photoemission indicates a pronounced non-trivial circular dichroism in the angular distribution of valence band photoemission [5]. I will discuss the chiral atomic structure

*Speaker

of Nb-doped CsV3Sb5 across the charge density wave transition, as determined from the X-ray photoemission diffraction pattern, as well as the chirality in the electronic bands.

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Friday, September the 26^{th} – 10h33

Electronic Structure And Edge States In The 2D Kagome Ta_2S_3 on Au(111)

Thais Chagas[1*], Alice Bremerich[1], Christoph Schuster[1], Pedro H. Rezende-Goncalves[2,3], Marcin Rosmus[2], Alessia Bardazzi[1], Dina Wilks[1], Samuel M. Vasconcelos[4], Alan C. R. Souza[3], Catherine Grover[1], Kai Mehlich[1], François Bertran[5], Chiara Bigi[5], Andrés F. Santander-Syro[2], Mario S. C. Mazzoni[3], Michael Rohlfing[4] and Carsten Busse[1]

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Kagome structures are an important model system in quantum physics as they combine topology and correlations. It constitutes the most frustrated 2D magnetic lattice, where the magnetic moments condense into a spin liquid at low temperature. The characteristic Kagome bands in this lattice consist of a Dirac cone that gives rise to massless Dirac fermions with high mobility and a flat band that, on the contrary, generates infinitely massive ones. The presence of these bands and their unique properties can lead to the emergence of exotic many-body states, including magnetism, superconductivity, and Wigner crystallization. In this work, we investigate the 2D Ta_2S_3 Kagome phase on Au(111) using scanning tunnelling microscopy (STM), angle-resolved photoemission spectroscopy (ARPES), and density functional theory (DFT). The edges of the island appear very bright in STM images as a consequence of an enhanced density of states. We also observe a pronounced dependence of atomic contrast on tunneling conditions, suggesting a complex electronic band structure near the Fermi level. Furthermore, we analyze the impact of growth parameters on defect formation.

*Speaker

Friday, September the 26^{th} – 10h51

Termination-Dependent ARPES Maps From Novel Magnetic Kagome Metals GdV_6Sn_6 and $GdMn_6Sn_6$

Robin P. Forster[1*], Honey Boban[1], Mohammed Qahosh[1], Xiao Hou[1], Yishui Zhou[2], Yixi Su[2], Claus M. Schneider[1] and Lukasz Plucinski[1]

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The magnetic Kagome metal GdV_6Sn_6 combines phenomena such as flat Kagome bands [1,2], local moments of the 4f electrons of Gd, and itinerant V 3d electrons [3], in a single material, providing a platform to study their complex magnetic and electronic interactions. We have performed termination-dependent micro-ARPES measurements with 20 μm real-space resolution at 20 K of paramagnetic GdV_6Sn_6 [4].

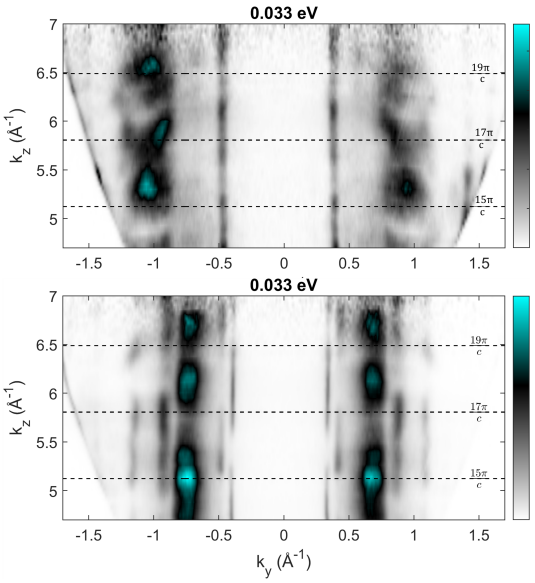

Figure: *A series of photon energy dependent ARPES spectra (from 75 eV to 200 eV) along M K Γ K M direction have been performed. After transforming hν into k_z, the cut at roughly Fermi-energy through series of scans of the Sn (upper spectra) and the Kagome (lower spectra) termination of* GdV_6Sn_6 *is presented.*

Surface and bulk states could be distinguished in the series of scans made over a range of photon energies. Subsequently, we have chosen $h\nu$ of 80 eV and 130 eV for detailed ARPES scans. In

*Speaker

addition, TEM measurements were conducted, which provide an insight into the crystal structure. Preliminary circular-dichroic ARPES maps exhibit multiple sign inversions that stem from a combination of initial state orbital angular momenta and photoemission final state scattering [5].

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Also presented as a poster

Friday, September the 26^{th} – 11h09

Imaging The Indirect-To-Direct Band-Gap Crossover In PbI_2

M. Rosmus[1*], A. Antezak[1], A. Ptok[2], F. Fortuna[1], C. P. Sonny Tsotezem[1], E. M. Staicu Casagrande[1], A. Momeni[1], A. Ouvrard[1], C. Bigi[3], M. Zonno[3], A. Ouerghi[4], H. Khemliche[1], A. F. Santander-Syro[1], E. Frantzeskakis[1]

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We present direct experimental evidence for a thickness-driven crossover from an indirect to a direct band-gap in PbI_2 thin films. Using angle-resolved photoemission spectroscopy (ARPES) performed on films grown by molecular beam epitaxy on graphene/SiC, we observe a shift of the valence band maximum (VBM) from a position between $\overline{\Gamma}$ and $\overline{\mathrm{M}}$ in monolayers to the $\overline{\Gamma}$ point in multilayers. This transition is accompanied by a dimensional crossover from a two-dimensional electronic structure in monolayers to three-dimensional dispersion in thicker films.

Our measurements are in excellent agreement with density functional theory calculations. The results identify the interlayer hybridization of iodine p_z orbitals as the driving mechanism for the band-gap transition. We further confirm that the VBM in multilayer PbI_2 resides at the A point of the bulk Brillouin zone, consistent with the emergence of a direct band-gap in the 2H polytype.

These findings provide a direct spectroscopic signature of band-gap tunability in a layered semiconductor, with implications for optoelectronic device applications.

*Speaker

Surface Science Unlocked

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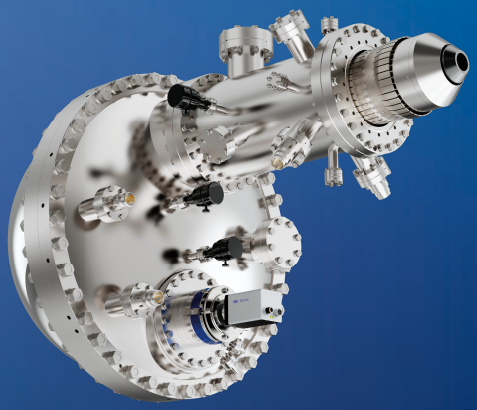

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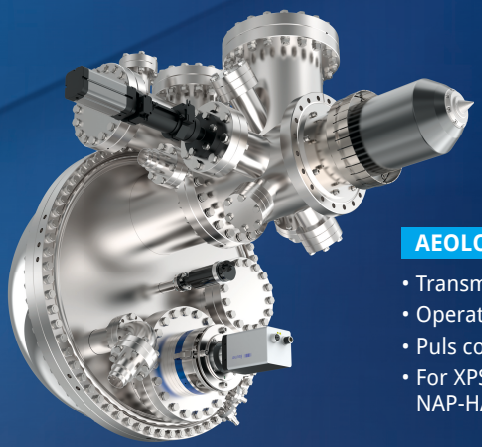

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Posters

High-Fermi Velocity Massless Carriers In A Triangular Lattice Of Sb Monolayer

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Two-dimensional (2D) quantum materials with high Fermi velocities are key candidates for ballistic transport and high-speed electronics. However, few 2D systems have demonstrated Fermi velocities exceeding that of graphene. Here, we report the successful synthesis of a triangular monolayer of antimony (Sb) on the wide-gap semiconductor SiC. Using combined spectro-microscopy and density functional theory, we reveal orbital filtering that isolates broad-bandwidth, massless p_x and p_y states, yielding a compensated Fermi surface with an ultrahigh Fermi velocity reaching 2.07×10^6 m/s–surpassing that of graphene. Linear dichroism measurements confirm the orbital polarization of these high-velocity bands. Consistent with triangular lattice physics, a valley Dirac cone emerges deep below the Fermi level due to enhanced Sb band filling. The coexistence of ultrafast charge carriers and Dirac features makes the triangular antimonene a compelling platform for next-generation quantum and high-speed electronic technologies.

*Speaker

Intercalation Of A Large Gap Quantum Spin Hall Insulator Into The Graphene/SiC Interface

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Bismuthene, a honeycomb lattice of bismuth atoms synthesized on a SiC(0001) substrate, is a topological insulator with a breakthrough bulk band gap of 800 meV due to giant spin-orbit coupling. The magnitude of this gap exposes bismuthene as a promising candidate for room temperature spintronic applications based on the quantum spin Hall effect. However, oxidation of bismuthene in air confines most experiments on this system to UHV conditions. Here, we demonstrate the intercalation of bismuthene below a single sheet of graphene. This protective layer effectively prevents bismuthene from oxidation, while it fully conserves its structural and topological properties as we readily demonstrate by scanning tunneling microscopy and photoemission spectroscopy. This paves the way for ex-situ experiments and ultimately brings bismuthene closer to the fabrication of spintronic devices.

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*Speaker

Investigations On Electron-Hole Dynamics In Bulk Molybdenum Disulphide Via Time- and Angle-Resolved Photoemission Spectroscopy

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TR-ARPES has emerged as one of the most powerful tools for investigating dynamical properties of quantum materials [1] and it is widely used on semiconductors of the family of Transition Metal Dichalcogenides. They offer an interesting subject of study beacause of their strong light-matter interaction and the possibility of modulating their electronic properties through strain, doping, or stacking with other materials. In this work, we perform measurements via time

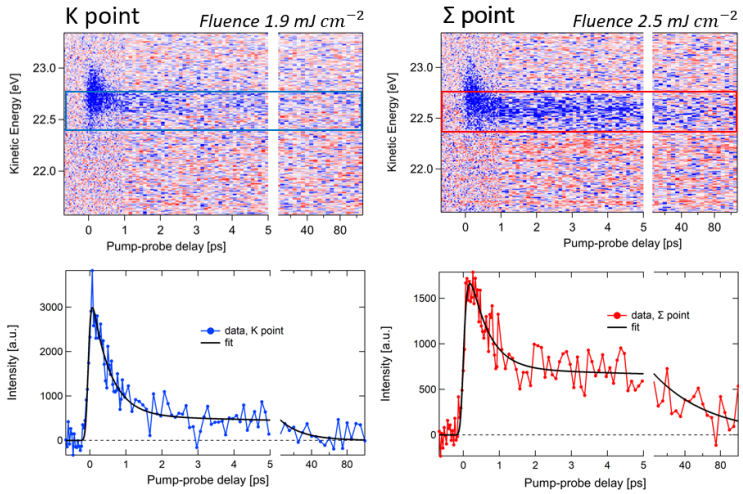

Figure: *Conduction Band at K and Σ valleys (pump at hν = 1.94 eV). Fits of transient intensities (down), from integration in energy of the angle-integrated differential maps (up), assuming a phenomenological double exponential decay. The corresponding energy ranges are indicated in blue and red lines. In the difference map, the colour scale refers to a gain (blue) and a loss (red) of photoelectrons with respect to before time zero mean value. For K valley the time constants from the fit are τ_1 = (0.4 ± 0.1) ps and τ_2 = (38 ± 11) ps, while for Σ valley are τ_1 = (0.6 ± 0.2) ps and τ_2 = (49 ± 13) ps.*

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and angle-resolved photoemission spectroscopy on molybdenum disulphide bulk system in 2H polytype, by using pump and probe laser pulses from the High Harmonic Generation setup at SPRINT laboratory (CNR-IOM, Trieste) [2]. The purpose is to understand hot electron relaxation processes at different pump photon energies of 1.94 eV and 3.1 eV, respectively resonant with A exciton and above-gap.
After resonant excitation, the photoemission signal arrives faster in K valley and is short-lived compared to that in Σ. The latter is characterised by a time decay constant of (63 $\pm$ 12) picoseconds, in a region close to the bottom of the conduction band (see figure). Moreover, the resonant pump produces a tail towards lower energies at time zero, only at K point, suggesting an electron-hole plasma effect. At short delays, the spectrum broadening towards higher energies is due to the above-gap pump that promotes electrons to upper energy levels, at both K and Σ point.
Finally, we perform multi-peak fitting from energy distribution curves in conduction and valence band at K, Σ and Γ points, to extract information on the time evolution of the valence band maximum and conduction band minimum.

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Photoelectron Diffraction Of Twisted Bilayer Graphene

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Twisted bilayer graphene (TBG), composed of two graphene layers rotated relative to each other, exhibits remarkable structural and electronic properties that strongly depend on the twist angle. The resulting moiré patterns modify the interlayer interactions and can give rise to novel phenomena such as flat electronic bands and correlated states [1].

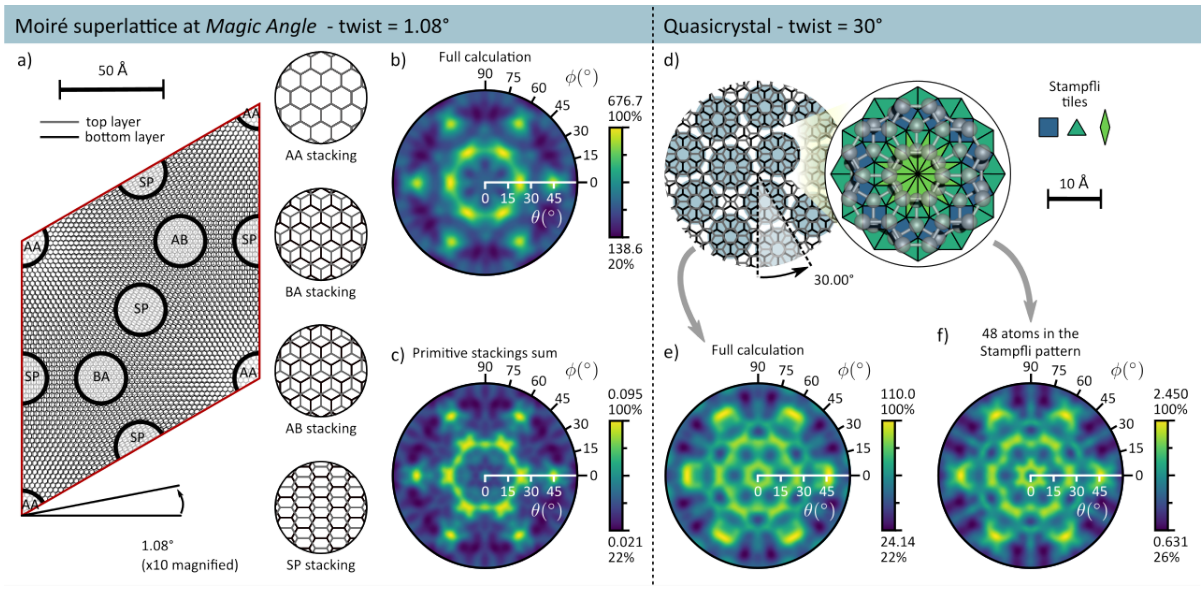

Figure: *a) Moiré supercell of twisted bilayer graphene (red parallelogram) formed at the magic angle (∼1.08°). (b) PED pattern of 1.08°-twisted BLG computed using full multiple scattering. (c) PED pattern from the incoherent sum of contributions from AA, AB, BA, and SP stackings. (d) Superlattice of 30°- twisted BLG forming a 12-fold symmetric quasicrystal; green regions indicate a 48- atom subset of the Stampfli tiling. (e) PED pattern of 30°-twisted BLG. (f) PED pattern from only the 48 atoms forming the Stampfli mosaic.*

Photoelectron diffraction (PED) is a powerful spectroscopic technique that combines elemental resolution with a high sensitivity to the local atomic arrangement at crystal surfaces, thus providing unique fingerprints of selected atomic sites in matter. Stimulated by the rapid innovation

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in the development of various analysis methods for probing the atomic and electronic structures of van der Waals (vdW) heterostructures of two-dimensional materials, we present a theoretical assessment of the capacity of PED for extracting structural properties such as stacking, twist angles and interlayer distances. We present in this communication a theoretical investigation of the capabilities of photoelectron diffraction (PED) to provide a PED phase diagram of the twisted BLG characterised by three distincts regimes. Near the magic values, at small twist angles, the PED captures precisely the proportions of areas associated with stacking found in primitive, i.e. untwisted, BLG (Figure (a)-(c)). Then, at intermediate twist angles, a moiré crystal regime is observed, in which the symmetries of commensurate moiré supercells are probed. Finally, at large twist angles, another quasi-moiré crystal regime reflects the characteristic tessellation of the Stampfli fractal tessellation observed for quasi-crystals with 12^{th}-order rotational symmetry (Figure (d)-(f)). These theoretical results will motivate future PED experiments with high angular, energy and spatial resolution to probe in depth the atomic structure of the vast and fascinating family of twisted, constrained and intercalated vdW materials [2].

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Cuprate-Like Electronic Structures In Infinite-Layer Nickelates With Substantial Hole Dopings

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To understand the underlying mechanism of superconductivity in infinite-layer nickelates, direct observation of its electronic structure is important. Here using Angle-Resolved Photoemission Spectroscopy we directly resolve the electronic structures of the parent compound $LaNiO_2$ and superconducting $La_{0.8}Ca_{0.2}NiO_2$. Their Fermi surfaces consist of a quasi-2D hole pocket and a 3D electron pocket at the Brillouin zone corner, whose volumes change upon Ca doping. The Fermi surface topology and band dispersion of the hole pocket closely resemble those observed in hole-doped cuprates. However, the cuprate-like band exhibits significantly higher hole doping in superconducting $La_{0.8}Ca_{0.2}NiO_2$ compared to superconducting cuprates, highlighting the disparities in the electronic states of the superconducting phase. Our observations highlight the novel aspects of the IL nickelates and pave the way toward the microscopic understanding of the IL nickelate family and its superconductivity.

*Speaker

Hybrid Setup For Photoemission Measurements And Experimental Data On Electronically Correlated Materials

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The hybrid setup for angle-resolved photoemission electron spectroscopy (ARPES) combines a hemispherical analyser and a time-of-flight (ToF) momentum microscope. This allows to perform advanced studies of electronically correlated systems over a broad energy and momentum ranges. This setup gives us an opportunity to measure with continuous and/or pulsed photon sources, including a helium discharge lamp or a pulsed laser setup. In the first case, the hemispherical analyser acts as a bandpass pre-filter. The setup is also designed to enable operando measurements, such as mechanical strain, allowing in situ probing of strain-induced modifications to the electronic band structure.

This work will present the technical characteristics of the experimental setup, as well as the plans for its future upgrade. The modernisation will involve installation of the spin branch and building a laser-based photon source with high-harmonic generation (HHG).

Experimental ARPES data for different Nb doped Kagome systems CsV_3Sb_5, measured with a helium discharge lamp will be presented.

*Speaker

Uniaxial Strain Effects On $PrNiO_2$ Thin Films Revealed By RIXS

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While hydrostatic pressure is a key parameter to achieve high-temperature superconductivity (SC) at extreme pressures, searching for SC near ambient conditions requires alternative tuning strategies. One of these parameters is chemical doping, which can effectively change the structure and electronic state, and another is the dimensionality, as in the case of infinite-layer (IL) nickelates. In these materials, the removal of the apical oxygen adjusts the Ni oxidation state toward the cuprate SC. The biaxial epitaxial strain induced by the choice of substrate during the film growth process can largely modify how the IL phase is stabilized, and the resulting strain significantly alters the electronic configuration of the Ni atoms, impacting magnetic properties, ground state energies, and superconducting transition temperatures (T_C) [1 – 3]. Notably for bilayer nickelates, strain combined with doping can simulate bulk high-pressure effects, elevating T_C to 40 K in $La_3Ni_2O_7$ thin films [4, 5] (compared to 80 K under hydrostatic pressure [6]). In this regard, it is of great interest to decouple the effect of externally applied strain from epitaxial strain on the electronic properties and to investigate the spectroscopic response as a function of applied mechanical stress. We employed Resonant Inelastic X-ray Scattering (RIXS) to investigate the effect of strain on the infinite-layer $PrNiO_2$ thin film by using a Razorbill ultra-high vacuum (UHV) strain cell. Contrary to substrate-induced strain (where compressive strain softens magnons [1]), we found that uniaxial compression increases magnon energies compared to as-grown samples. We conclude that uniaxial strain can be more effective in enhancing the magnetic exchange interaction, which is believed to promote higher TC [7].

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In-situ Combination Of RIXS And ARPES Based On Time-Of-Flight Photoelectron Detection

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Nowadays, the progress in solid-state physics requires correlating electronic structure and collective excitations to understand emergent electronic orders in quantum materials, such as unconventional superconductors, van der Waals heterostructures, antiferromagnets, and the recently discovered altermagnets.

The goal of our project is to develop an instrument that combines resonant inelastic X-ray scattering (RIXS) and angle-resolved photoemission spectroscopy (ARPES). This allows us to apply both methods to the same sample area without moving the sample or the photon footprint. For RIXS, we use an innovative approach that offers several advantages over traditional soft X-ray detection methods. This method converts scattered photons into electrons using a technique called photoelectron spectrometry for the analysis of X-rays (PAX). Time-of-flight photoelectron emission microscopy (ToF-PEEM) efficiently detects photoelectrons excited in the soft X-ray regime. This method enables simultaneous analysis of kinetic energy, as well as position or momentum in two dimensions. Combining these two methods in the same experiment provides unprecedented information on the electronic states (via ARPES) and phononic, magnonic, and electronic excitations (via RIXS) from an identical sample spot.

The presentation will cover the current state of the unique instrument, including its principles, benefits, challenges, and prospects. Additionally, we will discuss the initial experimental results obtained at the soft X-ray beamline P04 (DESY).

*Speaker

Spin Polaron Fingerprints In The Optical Conductivity Of Iridates

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Since the discovery of their exotic spin-orbital entangled insulating ground state, Ba_2IrO_4 and Sr_2IrO_4 have attracted considerable attention. Their low-energy electronic structure is usually described in terms of the so-called j_{eff} states, and their optical transport spectra are characterized by a peculiar double-peak structure. The two peaks, α and β, are conventionally attributed to excitations within the j_{eff} manifold and from the j_{eff} to the j_{eff} states, respectively.

In this work, we employ different numerical techniques to revisit this topic. We compare our simulations with the existing experiments, and we propose an alternative interpretation of the optical conductivity lineshape, based on the presence of spin-polaron quasiparticles within the j_{eff} bands.

We calculate the optical conductivity of both compounds within the dynamical mean-field theory of correlated electrons. We show that both α and β peaks display mixed orbital character, in contrast with the conventional interpretation. Subsequently, we calculate the spin-polaron spectral function via the self-consistent Born approximation. By this means, we demonstrate the polaronic nature of the low-energy features of the eigenspectrum and unveil the importance of these quasiparticles in shaping the absorption spectra.

*Speaker

Institutions

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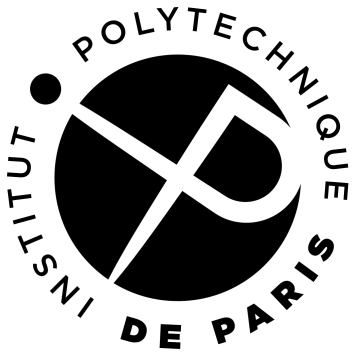

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